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Elementary Kinetics of Soot Oxidation by OH

By

David Eugene Edwards

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Committee in charge:
Professor Michael Frenklach, Chair
Professor William A. Lester Jr.
Professor Jyh-Yuan Chen

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Abstract

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The goal of this dissertation is to elucidate detailed pathways, products, and rates leading to soot oxidation by OH. Such information would supplement current soot modeling which has generally focused more on growth reactions. Indeed, OH oxidation of soot has received no detailed theoretical analysis. The results presented here are a first step to fill this gap in soot modeling.

Due to the presumed importance of oxyradical decomposition to soot oxidation, the thermal decomposition of armchair oxyradicals was pursued. A number of different armchair prototype reactions were investigated to determine how rates vary based on oxyradical location and prototype size. Potential energy surfaces were explored and thermal decomposition rates were calculated. The results indicated that armchair edge oxyradicals decompose at rates similar to zigzag edge oxyradicals. These results were used in subsequent OH oxidation study.

Next, OH oxidation was studied on a series of prototype soot surfaces to identify which edge sites would lead to rapid oxidation by OH. The potential energy surfaces of three different reactions were explored. The carbon radical site was identified as the most likely candidate for a single OH radical attack leading to CO expulsion. A phenanthrene radical was selected as the prototype structure for this site, and the kinetics of this most promising reaction, OH + phenanthrene radical, were explored. This system, including a number of barrierless reactions, was explored using both chemical-activation and thermal decomposition master-equation simulations. The results confirmed the assumption that oxyradicals are key intermediates; multiple oxyradicals were found, all leading to CO expulsion. The overall rate coefficient of phenanthrene radical oxidation by OH forming CO was found to be insensitive to pressure and temperature and was approximately 1×10^{14} cm^3 mol^{-1} s^{-1}. The OH + phenanthrene radical was also studied on the triplet surface. The rate in this case was found to be about a factor of 6 smaller than the singlet surface results.

The two principal processes involved in phenanthrene radical oxidation by OH were H atom migration/elimination followed by oxyradical decomposition. H atom migration/elimination made possible the relatively rapid rearrangement of the PAH edge, forming kinetically favorable oxyradicals which then decomposed. These same two processes are expected to be present in soot surface oxidation by OH. As a preliminary comparison of these theoretical results to soot oxidation experimental results, the collisional efficiency of OH with a phenanthrene radical was calculated and found to be a close match to the experimentally calculated collision efficiency of OH with a soot particle.

To Patti, without whose support and love none of this, and things of greater importance, would be worthwhile

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Chapter 1

Introduction

1.1 Motivation

Total world energy consumption during the year 2010 was 150,000 billion kWh, with 84% of this energy obtained through the burning of liquid fuels, coal, and natural gas [1]. Because of the well documented climate and health issues related to combustion, much effort has been expended to develop renewable energy sources and decrease dependence on fossil fuels. These efforts are critical to one day ending use of fossil fuels. Unfortunately, these greener sources have yet to overtake fossil fuels in energy production and provided only 11% of the world energy in 2010 [1]. Projections of the next thirty years show little change in this dependence, with recent reports estimating that by 2040 fossil fuels will still account for 78% of the world's energy sources, while renewables will have grown to only 15% [1]. While development of alternative sources of energy is important and ongoing, it is also apparent, due to the enduring nature of our dependence on fossil fuel, that research to understand and mitigate the negative impact of combustion is also a worthwhile goal.

Additionally, as greener sources of energy become prevalent, the need for combustion will likely not fade because carbon neutral fuels, such as biomass and biofuels, still require combustion to release the energy in the fuels. For example, the Joint BioEnergy Institute, of which UC Berkeley is a member, has the stated goal of "developing advanced biofuels—liquid fuels derived from the solar energy stored in plant biomass that can replace gasoline, diesel and jet fuels" [2]. These fuels still require combustion; however, in this situation the carbon for the fuel would come from the atmosphere, be formed into a biofuel, and then combusted, returning the carbon to the atmosphere. Because biofuels still rely on combustion, advances made to reduce pollutants for current fuels, would likely still be applicable to biofuels. Furthermore, the Joint BioEnergy Institute, for example, plan on not just making biofuels, but "transportation fuels identical to gasoline, diesel and jet fuel" [2]. If this goal is realized, pollution mitigation strategies and research on gasoline, diesel, and jet fuels performed now, would continue to play an important and relevant role even in a future free of fossil fuels.

The primary issues caused by combustion are related to the release of pollutants, such as NO_x, unburnt hydrocarbons, and particulate matter, as well as greenhouse gases such as CO_2. Mitigation of these combustion products is generally achieved by understanding the fundamental chemistry behind their formation which then informs better design of engines and combustion devices. For example, detailed understanding of NO_x formation and mechanisms have been developed [3], which in conjunction with catalytic converters have brought NOx emissions to acceptable levels. On the other hand, particulate matter, specifically soot, at a fundamental level, is less well understood [4,5]. My focus in this dissertation is to help bridge this gap in knowledge of fundamental soot processes.

As a greenhouse gas, a recent study estimated the climate forcing of soot to be second only to CO_2 [6]. The same study emphasized that due to the short lived nature of soot in the atmosphere, reductions in soot emissions could lead to a rapid effect on warming. In addition to harming the environment, Pope et al. [7] found that a reduction in particulate matter (of which soot is a main contributor) accounted for as much as 15% of the increased life expectancy they observed in their study areas. Soot has also been found to cause cancer [8]. Reducing soot emissions, which first requires understanding the life cycle of soot, including oxidation, would have a measurable impact on both human health and the environment.

In the following sections I will briefly review current understanding of soot formation, followed by oxidation.

1.2 Soot formation

Formation of soot comprises a number of sequential steps, including soot precursor formation, particle nucleation, and particle coagulation. Parallel to these steps are reactions taking place on the edge of PAHs and soot. These edge reactions include both the addition and removal of carbon, and are an active area of research. Detailed reviews of each of these processes and the current state of development for each process can be found in recent reviews of soot [4,5,9]. The focus of this dissertation is on edge reactions, and more details are presented next.

Initially, understanding of edge reactions was based on simple empirical models [10,11] that based growth on concentration of fuel or other gas phase species. The next major step was the introduction of the H-abstraction/C_2H_2-addition (HACA) mechanism [12-14]. The HACA mechanism treated soot and PAH surface reactions at the level of elementary reactions. Finally, current soot edge modeling is done with kinetic Monte Carlo (KMC) simulations of soot edge reactions on a nascent soot structure [15-18].

1.2.1 Kinetic Monte Carlo Model

A common question of the neophyte soot investigator is why KMC simulations are needed instead of the traditional mechanistic approach. Species in combustion mechanisms are generally well specified molecules with known properties and reaction rates, e.g. methane, ethane etc. In contrast, soot is a solid of amorphous shape and composed of 10^2–10^5 atoms. It is not feasible to definitively state the nature of soot or what the reactions, let alone the reaction rates, would be for all soot particles—each soot particle will be different and unique. For example, even if species were tracked for number of carbon and hydrogen atoms, as shown in Equation 1.1, it would still not account for the exponential number of isomers for each number of carbon atoms. It quickly becomes apparent that this traditional, i.e. CHEMKIN [19], approach would not work.

$$\mathrm{C}_{1,562}\mathrm{H}_{342} + \mathrm{C}_2\mathrm{H}_2 \longrightarrow \mathrm{C}_{1,564}\mathrm{H}_{344} \tag{1.1}$$

As a practical alternative, a KMC simulation is employed to track a single nascent soot particle and how it grows, or oxidizes, based on the edge reactions that are included in the simulation. At each time step, a reaction is stochastically selected from among the edge reactions included in the model. The reaction events available are also constrained by the availability of edge sites for each reaction. The reaction selected occurs, the geometry is updated, and then the process is repeated. The simulation can be run for a specified amount of time or until certain conditions are met. Certain parameters, such as soot growth rate, can be determined from the simulation. Additional details about KMC simulations are provided in work published from the Frenklach group [18,20] and others [16,17]. A key component affecting the accuracy of the KMC model is the edge reactions included in the model. Due to this importance, the discovery of possible reactions and the rates of those reactions are an important part of research in soot edge chemistry. One of the purposes of the results and reactions presented in this dissertation would be their inclusion in KMC models to increase the accuracy of the OH oxidation modeling of the simulation.

1.2.2 Growth Edge Reactions

Much of the studied soot edge reactions have focused on the growth of soot structures in the absent of oxygen. Previous studies from the Frenklach group have looked at migration [21] and collision of five-member rings [22], 5- and 6-member ring flip reactions [23], and embedded-ring migration [24]. However, less attention has been given to oxidation.

1.3 Soot Oxidation

The main focus of this dissertation work is on elucidating elementary soot edge reactions involving OH. Before providing the literature review of soot oxidation by OH, I define common PAH edge types and then explain in more detail the connection between PAH and soot edges.

1.3.1 PAH Edge Definitions

Polycyclic aromatic hydrocarbons (PAH) are fused aromatic rings without attached substituents. Some basic definitions related to both PAH and soot edges are shown in Figure 1.1. The two different edge forms, armchair and zigzag, and the two basic edge sites, $C_{surface}$● (read "C surface radical") and $C_{surface}$−H are shown. An oxyradical site is also included in Figure 1.1 because of the prominent role oxyradicals played in the dissertation results. Note that the definitions provided in the figure do not depend on the extent of the PAH structure, but only on the local structure.

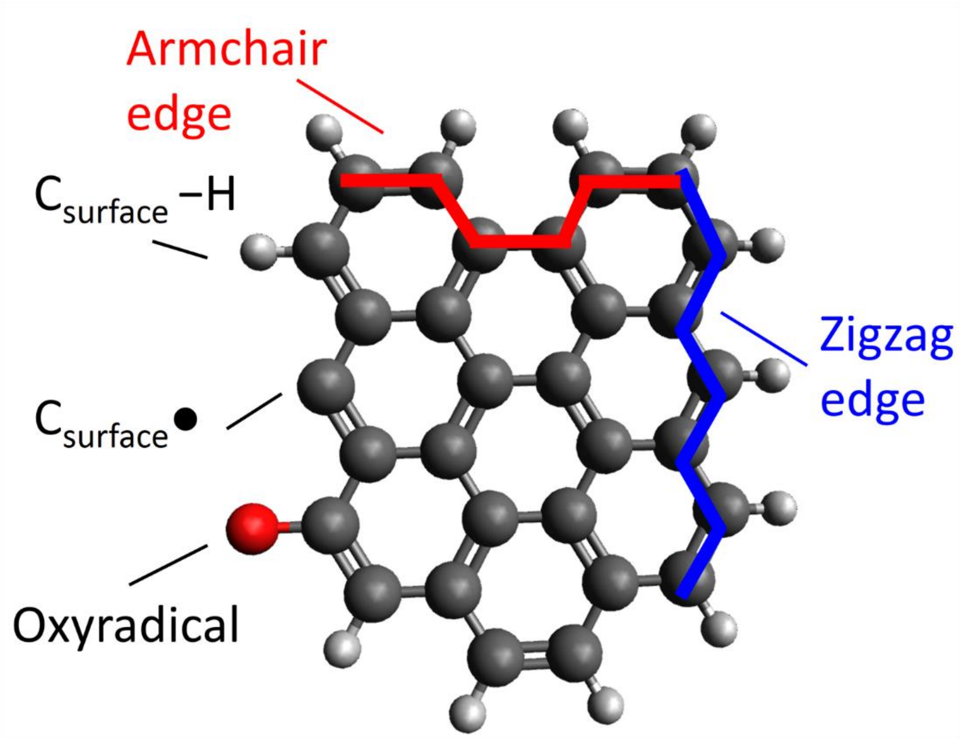


Figure 1.1. Example of a generic PAH structure, identifying the different edges and site types.

1.3.2 Connection between PAHs and Soot Edges

How are possible edge reactions identified? The key step is recognizing that the basic composition or building blocks of soot are PAH structures that coagulate to form a particle [4,5,25]. Figure 1.2 is a representation of a soot particle, highlighting how the edges are similar to PAH edges. Instead of studying reactions on actual soot surfaces, smaller, more computationally (or experimentally) tractable PAH molecules are used as prototypes. Because of this similarity, edge reactions of a relatively small PAH, such as anthracene or phenanthrene, are assumed to be the same as those occurring on soot edges. Based on this, reaction rates, pathways, and products found on these smaller PAH edge reactions are assumed to be the same for soot edges. For example, to study the detailed reaction of O_2 with an armchair $C_{surface}$–H soot edge site one might study the reaction of O_2 with phenanthrene. The results of the study of O_2 attacking phenanthrene could then be assumed to be the same as O_2 attacking an armchair $C_{surface}$–H site on a soot surface.

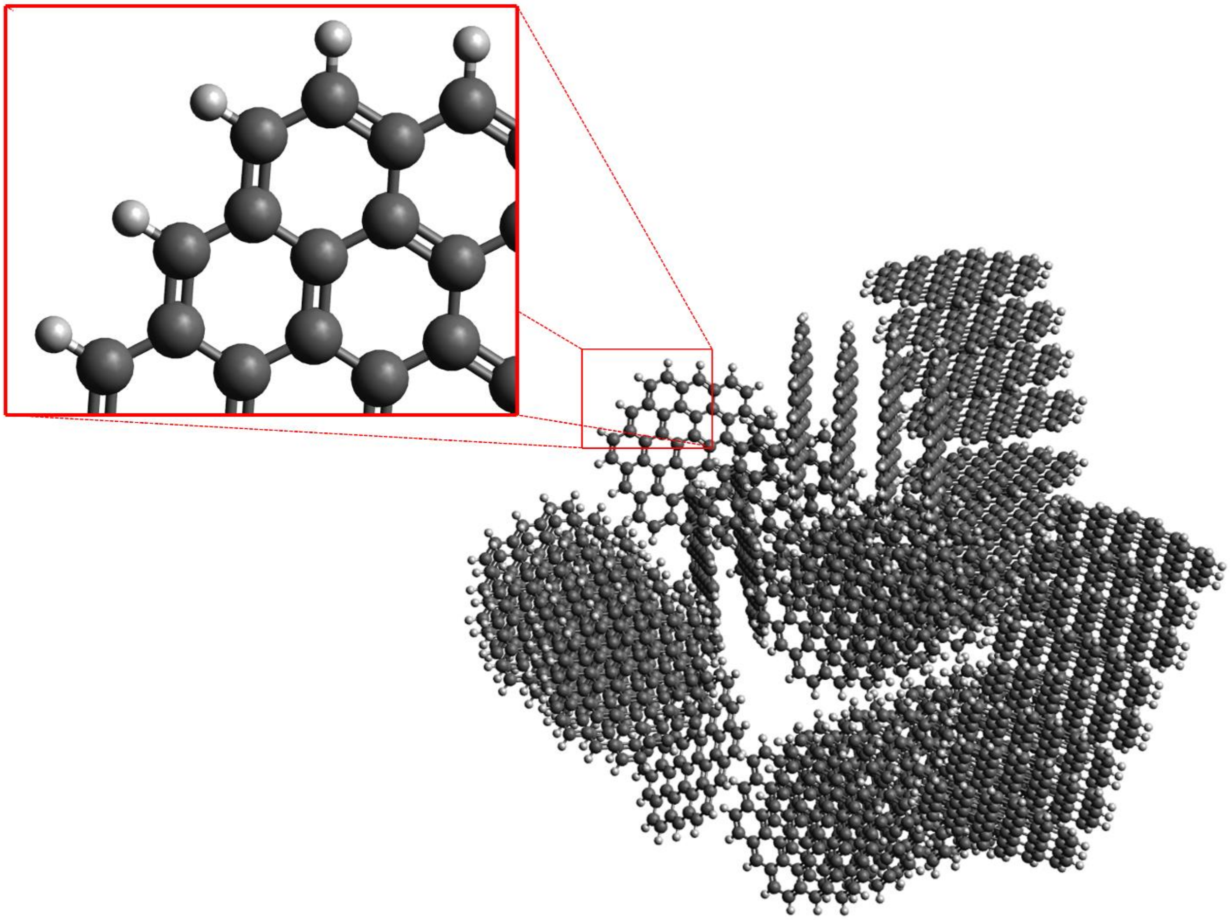


Figure 1.2. Representation of a soot particle composed of multiple PAH layers.

1.3.3 Literature Review of Soot Oxidation by OH

To my knowledge, no atomistically resolved pathways leading to the removal of carbon by OH from soot have been identified. As will be discussed next, however, there have been a number of experimental studies examining soot oxidation by OH.

Current laminar and turbulent models for soot oxidation by OH typically describe oxidation by an OH collision efficiency (η_{OH}) value of 0.13 [26,27], the lower value of the range reported in the experiments of Neoh et al. [28]. η_{OH} is defined by Neoh et al. as "the ratio of the … reaction rate to the collision rate from kinetic theory". In their experiments, Neoh et al. examined the oxidation of soot in a two-stage atmospheric pressure premixed system. Soot was formed in the first burner under rich conditions, and then oxidized in the secondary burner over slightly lean to slightly rich conditions. OH was found to be the principal oxidant of soot under these conditions. They reported η_{OH} values of 0.13–0.28. The lower value is obtained when the surface area of a soot particle was calculated using the diameters of the individual primary particles within the aggregates, while the higher value is obtained when the optical, or equivalent sphere, diameter is used for the soot aggregates. Generally the 0.13 value is used.

Roth et al. used shock tube experiments to study soot oxidation. They calculated collision efficiencies for NO and O [29,30], as well as for OH and O_2 [31]. η_{OH} was calculated as a fitting parameter to account for the observed CO formation. η_{OH} calculated in this way was 0.2. Another study, by Puri et al. [32,33], reported lower bounds for η_{OH} of 0.04 for methane and 0.05 for methane/butane flames. These authors initially reported η_{OH} decreasing with increasing temperature, but in a later communication [33] withdrew this conclusion. They also noted a trend of increasing η_{OH} with time.

Faeth and co-workers [34-36] performed a series of experimental studies examining soot oxidation by OH. They examined the oxidation rate of soot over the ranges of 0.1–8 atm and 1400–2350 K in diffusion and premixed flames burning a variety of fuels. They concluded that η_{OH}, over all of their experimental conditions, was roughly constant at 0.12, with an uncertainty (95 % confidence) of ± 0.03 [35]. Most of their data fall within this range, but some measurements were as low as 0.02 and as high as 0.4 for η_{OH}. Table 1.1 summarizes all of these experimental values and show that the collision efficiency of OH with soot is generally in the range of 0.1 to 0.2.

Table 1.1. Summary of the experimental work of different groups in calculating the collision efficiency of OH with soot.

Research group	η_{OH}
Neoh et al.	0.13-0.28
Puri et al.	≥0.04
Roth et al.	0.2
Faeth et al.	0.09-0.15

1.4 Objective

The objective of my dissertation is to theoretically investigate the detailed pathways, products, and rates of soot oxidation by OH. This objective is met through the following organization of the dissertation. Chapter 2 describes the methodology used in calculating rates and exploring pathways. Chapter 3 describes the results of armchair oxyradical decomposition. Oxyradical decomposition was studied first because of the believed (and for the reactions studied in this dissertation confirmed) importance of oxyradical decomposition to soot oxidation. Chapter 4 contains the main results of this work, the energetics and kinetics of soot oxidation by OH, found primarily through the investigation of the prototype reaction of OH with a phenanthrene radical. Chapter 5 contains the analysis of the OH + phenanthrene radical reaction on the triplet surface. Finally, Chapter 6 finishes with general conclusions as well as recommendations for further research.

Chapter 2

Methodology

2.1 Quantum Chemistry Calculations

Density functional theory (DFT) was employed to calculate potential energy surfaces (PESs) of all stable species and transition states for the systems examined in Chapters 3, 4 and 5. Geometry optimization and vibrational frequency calculations were performed to identify all stationary points on the reaction pathways generally using the B3LYP hybrid functional [37,38] and a 6-311G(d,p) basis set [39]. Zero-point energies (ZPE) and vibrational frequencies were scaled by a factor of 0.967 [40]. The bond dissociation energy of several barrierless reactions were also calculated using the CBS-QB3 level of theory [41]. In a few instances, the M06-2X functional [42] was used; those instances are stated below. Transition states were confirmed to connect the reactant and product species by inspection of the normal mode for the single imaginary frequency of each saddle point. In addition, the transition structures were slightly perturbed along both directions of the negative frequency and then allowed to relax to the reactant and product. This provided additional confirmation connecting the reactant and product species. All the quantum-chemical calculations were carried out using the Gaussian 03 [43] and 09 [44] program packages.

2.2 Reaction Rate Calculations

2.2.1 Master Equation Modeling

The rate coefficients of the systems studied were computed using the MultiWell suite of codes [45,46]. MultiWell solves the one-dimensional time-dependent energy-transfer master equations for a multi-well and multi-channel unimolecular reaction system using the Monte Carlo stochastic method. Microcanonical rate coefficients for the elementary reactions of these systems were calculated with MultiWell at the Rice-Ramsperger-Kassel-Marcus (RRKM) level of theory. This approach, including the selected quantum chemistry level of theory, is estimated to produce rate coefficients to within an order-of-magnitude accuracy, appropriate for the exploratory nature of this dissertation. Previously, this approach was used and found reasonable agreement with available experimental data [47]. The most recent available MultiWell versions were used for the calculations. A major bug affecting MultiWell versions 2011 and earlier was fixed for all later versions [48]. The work reported here used versions 2011.3 and 2013[49,50], and are not affected by this bug. I wrote a Matlab program to extract the species fractions, to extract the elementary high-pressure rate constants and to manage the MultiWell runs. The code is provided in Appendix D.

The key inputs to MultiWell—reaction barriers, frequencies, and moments of inertia—were determined from quantum chemistry calculations. Following Gilbert and Smith [51], the real frequencies were examined by graphically visualizing the associated normal mode vibrations to identify internal rotational modes. All internal rotors were treated as 1-D hindered rotors. The rotational potentials were obtained by performing a relaxed potential energy surface scan. The code I wrote to extract the potential energy values for hindered rotors from the Gaussian calculation is provided in Appendix D.

Reaction rates were computed at temperatures ranging from 1500 to 2500 K and pressures from 0.01 to 10 atm. Argon was chosen as the bath gas collider. The exponential-down model with $\langle \Delta E \rangle_{\mathrm{down}}$ = 260 cm^{-1} was used to describe the collisional energy transfer [52]. Lennard-Jones parameters were estimated from an empirical correlation [53]. The exact count, with an energy grain size of 10 cm^{-1} for the low energy spacing, was employed to determine the density of states. For each set of initial conditions, the number of trials was varied to keep statistical error below 5 %.

Two primary types of MultiWell simulations can be performed, thermal decomposition and chemical decomposition. Determining rates from each type of simulation will be discussed in detail below, but first a discussion related to how the $\langle \Delta E \rangle_{\mathrm{down}}$ parameter was selected follows.

2.2.2 $\langle \Delta E \rangle_{\mathrm{down}}$ Parameter

As described above, a constant $\langle \Delta E \rangle_{\mathrm{down}}$ = 260 cm^{-1} was used. One could consider using a temperature-dependent $\langle \Delta E \rangle_{\mathrm{down}}$ expression, such as Equation 4.1 from Hippler et. al.[54],

$$-\langle \Delta E \rangle \simeq \frac{\langle \Delta E \rangle_{\mathrm{down}}^2}{\langle \Delta E \rangle_{\mathrm{down}} + kT} \tag{2.1}$$

Using $\langle \Delta E \rangle$ = –130 cm^{-1} from the above cited reference produces $\langle \Delta E \rangle_{\mathrm{down}}$ values of 439 to 545 cm^{-1} for the temperature range of 1500 to 2500 K, respectively.

Figure 2.1 compares the phenoxy decomposition rates calculated using $\langle \Delta E \rangle_{\mathrm{down}}$ = 260 cm^{-1} with those computed with Equation 2.1. The rate coefficients calculated using the constant $\langle \Delta E \rangle_{\mathrm{down}}$ value are closer to the experimental results than those calculated using Equation 2.1. This observation can be further supported by the work on the decomposition of phenoxy by Carstensen and Dean [55]. These authors used a constant $\langle \Delta E \rangle_{down}$ with even a lower value, 200 cm^{-1}. Also, in another study [56] Golden reported lower values of $\langle \Delta E \rangle_{down}$, albeit for a smaller system than phenoxy, yet smaller than prior literature recommendations.

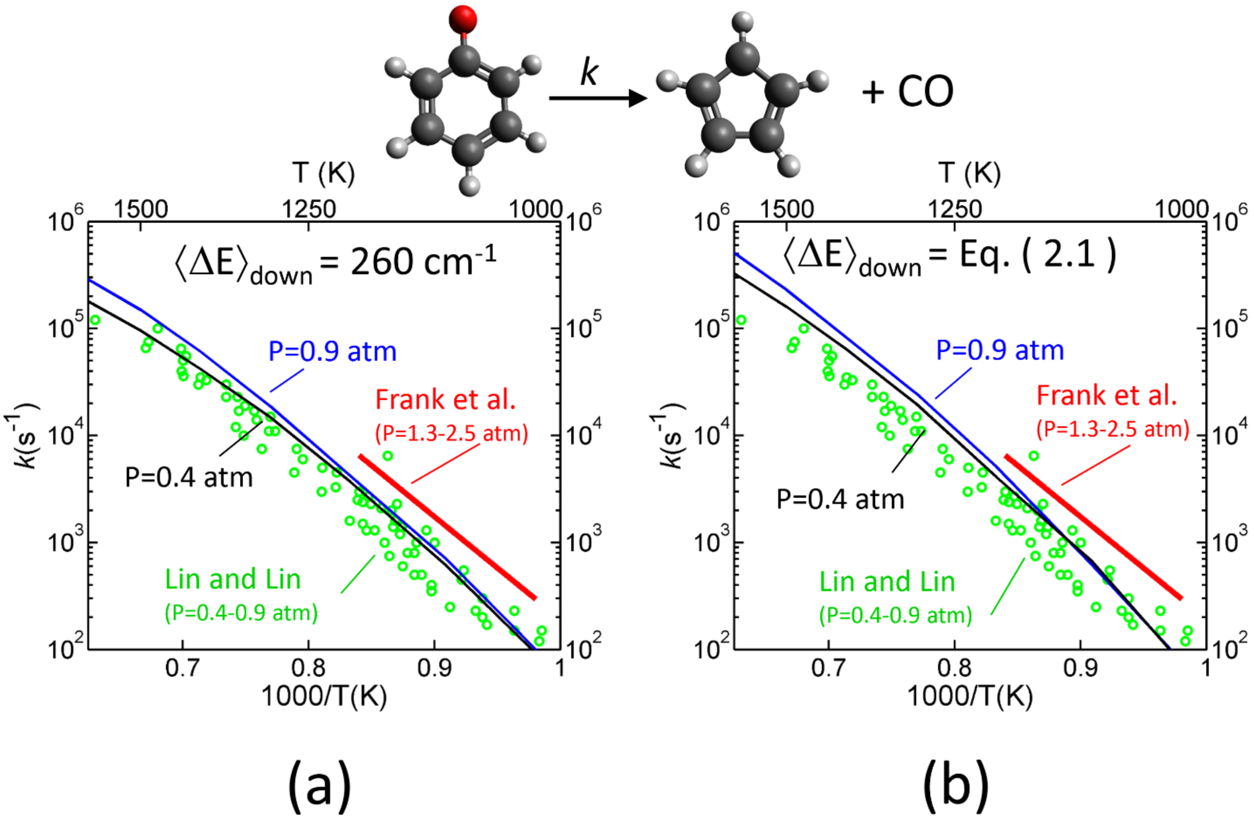


Figure 2.1. Calculation of the thermal decomposition rate coefficient of phenoxy, based on calculations from You et al. [47]. (a) calculated with a constant $\langle \Delta E \rangle_{down}$ value of 260 cm^{-1}. (b) calculated with a variable $\langle \Delta E \rangle_{down}$, calculated using Equation 2.1. The green circles are experimental results from Lin and Lin [57] and the solid red lines are the results from Frank et al. [58]. The blue and black lines are MultiWell calculations at the indicated pressures.

Based on all above observations and to maintain continuity with previous MultiWell calculations performed in the Frenklach group, I decided to use $\langle \Delta E \rangle_{down}$ = 260 cm^{-1}. In some instances, for comparison, calculations using Equation 2.1 to define $\langle \Delta E \rangle_{down}$ were performed and will be discussed in subsequent chapters.

2.2.3 Determining Thermal Decomposition Rate Coefficients

The thermal decomposition rate coefficients, calculated using MultiWell, are derived from the exponential decay of the reactant molecule after a period of initial relaxation [48,52]. A MultiWell simulation is started with a thermally activated initial energy distribution. After a period of initial relaxation, the average value of the internal energy approaches thermal equilibrium, and the reactant molecule began to decompose exponentially. This is shown in Figure 2.2. The PES pathways used in this calculation is shown below in Figure 3.2. The green line is the average internal energy of the reactant, while the blue and red lines are the reactant and product species fractions, respectively. The slope of the decay of the reactant on a semi-log plot yielded the rate coefficient of interest. If the system contains multiple products, the rate of formation of each product is calculated by multiplying the accumulated product species fraction by the decomposition rate of the reactant.

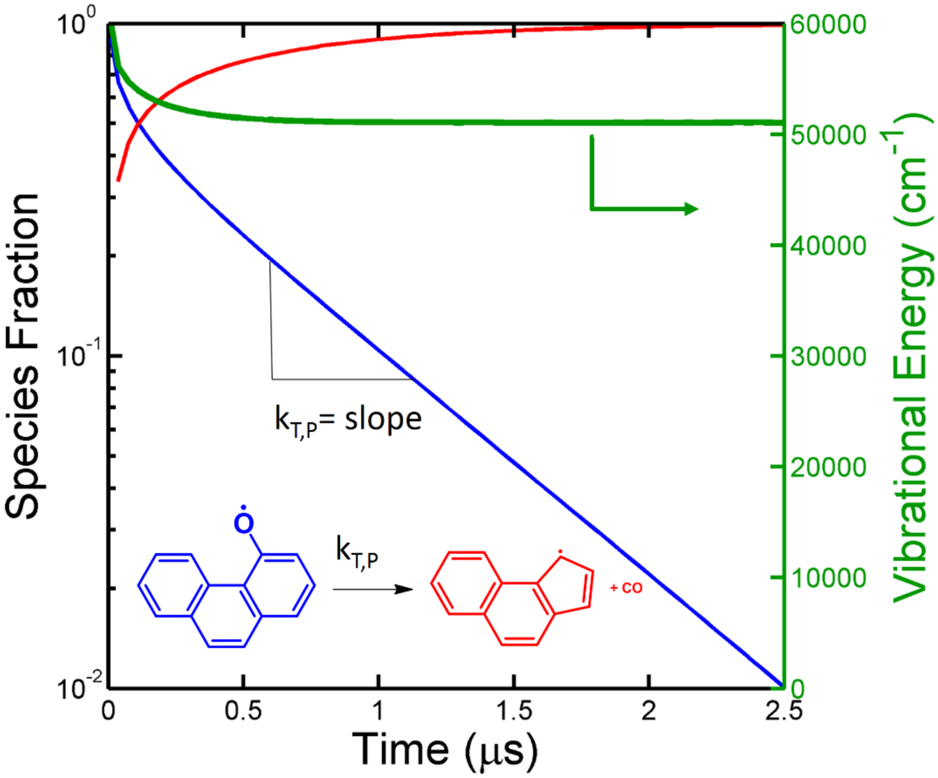


Figure 2.2. Representative example demonstrating how pressure and temperature dependent thermal decomposition rates are calculated in MultiWell. The green line, plotting the internal energy of the reactant with time, is associated with the right axis. After the internal energy (green line) becomes constant, the slope of the reactant (blue line) is calculated and is the temperature and pressure dependent rate constant for the reaction. The red line is the product specie fraction.

A key part of the analysis of a MultiWell thermal decomposition simulation is noting if there is significant accumulation of any intermediates. In the example shown in Figure 2.2, there was no accumulation of species fraction for any intermediate. If there is accumulation, a number of scenarios may exist. The accumulating intermediate may be in partial equilibrium. It may also suggest that there is no single phenomenological, time-independent rate constant that can describe that system. Rather the system would be described as a multi-step process with finite rates among wells. Another approach would be to describe the overall rate constant as being time-dependent. Generally, the thermal decomposition rates calculated in this dissertation did not have appreciable accumulation of intermediate species. For each case discussed in subsequent chapters, specific details are provided.

2.2.4 Determining Chemical Activation Rate Coefficients

The chemical-activated rate coefficients were derived from the accumulated species fractions of the products, as have been done previously [23] in the Frenklach group. The accumulated species fractions were found by running a MultiWell simulation starting with a chemical-activated initial energy distribution for the initial adduct. The species fractions were found after the average energy of the initial adduct reached 5% of the steady state value—indicating the end of the chemically-activated simulation. The product formation rates were calculated by multiplying the species fraction of the products by the high-pressure reaction rate of the adduct formation reaction. Figure 4.14 and Figure 4.15 in Section 4.2.3 below demonstrate this procedure and show how the species fractions are identified.

If at the end of the chemically-activated simulation, there is accumulation of intermediates, this suggests that chemical-activation was insufficient to drive the reaction through to product. In this case, the thermal decomposition of the accumulated intermediate is calculated. Additional details and examples of this situation are discussed in Chapter 4.

2.2.5 Barrierless Reaction Rate Calculations

Rate coefficients of barrierless reactions were calculated using the variable reaction coordinate (VRC) approach, as implemented in VariFlex [59]. Briefly, the VRC approach separates the transition state's degrees of freedom into "conserved" and "transitional" modes. The conserved modes have little change over the reaction process and are treated as rigid rotors or harmonic oscillators by directly computing the corresponding sums of states. The transitional modes are treated classically through a phase-space integral. The partition function of the transition state is then calculated through a convolution of these two modes. The bond length associated with the barrierless reaction is varied, and the contribution of the transitional modes to the partition function recalculated, until a minimum reaction rate is found [60]. The microcanonical rate constants calculated in this manner are entered into MultiWell using the .rke file format, as described in the MultiWell manual. This allows for the direct inclusion of barrierless reactions into a MultiWell simulation.

The VariFlex inputs are similar to MultiWell, with matching energy grain sizes and maximum energy. A Morse [61] or Varshni [62,63] potential was fit to a PES scan performed at the B3LYP/6-311G(d,p) level for each barrierless reaction. The potential form with the best fit was used in the barrierless reactions.

Further details about which form is used and limitations of VariFlex are provided in Chapter 4.

Chapter 3

Armchair Oxyradicals

In this chapter the results of investigation into armchair oxyradical decomposition are presented. The main focus of this dissertation is soot oxidation by OH, however, due to the assumed prominence of oxyradicals on soot oxidation pathways, I investigated their decomposition first. The usefulness of this approach will be confirmed in Chapter 4 when oxyradicals were found to play a key role.

First, before discussing my work, I will review recent work completed by the Frenklach group on oxyradicals.

3.1 Zigzag Edge Oxyradical Decomposition

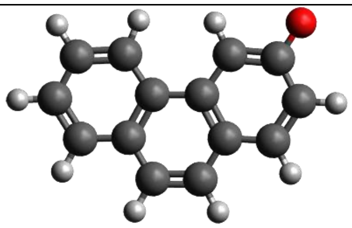
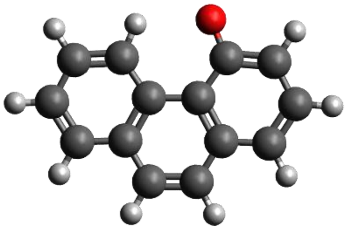
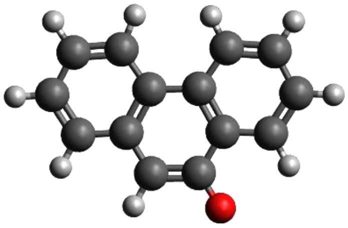
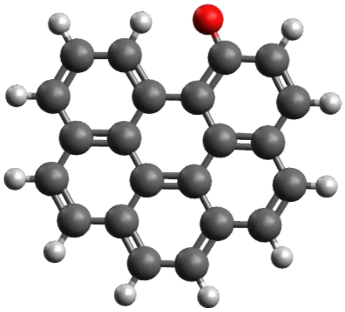
As discussed above, oxyradicals are assumed to be key intermediates of soot oxidation. Because of this, the Frenklach group initially examined the thermodynamic stability of graphene-edge oxyradicals, located at both zigzag and armchair sites [64,65] to gain insight into the role oxyradicals may play in soot formation. It turned out that thermodynamic stability varies substantially at different O chemisorbed sites, and this variability can be explained and correlated with substrate aromaticity. Next the group studied the kinetics of graphene zigzag edge oxyradical decomposition [47]. The results indicated that the rate of decomposition varies with the location of the O chemisorbed site on the zigzag edge. The principal conclusion, combining the thermodynamic [64,65] and kinetic results [47], is that only the outer rings of a zigzag edge are able to undergo oxidation, similar to phenoxy decomposition [55,66,67], whereas the inner rings resist oxidation in combustion environments. The next question was how armchair edge oxyradicals decompose and compare to zigzag edges. That investigation forms this chapter.

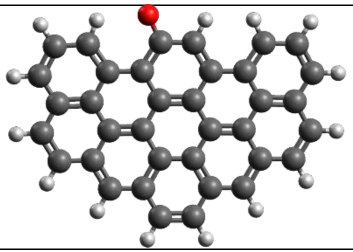
In this Chapter, I present the continuation of this oxyradical investigation to armchair edge oxyradical decomposition [52]. First the prototype PAHs are defined, then the PES are presented, followed by the computed rate coefficients and finally conclude with the implications of these findings for soot oxidation.

3.2 Armchair Prototypes

To study the decomposition of armchair edge oxyradicals, five molecules were selected as prototypes. These structures are displayed in Table 3.1. Phenanthrene oxyradicals I and II were selected to examine the differences in decomposition rate between the two principal armchair sites. Phenanthrene oxyradical III was included to provide comparison with the previously studied zigzag edge decomposition [47]. Benzoperylene oxyradical and the extended-armchair oxyradical have oxygen located on an armchair site that is the same as in phenanthrene II, but part of a larger substrate. The intent of including these larger substrates is to examine if and by how much the decomposition rate for the same edge site changes with substrate size.

Table 3.1. Armchair Oxyradical Structures

Specie Name	Structure
Phenanthrene I	
Phenanthrene II	
Phenanthrene III	
Benzoperylene	

Specie Name	Structure
Extended Armchair	

3.3 PES Results

Decomposition routes for phenanthrene oxyradicals I, II, and III, shown in Figure 3.1, Figure 3.2, and Figure 3.3, respectively, decompose via similar pathways and intermediates. The three pathways each contain a cyclic intermediate **2**, and all have at least one ring-opening intermediate **5**. For phenanthrene oxyradical I, two five-member rings with attached CO, intermediates **3** and **7**, were found. For phenanthrene oxyradicals II and III, only one such intermediate, **3**, was discovered. An additional channel was found for phenanthrene oxyradical II, namely **TS 2**-**4**, which connects intermediate **2** directly to product **4**.

These three systems are similar to those computed for the decomposition of pentacene corner oxyradicals [47], which also included the cyclic (**2**), attached-CO (**3**), and ring-opening (**5**) intermediates. Furthermore, the products of decomposition are also comparable in that all contain a five-member ring. Barrier energies of the corner-pentacene and phenanthrene oxyradical decomposition pathways are also very close to each other, often within 3-4 kcal/mol. Such parallels in the reaction pathways indicate that the armchair-edge and corner zigzag-edge decompositions are comparable and could be classified as equivalent types of oxidation reactions.

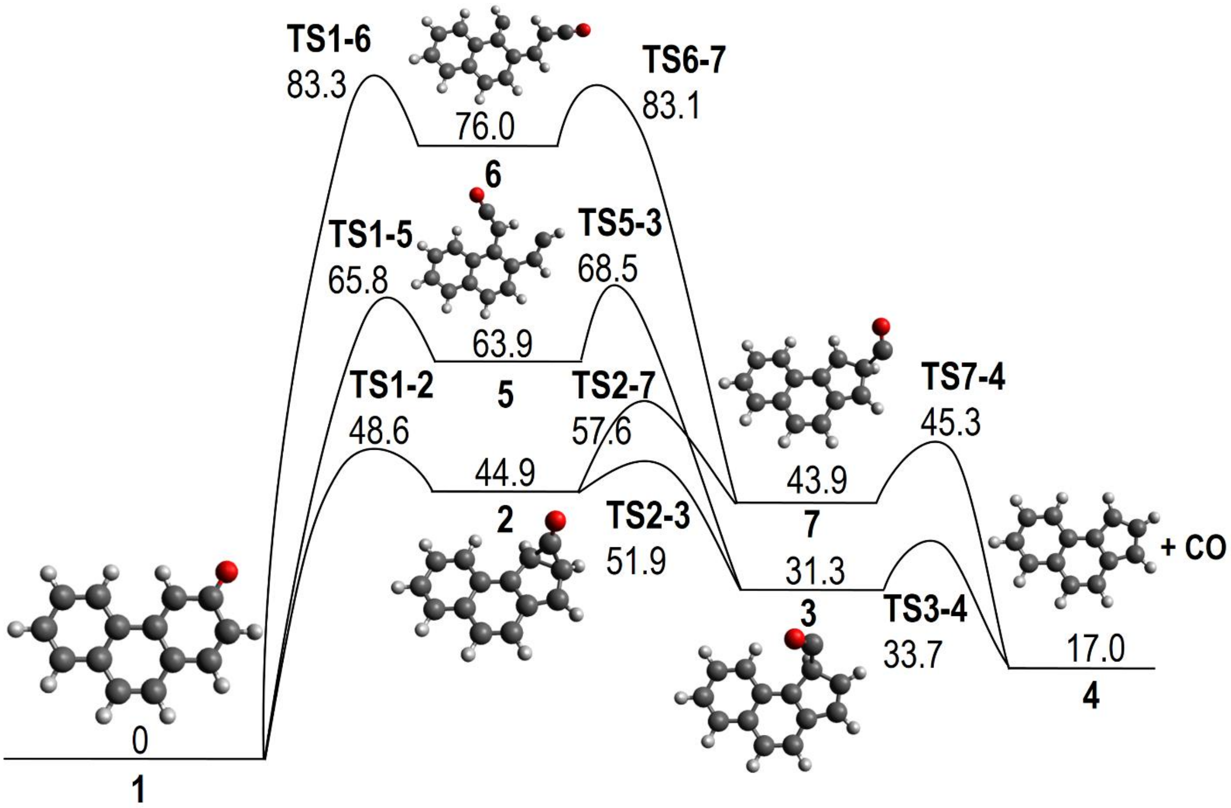


Figure 3.1. Minimum potential energy paths for the thermal decomposition of the phenanthrene I oxyradical, at the B3LYP/6-311G(d,p) level. Energies are in kcal/mol at 0 K relative to the reactant and include ZPE.

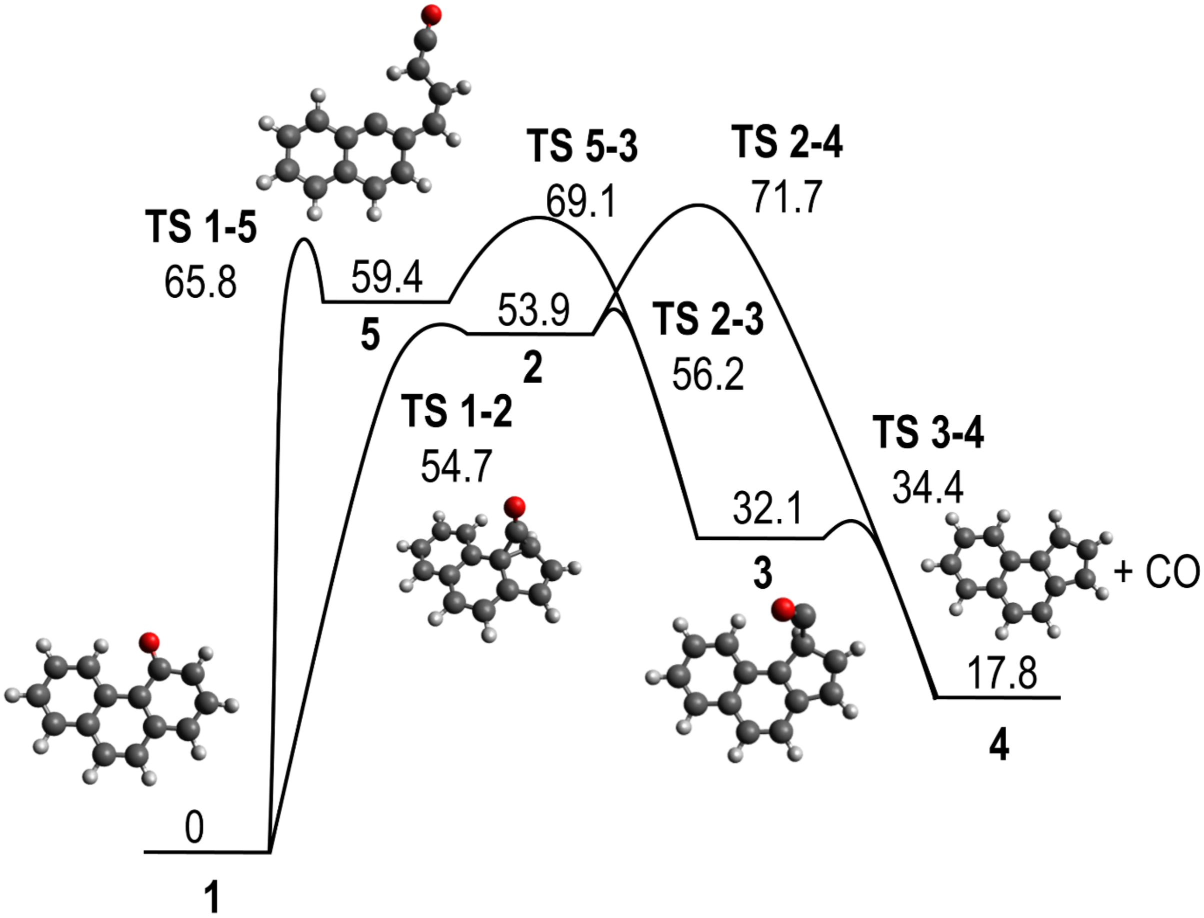


Figure 3.2. Minimum potential energy paths for the thermal decomposition of the phenanthrene II oxyradical, at the B3LYP/6-311G(d,p) level. Energies are in kcal/mol at 0 K relative to the reactant and include ZPE.

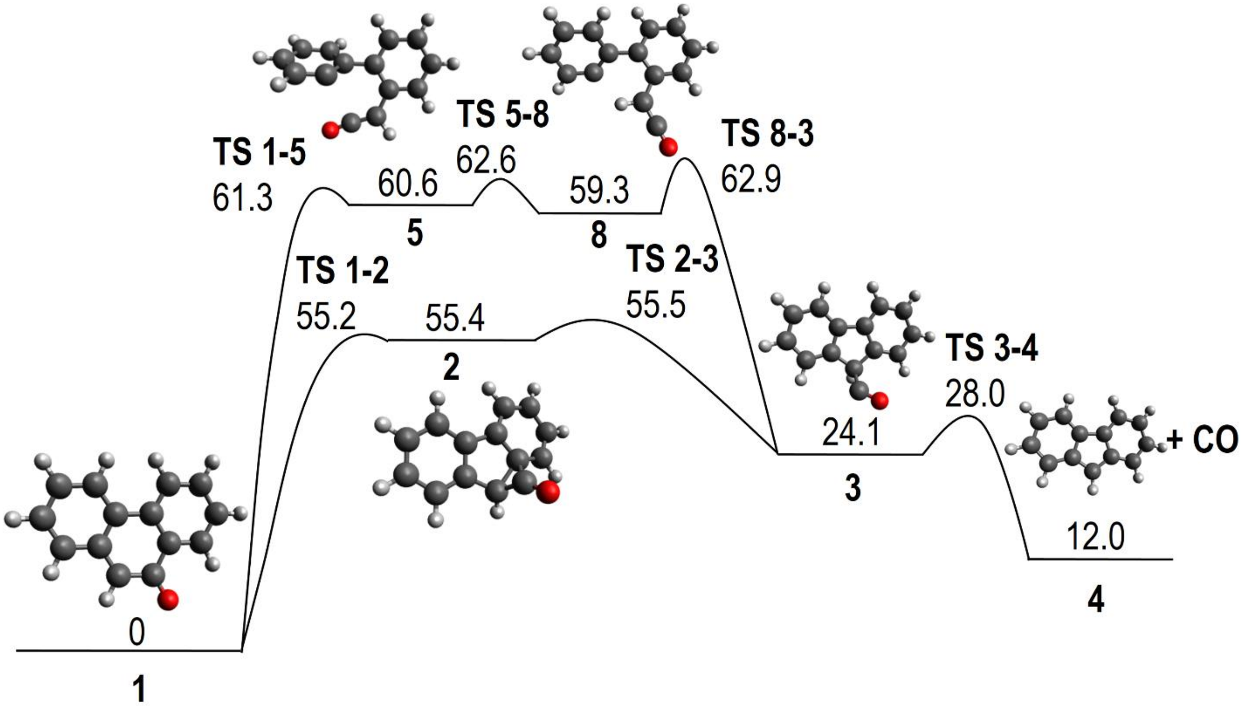


Figure 3.3. Minimum potential energy paths for the thermal decomposition of the phenanthrene III oxyradical, at the B3LYP/6-311G(d,p) level. Energies are in kcal/mol at 0 K relative to the reactant and include ZPE.

Phenanthrene oxyradicals I, II, and III are all made up of a single row of six-member rings. To test the influence of substrate size on decomposition kinetics, the benzoperylene and extended-armchair oxyradicals were studied; both have oxygen on a site similar to that in phenanthrene II. The phenanthrene II and benzoperylene decomposition pathways, shown in Figure 3.2 and Figure 3.4, respectively, contain the same intermediates, but the energy of the highest transition state barrier along the lowest potential energy path (**TS 1**-**2**) is larger by 7 kcal/mol for benzoperylene. Furthermore, the benzoperylene ring-opening barrier (**TS 1**-**5**) is 13.5 kcal/mol higher than the similar phenanthrene II barrier. As shown in the next section, these higher barriers lead to an almost tenfold slower decomposition rate for benzoperylene oxyradical relative to phenanthrene II oxyradical. The extended-armchair decomposition pathway differs from the phenanthrene II and benzoperylene pathways. The extended-armchair pathway, shown in Figure 3.5, does not contain the cyclic intermediate **2**, but it does have the ring-opening intermediate **5**. In this case, rather than proceeding from **1** to **2** to **3** as with the other structures, the extended-armchair oxyradical reacts directly from **1** to **3**. The difference in potential energy between the highest barrier on the lowest energy path of the extended-armchair (**TS 1**-**3**) and that of benzoperylene (**TS 1**-**2**) is 2.8 kcal/mol. This difference is counteracted by a 11.7 kcal/mol higher ring-opening barrier (**TS 1**-**5**) of benzoperylene compared to that of the extended-armchair. These opposing trends nearly cancel and, as shown in the next section, the extended-armchair and benzoperylene oxyradicals decompose at similar rates.

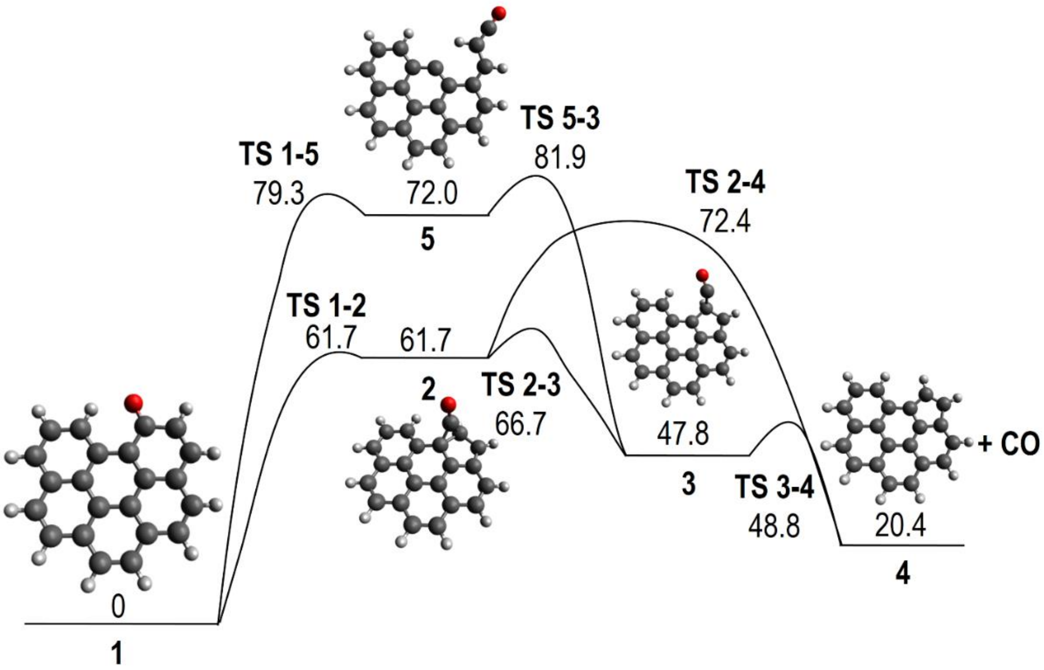


Figure 3.4. Minimum potential energy paths for the thermal decomposition of the benzoperylene oxyradical, at the B3LYP/6-311G(d,p) level. Energies are in kcal/mol at 0 K relative to the reactant and include ZPE.

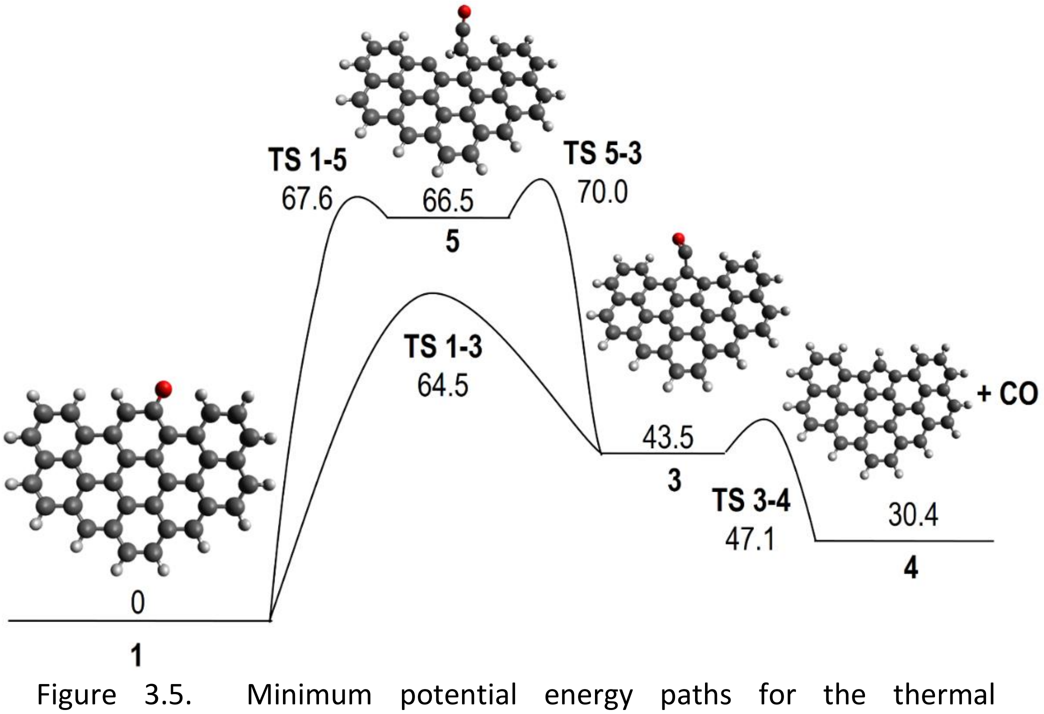
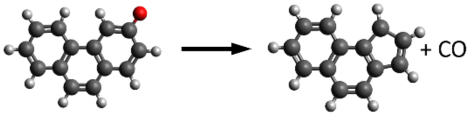


Figure 3.5. Minimum potential energy paths for the thermal decomposition of the extended armchair oxyradical, at the B3LYP/6-311G(d,p) level. Energies are in kcal/mol at 0 K relative to the reactant and include ZPE.

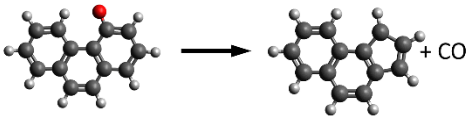
For all molecular structures, the zero-point energies, expectation values of the S^2 operator, vibrational frequencies, rotational constants, and the Cartesian coordinates for all optimized structures are included in Appendix A, Table A.6 and Table A.7.

3.4 Reaction Rate Coefficients

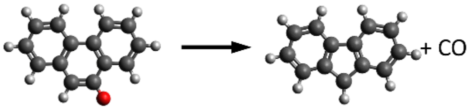
The main results of this chapter are reaction rates, based on the above PESs, calculated for the following five reactions:



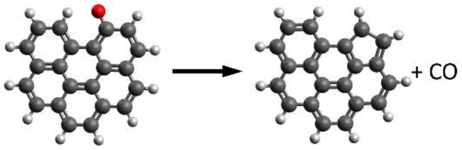
(R3.1)



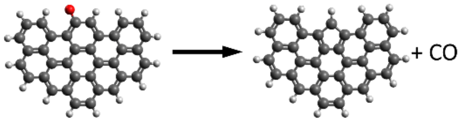
(R3.2)



(R3.3)



(R3.4)



(R3.5)

The principal products of oxyradical decompositions were the attached (embedded) five-member ring and CO. The accumulation of other species was negligible for the conditions studied.

The rate coefficients at specific values of pressure and temperature were computed by solving the master equations using the MultiWell suite of codes. The computed values of the rate coefficients of Reactions R3.1−R3.5 for a matrix of temperatures and pressures are reported in Table 3.2−Table 3.6 and in graphical form in Figure 3.6. These were computed employing a constant $\langle \Delta E \rangle_{\text{down}}$. For the purpose of comparison, the rate coefficients were also calculated using the temperature-dependent $\langle \Delta E \rangle_{\text{down}}$ expression Equation 2.1; these values are reported in Table 3.7−Table 3.11. All other references in this dissertation to the rates of Reactions R3.1−R3.5 were calculated using the constant $\langle \Delta E \rangle_{\text{down}}$ value. The average difference between the rate coefficients calculated using the two approaches, a constant $\langle \Delta E \rangle_{\text{down}}$ and temperature-dependent $\langle \Delta E \rangle_{\text{down}}$, was a factor of 2 and the maximum difference was a factor of 3.3. I would expect these differences to be larger for smaller systems which have greater pressure dependence. On the other hand, for larger systems the sensitivity to $\langle \Delta E \rangle_{\text{down}}$ would be expected to decrease. For example, the average difference between the two $\langle \Delta E \rangle_{\text{down}}$ calculations for phenanthrene II was a factor of 2.2, while for benzoperylene and the extended-armchair the difference decreased with size to a factor of 1.8 and 1.5, respectively. All of these reactions displayed similar pressure and temperature dependence.

Table 3.2. Rate coefficients (in s^{-1}) of the decomposition of phenanthrene oxyradical I, Reaction R3.1, using $\langle \Delta \mathrm{E} \rangle_{\text{down}} = 260\ \mathrm{cm}^{-1}$.

	P(atm)				
T(K)	0.01	0.1	1	10	k_∞
1500	2.7E+04	1.2E+05	3.7E+05	8.0E+05	1.3E+06
1600	3.8E+04	1.9E+05	7.1E+05	1.9E+06	4.1E+06
1700	4.9E+04	2.7E+05	1.2E+06	3.6E+06	1.1E+07
1800	6.1E+04	3.5E+05	1.7E+06	6.0E+06	2.7E+07
1900	7.3E+04	4.3E+05	2.2E+06	9.1E+06	6.2E+07
2000	8.3E+04	5.1E+05	2.8E+06	1.3E+07	1.3E+08
2100	9.4E+04	5.9E+05	3.4E+06	1.6E+07	2.6E+08
2200	1.0E+05	6.7E+05	3.9E+06	2.0E+07	4.8E+08
2300	1.1E+05	7.4E+05	4.5E+06	2.4E+07	8.6E+08
2400	1.2E+05	8.1E+05	5.0E+06	2.8E+07	1.5E+09
2500	1.3E+05	8.7E+05	5.5E+06	3.1E+07	2.4E+09

Table 3.3. Rate coefficients (in s^{-1}) of the decomposition of phenanthrene oxyradical II, Reaction R3.2, using $\langle \Delta \mathrm{E} \rangle_{\text{down}} = 260\ \mathrm{cm}^{-1}$.

	P(atm)				
T(K)	0.01	0.1	1	10	k_∞
1500	1.2E+04	4.2E+04	1.1E+05	1.7E+05	2.4E+05
1600	1.9E+04	8.0E+04	2.5E+05	5.2E+05	8.9E+05
1700	2.7E+04	1.3E+05	4.8E+05	1.2E+06	2.9E+06
1800	3.5E+04	1.8E+05	7.8E+05	2.4E+06	8.2E+06
1900	4.4E+04	2.4E+05	1.2E+06	4.2E+06	2.1E+07
2000	5.2E+04	3.1E+05	1.6E+06	6.4E+06	5.1E+07
2100	6.0E+04	3.7E+05	2.0E+06	8.9E+06	1.1E+08
2200	6.9E+04	4.3E+05	2.4E+06	1.2E+07	2.4E+08

2300	7.6E+04	4.9E+05	2.9E+06	1.5E+07	4.7E+08
2400	8.3E+04	5.4E+05	3.3E+06	1.8E+07	8.9E+08
2500	8.9E+04	6.0E+05	3.7E+06	2.1E+07	1.6E+09

Table 3.4. Rate coefficients (in s^{-1}) of the decomposition of phenanthrene oxyradical III, Reaction R3.3, using $\langle \Delta E \rangle_{down}$ = 260 cm^{-1}.

	P(atm)				
T(K)	0.01	0.1	1	10	k_∞
1500	1.2E+04	4.7E+04	1.3E+05	2.2E+05	3.3E+05
1600	2.0E+04	8.8E+04	2.9E+05	6.4E+05	1.2E+06
1700	2.8E+04	1.4E+05	5.5E+05	1.5E+06	3.7E+06
1800	3.7E+04	2.0E+05	8.8E+05	2.9E+06	1.0E+07
1900	4.6E+04	2.6E+05	1.3E+06	4.8E+06	2.5E+07
2000	5.5E+04	3.3E+05	1.7E+06	7.2E+06	5.7E+07
2100	6.2E+04	3.9E+05	2.2E+06	9.9E+06	1.2E+08
2200	7.1E+04	4.5E+05	2.6E+06	1.3E+07	2.4E+08
2300	7.9E+04	5.1E+05	3.1E+06	1.6E+07	4.4E+08
2400	8.6E+04	5.7E+05	3.5E+06	1.9E+07	7.7E+08
2500	9.2E+04	6.3E+05	3.9E+06	2.2E+07	1.3E+09

Table 3.5. Rate coefficients (in s^{-1}) of the decomposition of the benzoperylene oxyradical, Reaction R3.4, using $\langle \Delta E \rangle_{down}$ = 260 cm^{-1}.

	P(atm)				
T(K)	0.01	0.1	1	10	k_∞
1500	3.0E+03	6.6E+03	9.1E+03	1.0E+04	1.2E+04
1600	6.5E+03	1.9E+04	3.3E+04	4.0E+04	5.1E+04
1700	1.1E+04	4.1E+04	9.5E+04	1.4E+05	1.8E+05
1800	1.7E+04	7.2E+04	2.1E+05	3.7E+05	5.6E+05
1900	2.4E+04	1.1E+05	3.9E+05	8.9E+05	1.5E+06
2000	3.1E+04	1.6E+05	6.2E+05	1.7E+06	3.9E+06
2100	3.8E+04	2.0E+05	8.9E+05	2.9E+06	9.0E+06
2200	4.5E+04	2.5E+05	1.2E+06	4.4E+06	2.0E+07
2300	5.1E+04	3.0E+05	1.5E+06	6.2E+06	4.0E+07
2400	5.7E+04	3.5E+05	1.9E+06	8.2E+06	7.7E+07
2500	6.4E+04	4.0E+05	2.2E+06	1.0E+07	1.4E+08

Table 3.6. Rate coefficients (in s^{-1}) of the decomposition of the extended-armchair oxyradical, Reaction R3.5, using $\langle\Delta E\rangle_{down}$ = 260 cm^{-1}.

	P(atm)				
T(K)	0.01	0.1	1	10	k_∞
1500	3.3E+03	6.4E+03	8.3E+03	8.4E+03	1.3E+04
1600	7.6E+03	2.0E+04	3.2E+04	3.7E+04	5.4E+04
1700	1.4E+04	4.5E+04	9.7E+04	1.3E+05	1.9E+05
1800	2.1E+04	8.2E+04	2.3E+05	3.7E+05	5.9E+05
1900	2.9E+04	1.3E+05	4.3E+05	9.0E+05	1.6E+06
2000	3.7E+04	1.8E+05	7.0E+05	1.8E+06	4.0E+06
2100	4.5E+04	2.4E+05	1.0E+06	3.2E+06	9.2E+06
2200	5.4E+04	2.9E+05	1.4E+06	4.9E+06	1.9E+07
2300	6.2E+04	3.5E+05	1.8E+06	6.9E+06	3.9E+07
2400	6.9E+04	4.1E+05	2.1E+06	9.2E+06	7.2E+07
2500	7.7E+04	4.7E+05	2.6E+06	1.2E+07	1.3E+08

Table 3.7. Rate coefficients (in s^{-1}) of the decomposition of phenanthrene oxyradical I, Reaction R3.1, using the temperature-dependent $\langle\Delta E\rangle_{down}$ expression.

	P(atm)			
T(K)	0.01	0.1	1	10
1500	5.2E+04	2.1E+05	5.6E+05	9.7E+05
1600	8.1E+04	3.6E+05	1.2E+06	2.5E+06
1700	1.1E+05	5.5E+05	2.1E+06	5.5E+06
1800	1.5E+05	7.7E+05	3.2E+06	1.0E+07
1900	1.8E+05	1.0E+06	4.6E+06	1.6E+07
2000	2.2E+05	1.3E+06	6.2E+06	2.4E+07
2100	2.6E+05	1.5E+06	7.9E+06	3.3E+07
2200	3.0E+05	1.8E+06	9.5E+06	4.3E+07
2300	3.4E+05	2.1E+06	1.1E+07	5.4E+07
2400	3.7E+05	2.3E+06	1.3E+07	6.5E+07
2500	4.1E+05	2.6E+06	1.5E+07	7.6E+07

Table 3.8. Rate coefficients (in s^{-1}) of the decomposition of phenanthrene oxyradical II, Reaction R3.2, using the temperature-dependent $\langle \Delta E \rangle_{down}$ expression.

	P(atm)			
T(K)	0.01	0.1	1	10
1500	2.1E+04	6.7E+04	1.4E+05	2.0E+05
1600	3.8E+04	1.4E+05	3.8E+05	6.4E+05
1700	5.8E+04	2.5E+05	8.0E+05	1.7E+06
1800	8.2E+04	3.9E+05	1.4E+06	3.8E+06
1900	1.1E+05	5.5E+05	2.3E+06	7.1E+06
2000	1.4E+05	7.3E+05	3.3E+06	1.2E+07
2100	1.7E+05	9.3E+05	4.5E+06	1.8E+07
2200	2.0E+05	1.1E+06	5.8E+06	2.5E+07
2300	2.3E+05	1.4E+06	7.2E+06	3.3E+07
2400	2.6E+05	1.6E+06	8.7E+06	4.2E+07
2500	2.8E+05	1.8E+06	1.0E+07	5.1E+07

Table 3.9. Rate coefficients (in s^{-1}) of the decomposition of phenanthrene oxyradical III, Reaction R3.3, using the temperature-dependent $\langle \Delta E \rangle_{down}$ expression.

	P(atm)			
T(K)	0.01	0.1	1	10
1500	2.3E+04	7.8E+04	1.8E+05	2.5E+05
1600	4.1E+04	1.6E+05	4.6E+05	8.3E+05
1700	6.2E+04	2.8E+05	9.4E+05	2.1E+06
1800	8.7E+04	4.3E+05	1.7E+06	4.5E+06
1900	1.2E+05	6.0E+05	2.6E+06	8.3E+06
2000	1.5E+05	8.0E+05	3.7E+06	1.4E+07
2100	1.7E+05	1.0E+06	5.0E+06	2.0E+07
2200	2.1E+05	1.2E+06	6.4E+06	2.7E+07
2300	2.4E+05	1.4E+06	7.9E+06	3.6E+07
2400	2.7E+05	1.7E+06	9.4E+06	4.5E+07
2500	3.0E+05	1.9E+06	1.1E+07	5.5E+07

Table 3.10. Rate coefficients (in s^{-1}) of the decomposition of the benzoperylene oxyradical, Reaction R3.4, using the temperature-dependent $\langle \Delta E \rangle_{down}$ expression.

	P(atm)			
T(K)	0.01	0.1	1	10
1500	4.5E+03	8.2E+03	1.0E+04	1.0E+04
1600	1.1E+04	2.6E+04	4.0E+04	4.4E+04
1700	2.1E+04	6.4E+04	1.2E+05	1.5E+05
1800	3.5E+04	1.3E+05	3.0E+05	4.5E+05
1900	5.0E+04	2.1E+05	6.1E+05	1.1E+06
2000	6.9E+04	3.1E+05	1.1E+06	2.4E+06
2100	8.8E+04	4.3E+05	1.7E+06	4.4E+06
2200	1.1E+05	5.6E+05	2.4E+06	7.3E+06
2300	1.3E+05	6.9E+05	3.2E+06	1.1E+07
2400	1.5E+05	8.3E+05	4.0E+06	1.5E+07
2500	1.7E+05	9.7E+05	4.9E+06	2.0E+07

Table 3.11. Rate coefficients (in s^{-1}) of the decomposition of the extended-armchair oxyradical, Reaction R3.5, using the temperature-dependent $\langle \Delta E \rangle_{down}$ expression.

	P(atm)			
T(K)	0.01	0.1	1	10
1500	4.7E+03	7.9E+03	8.8E+03	8.9E+03
1600	1.2E+04	2.7E+04	3.7E+04	4.0E+04
1700	2.3E+04	6.6E+04	1.2E+05	1.4E+05
1800	3.7E+04	1.3E+05	3.0E+05	4.3E+05
1900	5.3E+04	2.1E+05	6.2E+05	1.1E+06
2000	7.0E+04	3.1E+05	1.1E+06	2.3E+06
2100	8.5E+04	4.2E+05	1.6E+06	4.3E+06
2200	9.9E+04	5.2E+05	2.2E+06	6.9E+06
2300	1.1E+05	6.2E+05	2.9E+06	1.0E+07
2400	1.2E+05	7.0E+05	3.5E+06	1.3E+07
2500	1.3E+05	7.7E+05	4.0E+06	1.7E+07

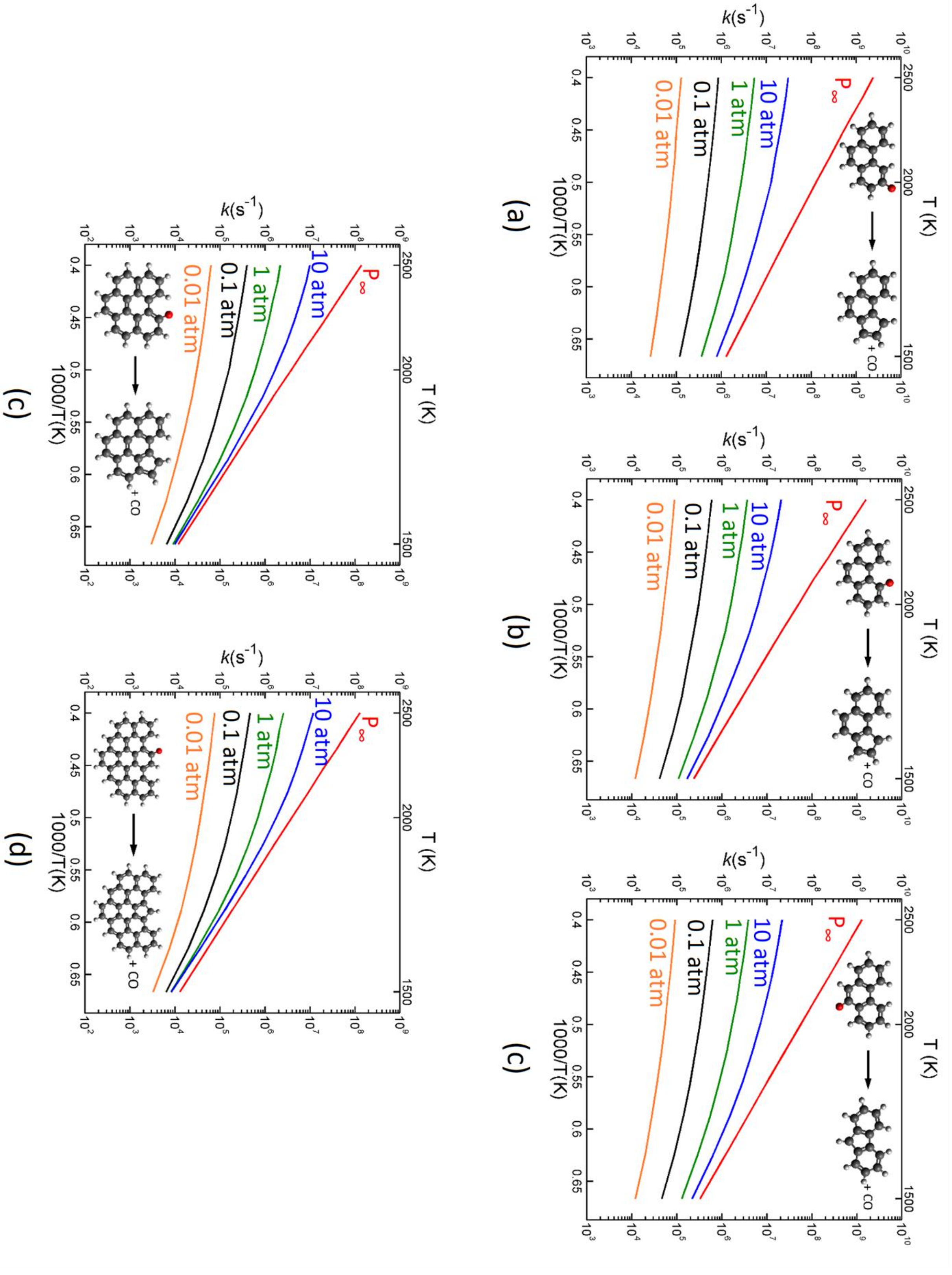


Figure 3.6. Thermal decomposition rate coefficients of Reactions R3.1−R3.5, shown in subpanels (a)−(d) respectively.

In observing the pressure dependence, it was desirable to calculate the high-pressure-limit rate coefficients for each of the overall Reactions R3.1–R3.5. To accomplish this aim, it was assumed that all intermediates of an individual reaction system were in steady state. The derived expressions, including tables of the high-pressure elementary reaction rates, are included in Appendix A Section A.1. The high-pressure rates reported above in Table 3.2–Table 3.11 and Figure 3.6 were calculated in this way. The fitted Arrhenius expressions for the high-pressure-limit rate coefficients of reactions R3.1–R3.5 are presented in Table 3.12.

Table 3.12. High-pressure-limit rate coefficients.

Reaction	Rate coefficient (s^{-1})
R3.1	$1.08\times10^{2}T^{3.28}\exp(-21866/T)$
R3.2	$4.00\times10^{-2}T^{4.38}\exp(-24624/T)$
R3.3	$6.42\times10^{10}T^{1.00}\exp(-29183/T)$
R3.4	$3.78\times10^{4}T^{2.59}\exp(-30151/T)$
R3.5	$4.47\times10^{12}T^{0.39}\exp(-33796/T)$

Inspection of rate coefficients computed for the three phenanthrene oxyradicals, displayed together in Figure 3.7, indicate that phenanthrene I, with oxygen farthest to the outside, decomposed faster than phenanthrene II, while the latter decomposed about as fast as phenanthrene III. The correlation of these rates with the molecular structure of the three phenanthrene oxyradicals was rationalized by counting “free edges”, a concept introduced in a previous study [47]. A “free edge” classifies the connectivity of the C-O site in the context of the multi-ring aromatic structure. For example, in phenanthrene I, C-O is connected, on both sides, to carbon atoms that are members of only one ring; each of these edges were then classified as free edges. On the other hand, C-O in phenanthrenes II and III is connected on one side to a C atom that is a member of two rings, and on the other side to a C atom that is a member of one ring. Therefore, phenanthrenes II and III contain only one free edge, with the non-free edge connected to the carbon atom that is a member of two rings. Using this simple structural classification enabled the rationalization of the relative ordering of the decomposition rates among phenanthrene oxyradicals I, II, and III. Phenanthrene I has two free edges and decomposed fastest, whereas II and III, each having just one free edge, decomposed slower than I and at nearly comparable rates.

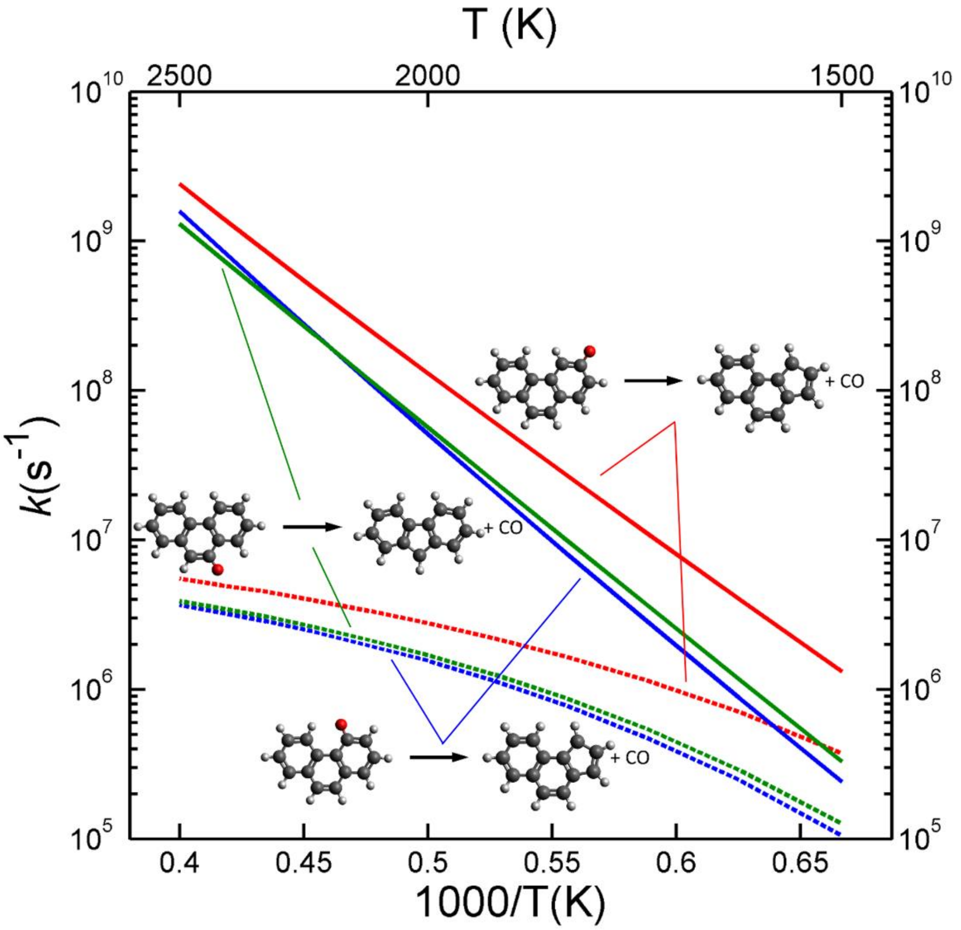


Figure 3.7. Rate coefficients of the decomposition of phenanthrene oxyradicals I (red), II (blue) and III (green). The solid lines are the high-pressure-limit values and the dashed lines are the rate coefficients at 1 atm.

Figure 3.8 compares the decomposition rates of phenanthrene II, benzoperylene, and the extended-armchair oxyradicals. Inspection of these findings indicated that the increase in substrate size, from phenanthrene to benzoperylene, reduced the computed reaction rate, whereas the rate seemed to level off with further increase in size, from benzoperylene to the extended-armchair oxyradical. The benzoperylene oxyradical decomposed nearly an order of magnitude slower than the phenanthrene II oxyradical. This was primarily due to the higher potential energy of **TS 1**-**2** and **TS 1**-**5** in the benzoperylene pathway compared to those in the phenanthrene II pathway. Comparing the extended-armchair energetics to that of benzoperylene indicated that although the lowest energy path for the extended-armchair had a higher barrier (**TS 1**-**3**) than benzoperylene (**TS 1**-**2**), it had a substantially lower barrier to ring-opening, thus making its decomposition rate competitive with that of benzoperylene oxyradical decomposition. These results indicate that benzoperylene may be sufficiently large to represent an armchair-edge reaction for an arbitrarily large graphene substrate.

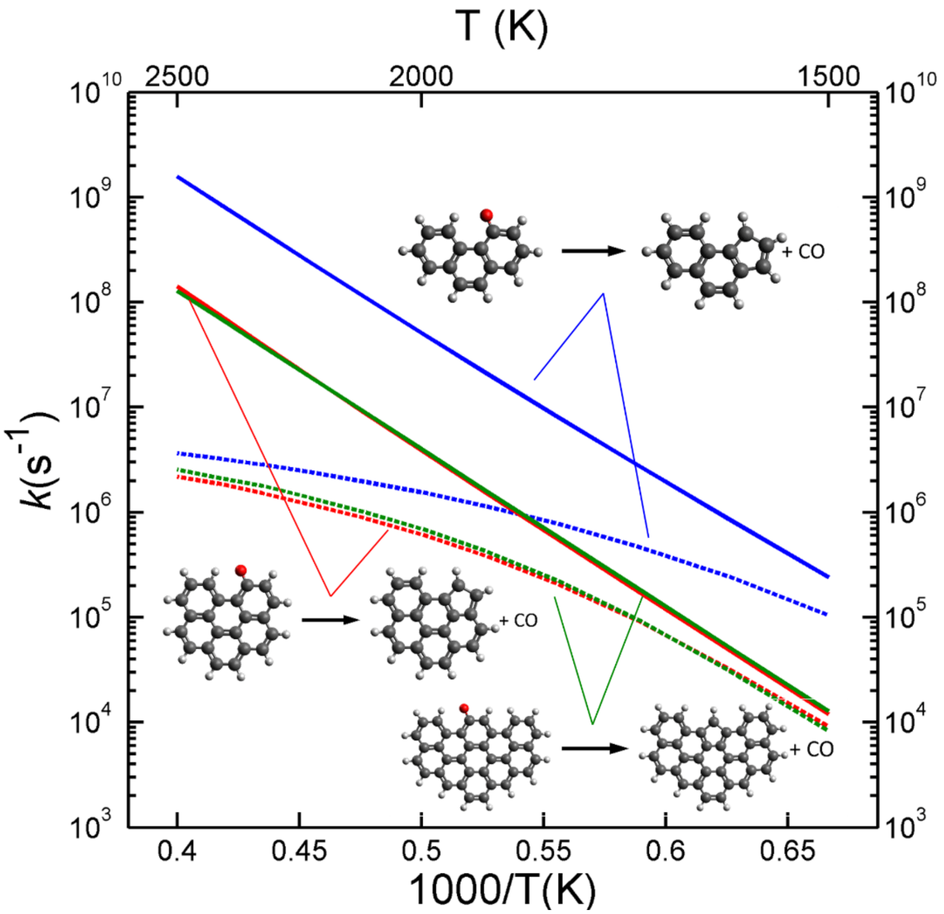


Figure 3.8. Rate coefficients of the decomposition of phenanthrene oxyradical II (blue), benzoperylene oxyradical (red), and the extended-armchair oxyradical (green). The solid lines are the high-pressure-limit values and the dashed lines are the rate coefficients at 1 atm.

Finally, comparing the decomposition rates of the armchair-edge and zigzag-edge oxyradicals highlighted the resemblance between the decomposition rates of the armchair and corner zigzag edges. Figure 3.9 displays the decomposition rates of phenanthrene I and II as well as those of pentacene I and II from a previous study [47]. Focusing first on the 1-atm results displayed in Figure 3.9, strong correlation between the phenanthrene and pentacene decomposition rates were observed, namely phenanthrene I and pentacene I decomposition rates (both in red) were very close to one another, as were the decomposition rates of phenanthrene II and pentacene II (both in blue). Structurally, phenanthrene I is similar to pentacene I—both have free edges on each side of the C-O bond. Likewise, phenanthrene II structurally resembles pentacene II, with a free edge on only one side of the C-O bond. Again, the structures with the same number of free edges decomposed at similar rates, and the structures with two free edges decomposed faster than those with one free edge. At the high-pressure limit, however, the correlation between the pentacene and phenanthrene oxyradical decomposition rates was weaker. The general trend within the different types of molecules still held, as oxyradical structures with more free edges decomposed at a faster rate than those with just one free edge. This “free-edge” analysis rationalizes one of the key results of this chapter, namely, that phenanthrene oxyradicals and corner pentacene oxyradicals decompose at similar rates.

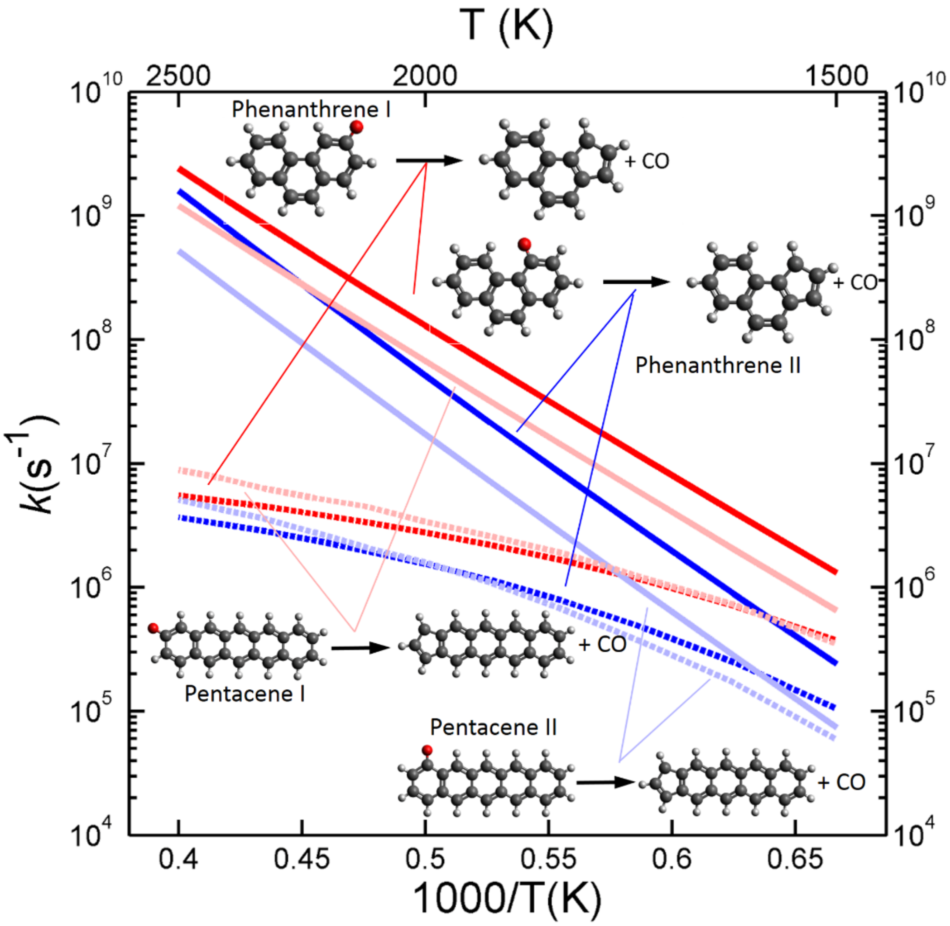


Figure 3.9. Rate coefficients of the decomposition of phenanthrene oxyradicals I and II (dark lines) and pentacene oxyradicals I and II (light lines) [47]. Red indicates a structure with two free edges while blue indicates a structure with one. The solid lines are the high-pressure-limit values and the dashed lines are the rate coefficients at 1 atm.

Branching ratios were also calculated for the ring-opening and cyclic pathway rates for reactions R3.1-R3.5, i.e., $k_{1\to2}/k_{1\to5}$ for R3.1-R3.4 and $k_{1\to3}/k_{1\to5}$ for R3.5. They are reported in Table 3.13–Table 3.17 for a range of temperatures and pressures. The ring-opening pathway generally dominates for reactions R3.2, R3.3, and R3.5, and the cyclic pathway dominates for reactions R3.1 and R3.4. The competitiveness of the ring-opening pathway is due to the higher entropy of the ring-opening transition structure compared to the cyclic pathway. The pressure dependent ratios were calculated using the MultiWell .flux file, while the high-pressure limit values were calculated using the elementary high-pressure rates.

Table 3.13. Branching ratios $k_{1\rightarrow2}/k_{1\rightarrow5}$ for phenanthrene oxyradical I. (The reaction path 1→6 did not exceed 30 % of 1→5).

	P(atm)				
T(K)	0.01	0.1	1	10	Hi-P
1500	189.3	76.5	36.8	21.8	15.8
1600	173.9	68.2	31.2	17.2	11.0
1700	163.1	62.6	27.7	14.5	7.6
1800	155.0	58.5	25.3	12.6	5.7
1900	147.9	55.1	23.3	11.3	4.2
2000	143.2	52.9	22.0	10.4	3.2
2100	138.9	50.7	20.8	9.7	2.6
2200	136.8	48.9	20.0	9.1	2.2
2300	132.6	47.6	19.3	8.7	1.8
2400	130.0	46.7	18.9	8.3	1.5
2500	127.9	45.6	18.2	8.1	1.3

Table 3.14. Branching ratios $k_{1\rightarrow2}/k_{1\rightarrow5}$ for phenanthrene oxyradical II.

	P(atm)				
T(K)	0.01	0.1	1	10	Hi-P
1500	1.9	1.2	0.8	0.7	0.6
1600	1.8	1.1	0.7	0.5	0.4
1700	1.6	1.0	0.6	0.5	0.3
1800	1.5	0.9	0.6	0.4	0.3
1900	1.4	0.8	0.5	0.4	0.2
2000	1.3	0.8	0.5	0.3	0.2
2100	1.3	0.8	0.5	0.3	0.2
2200	1.2	0.7	0.5	0.3	0.1
2300	1.2	0.7	0.4	0.3	0.1
2400	1.1	0.7	0.4	0.3	0.1
2500	1.1	0.6	0.4	0.3	0.1

Table 3.15. Branching ratios $k_{1\rightarrow2}/k_{1\rightarrow5}$ for phenanthrene oxyradical III.

	P(atm)				
T(K)	0.01	0.1	1	10	Hi-P
1500	1.0	0.8	0.7	0.6	0.5
1600	1.0	0.7	0.6	0.5	0.5
1700	0.9	0.7	0.6	0.5	0.4
1800	0.9	0.7	0.6	0.5	0.4
1900	0.9	0.7	0.5	0.4	0.3
2000	0.9	0.7	0.5	0.4	0.3
2100	0.8	0.6	0.5	0.4	0.3
2200	0.8	0.6	0.5	0.4	0.3
2300	0.8	0.6	0.5	0.4	0.3
2400	0.8	0.6	0.5	0.4	0.2
2500	0.8	0.6	0.5	0.4	0.2

Table 3.16. Branching ratios $k_{1\rightarrow2}/k_{1\rightarrow5}$ for the benzoperylene oxyradical.

	P(atm)				
T(K)	0.01	0.1	1	10	Hi-P
1500	18.3	12.2	9.9	9.2	8.6
1600	15.7	9.8	7.2	6.3	5.8
1700	14.0	8.3	5.7	4.6	4.2
1800	12.8	7.4	4.8	3.6	3.2
1900	11.9	6.7	4.2	3.0	2.5
2000	11.2	6.2	3.8	2.6	1.8
2100	10.7	5.8	3.5	2.3	1.4
2200	10.2	5.5	3.2	2.1	1.2
2300	9.8	5.3	3.1	1.9	1.0
2400	9.5	5.1	2.9	1.8	0.8
2500	9.2	4.9	2.8	1.7	0.7

Table 3.17. Branching ratios $k_{1\rightarrow3}/k_{1\rightarrow5}$ for the extended armchair oxyradical.

	P(atm)				
T(K)	0.01	0.1	1	10	Hi-P
1500	0.4	0.4	0.4	0.4	0.4
1600	0.4	0.4	0.4	0.3	0.3
1700	0.4	0.4	0.3	0.3	0.3
1800	0.4	0.3	0.3	0.3	0.3
1900	0.4	0.3	0.3	0.3	0.3
2000	0.4	0.3	0.3	0.3	0.3
2100	0.4	0.3	0.3	0.3	0.3
2200	0.4	0.3	0.3	0.3	0.3
2300	0.4	0.3	0.3	0.3	0.3
2400	0.3	0.3	0.3	0.3	0.2
2500	0.3	0.3	0.3	0.3	0.2

3.5 Correlation with Aromaticity

This chapter concludes by identifying potentially useful correlations between a simple geometric measure and the kinetics of oxyradical decomposition. These correlation could lead to practical rules for predicting oxyradical decomposition rate coefficients for arbitrary size and shape aromatics, thereby supplementing and enhancing models of soot oxidation.

3.5.1 Introduction to Aromaticity and HOMA

Polyaromatic hydrocarbons are structurally related to the benzene molecule. This connection implies strong similarity in electronic structure that characterizes aromatic systems, namely, that of delocalized bonding. However, in the analysis of chemical properties of prototype structures used to represent soot edges, this connection is rarely exploited. Such a connection can lead to formulation of simple quantitative or semi-quantitative predictive models that appeals to chemical intuition and help to rationalize properties of soot.

Aromaticity can be defined as the extra stabilization of a system featuring delocalized bonds with respect to a fictitious system with completely localized bonds. In practice, assessment of the resonance energy is a difficult task, especially for molecules that require multiple Kekule structures in the resonance description. Multiple measures of aromaticity have been proposed in order to simplify the task and connect the analysis to observable properties [68-70].

Considering the computational challenges associated with theoretical treatment of large PAHs it is reasonable to choose the simplest model of aromaticity that utilizes the observation that aromatic bonding is strongly associated with equalization of bond lengths due to formation of a delocalized bonding framework. In the Harmonic Oscillator Model of Aromaticity (HOMA) [71], one evaluates the mean deviation of bond lengths in a system under consideration with respect to bond lengths in benzene. It is further scaled such that HOMA = 0 for the Kekule form of benzene and HOMA = 1 for the aromatic form. Figure 3.10 details the formulation and limiting cases of HOMA.

Harmonic Oscillator Measure of Aromaticity

$$\text{HOMA} = 1 - \frac{257.7}{n} \sum_{i=1}^{n} \left(r_{\text{CC}} - r_{\text{CC-aromatic}} \right)^2$$

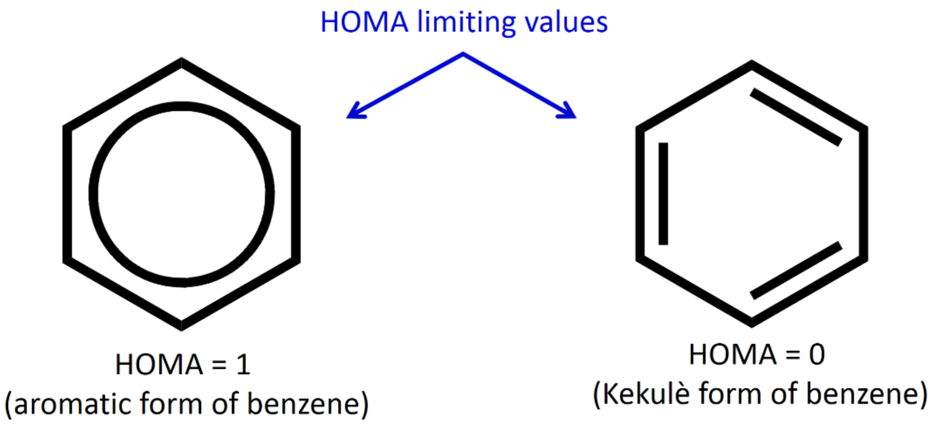


Figure 3.10. Definition of HOMA and example of limiting cases. Where n = 6 for the six-member rings of PAH.

3.5.2 Correlations with Aromaticity

Previous studies of the Frenklach group [64,65] demonstrated that a simple correlation exists between cumulative HOMA of oxyradicals and their relative thermodynamic stability. The origin of this relationship is fragmentation of the delocalized π-bonding framework due to its disruption upon chemisorption of an O atom at a graphene radical site. It is likely that the same reasoning applies to energetic characteristics of oxyradical decomposition. In the present case, HOMA was used for reactivity analysis for reaction kinetics. Considering the diversity of factors controlling reaction kinetics, for example, the multiple intermediates and transition states, the range of analyzed characteristics was narrowed down to a single one, namely the relative energy of the first transition state leading to the cyclic structure. Barrier height is a relative value, so it is logical to consider its relationship to a relative descriptor of aromatic bonding, which can be defined as:

$$\Delta\mathrm{HOMA} = \sum_{i=\mathbf{2}}^{n} \left(\mathrm{HOMA}_{\mathrm{TS},i} - \mathrm{HOMA}_{\mathrm{reactant},i} \right) \tag{3.1}$$

ΔHOMA is calculated as the summation of the change in HOMA for each ring in a PAH between transition structure and reactant, excluding the ring with the attached oxygen (hence the summation starts from two not one). The oxyradical ring is left out because aromaticity is completely destroyed in that ring in the transition structure and so $\mathrm{HOMA}_{\mathrm{TS}}$ is not well defined. ΔHOMA essentially measures how the reaction changes the aromaticity of the rings in the PAH. A simple correlation in the data can be seen by plotting (Figure 3.11) the results obtained in the present chapter and previous [47] studies. The largest barrier height is associated with the most negative ΔHOMA, thus suggesting that CO expulsion should proceed via the route that involves the smallest rearrangement of the conjugated bonding framework. In addition, to demonstrate that this barrier height corresponds with rates, the correlation between ΔHOMA and the thermal decomposition of the oxyradical at 2000 K and the high pressure limit are shown in Figure 3.12. These correlations are not perfect; for instance, the benzoperylene point falls from this general trend. A possible explanation is that benzoperylene is the only two row structure, while the other points are all single row structures. The extended armchair structure was not included in the correlation because it did not have the common transition structure going from reactant to the cyclic intermediate.

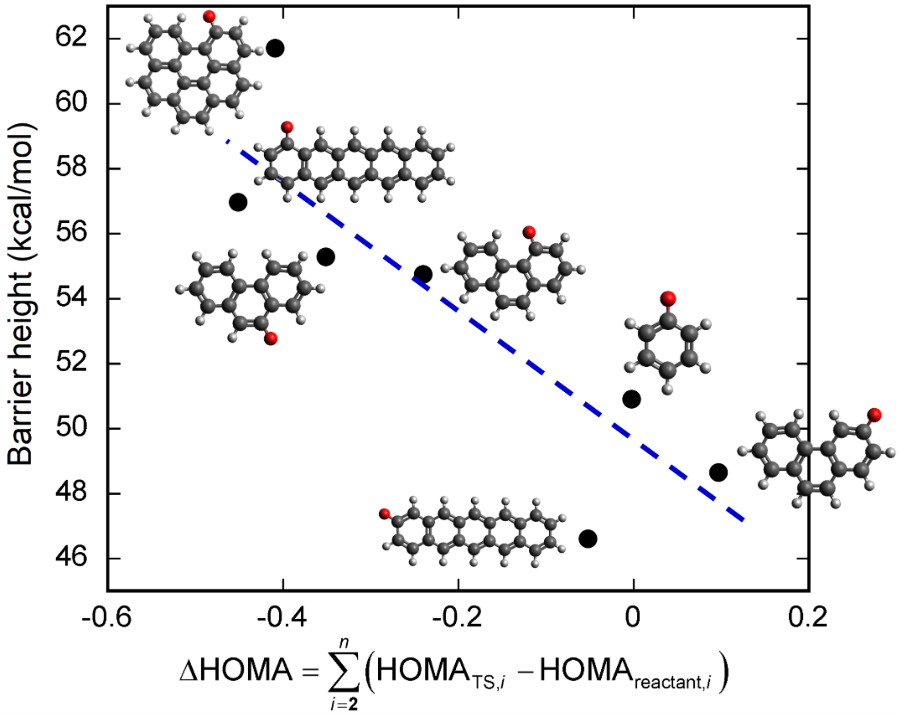


Figure 3.11. First barrier heights (**TS 1-2**) of oxyradical decompositions against ΔHOMA. Phenoxy and pentacene structures are from [47].

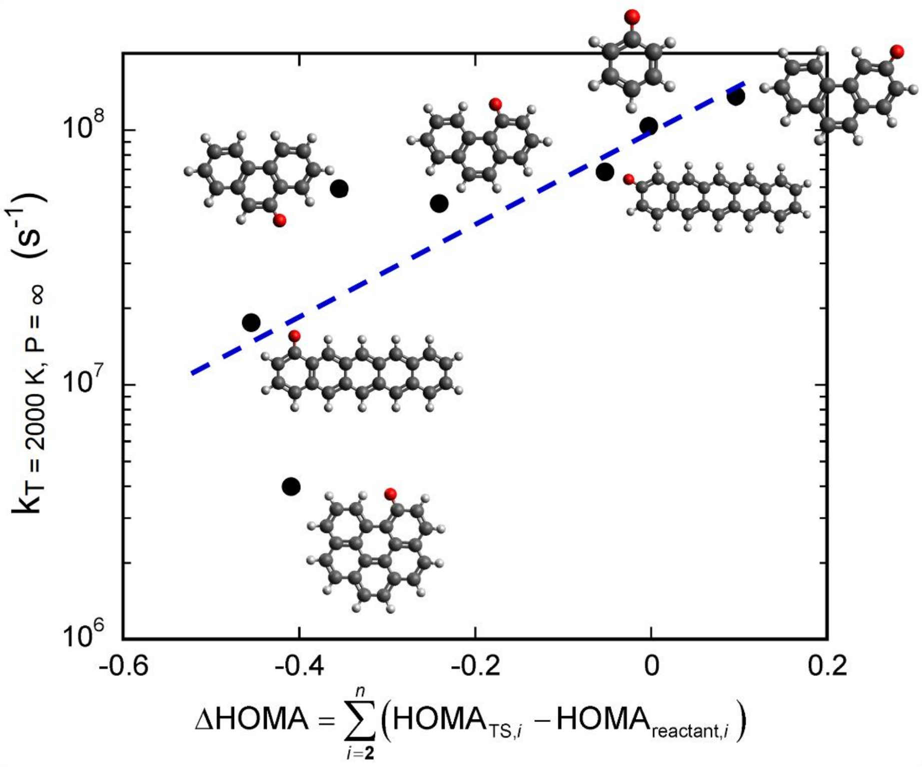


Figure 3.12. Oxyradical decomposition rates against ΔHOMA. Phenoxy and pentacene structures are from [47].

An improvement to the correlation shown in Figure 3.11, is made if another independent variable is considered, $HOMA_{oxyradical\ ring}$. This additional variable is the HOMA value of the reactant ring with oxygen attached. This improved correlation is shown in Figure 3.13. As would be expected, reactions that destroy aromaticity correlate with higher barriers.

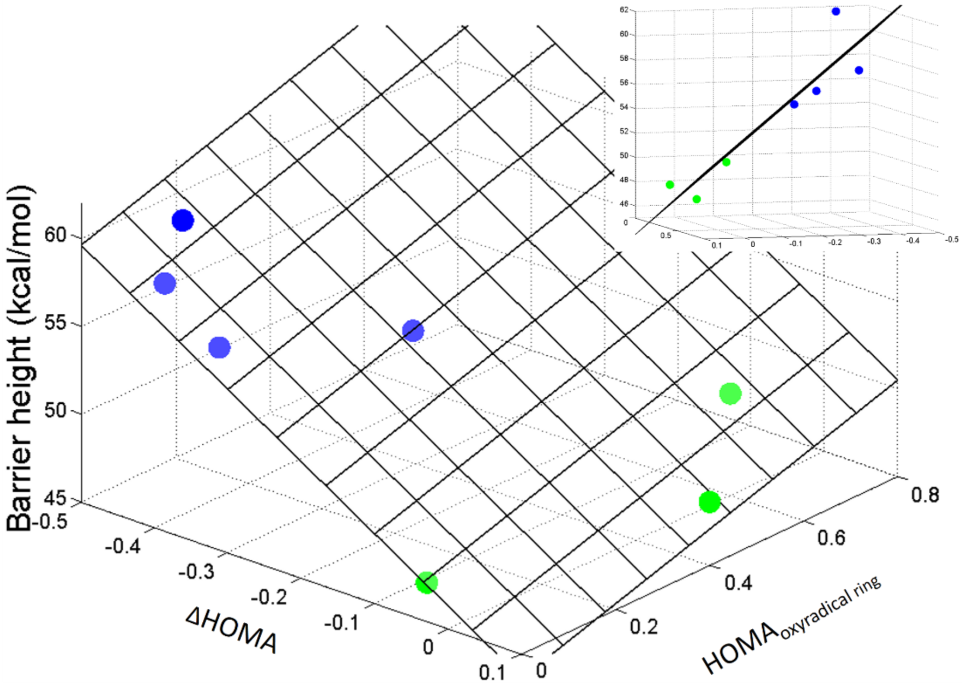


Figure 3.13. First barrier heights (**TS 1-2**) of oxyradical decompositions against ΔHOMA and $HOMA_{oxyradical\ ring}$. The blue points are PAHs with one free edge, while the green are PAHs with two free edges. The insert is a rotated view showing how the points deviate from the best fit plane.

Future work in these correlations would focus on adding additional oxyradicals to the correlation, especially multi-layer PAHs. Another area would be to verify the same correlations using lower-level theory for the electronic structure calculations. Currently to calculate ΔHOMA, quantum chemistry calculations on both the reactant and transition structure are performed. These same calculations also yield the barrier height, making the ΔHOMA correlation redundant. A lower level of theory, such as a semi-empirical method [72], may not calculate the energy accurately, but may be able to accurately calculate HOMA values. In this situation, these correlations with aromaticity would be very useful and could be used to predict barrier heights and rates for larger PAHs or unusual soot geometries.

3.6 Summary

The energetics and kinetics of the thermal decomposition of five graphene armchair-edge oxyradicals were investigated in this Chapter. In all cases studied, the computed decomposition rates were both temperature and pressure dependent. The extent of the pressure dependence, especially at higher temperatures, was substantial even for the largest molecular substrate studied, an eleven-ring PAH. Also noteworthy was the influence of substrate size on computed rates. In going from the three-ring phenanthrene II structure to the six-ring benzoperylene structure the thermal decomposition rate decreased by nearly an order-of-magnitude. Yet the change seemed to level off going from the benzoperylene structure to the eleven-ring extended armchair geometry. This may imply that two-layered PAHs may be sufficiently large to represent a soot edge.

Applying the concept of "free edges" for PAHs [47], the trends described in this chapter for computed decomposition rates with oxyradical location on PAHs were rationalized. Oxyradicals with more free edges decomposed at faster rates than those with a fewer number of free edges. This relationship held strongest within oxyradicals of similar structures (e.g., different phenanthrene oxyradicals), and was weaker in explaining the relative rates between different structures (e.g., phenanthrene versus pentacene oxyradicals).

The kinetic stability of graphene-edge oxyradicals, was shown to be correlated with change in aromaticity during the initial, typically rate-controlling, step of oxyradical decomposition. This correlation, together with a recently-established similar scaling for thermodynamic stability [64,65], could lead to practical rules for predicting oxidation rate coefficients for arbitrary size and shape aromatics, thereby supplementing and enhancing models of soot oxidation.

The potential energy pathways and overall decomposition rates computed in the present chapter for armchair edge oxyradicals are very similar to those obtained in a previous study [47] for corner zigzag edge oxyradicals. Figure 3.14 below, summarizes the high-pressure rates for these oxyradical decompositions. This similarity between edges implies that for an arbitrary shaped PAH, oxidation should predominantly remove armchair and corner-zigzag sites, leaving resistant-to-oxidation [47] inner zigzag sites essentially intact. Considering that the growth of both armchair and zigzag edges proceed at effectively the same rate [73,74], this conclusion suggests that there would be a proliferation of zigzag-edge surfaces on soot particles formed in flame environments.

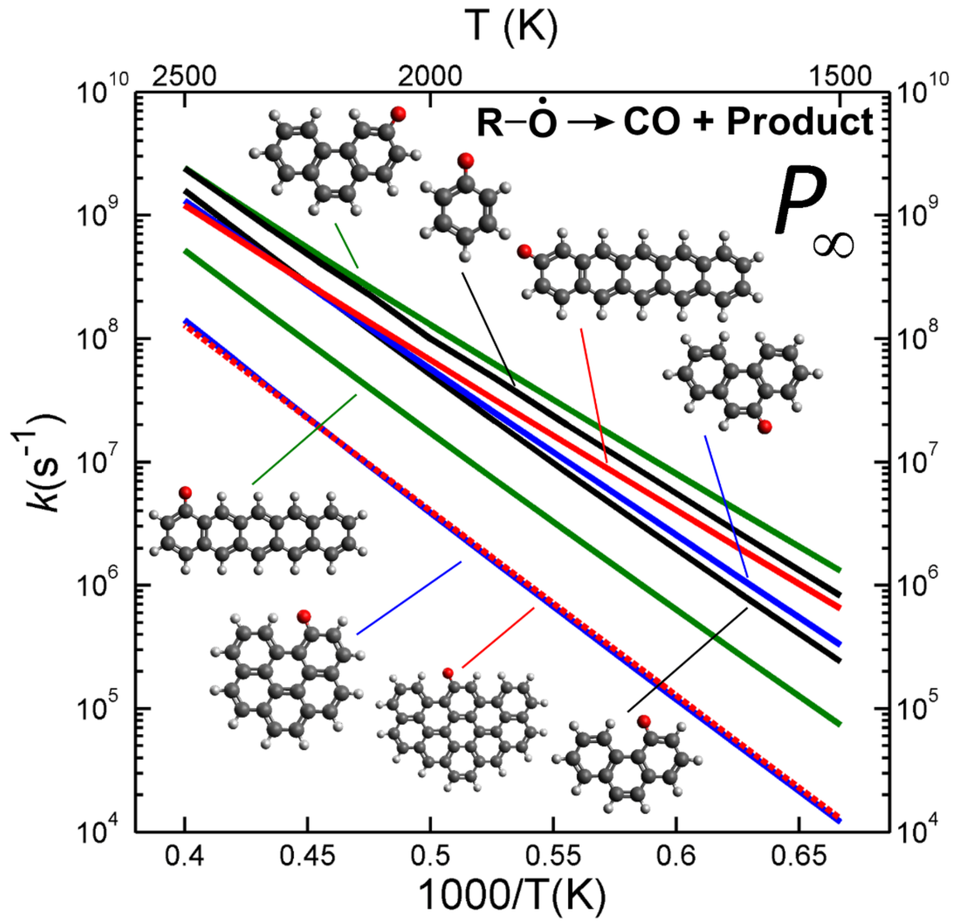


Figure 3.14. Summary of high-pressure rate coefficients for all oxyradical decompositions studied here and in previous work [47].

Chapter 4

Detailed Pathways of PAH Oxidation by OH

The main results of this dissertation are presented in this chapter, namely investigation of possible pathways of PAH oxidation by OH leading to prototype reactions of soot oxidation by OH. An important principle guiding the investigation reported in this Chapter was that OH oxidation pathways must be commensurate with the fast soot oxidation rates observed experimentally. To this end I computed PESs of OH reacting with three types of PAH edge sites to explore possible pathways leading to CO expulsion. The kinetics of the most promising reaction, OH reacting with a phenanthrene radical, were then calculated by solving energy-transfer master equations.

4.1 PES Results

Three PAH edge sites were investigated as possible prototypes of soot surface sites for reaction with OH: $C_{surface}$–H, $C_{surface}$●, and a benzene-phenol complex. For these three systems, pathways leading to CO expulsion were only found for OH attacking a $C_{surface}$● site. For this latter case, hydrogen migration and expulsion were key steps that opened up the CO eliminating pathways.

For all of the molecular structures discussed below, Appendix B contains the zero-point energies, expectation values of the S^2 operator, vibrational frequencies, rotational constants, high-pressure elementary reaction rates and the Cartesian coordinates for all optimized structures.

4.1.1 OH + $C_{surface}$–H

Benzene was selected as a prototype for the $C_{surface}$–H soot surface site. The PES for this system, shown in Figure 4.1, identified two main products, H_2O and phenol. There were no pathways leading to CO expulsion. Prior theoretical studies of the same reaction [75,76] also did not identify any major channels leading to CO expulsion. It is likely that phenol (**9**) would decompose to release CO, however, the formation of **9** is expected to be minor compared to the H-abstraction channel leading to **6**.

I concluded, therefore, that OH reacting with a $C_{surface}$–H edge site does not lead to CO expulsion at a rate fast enough to explain the observed collision efficiency.

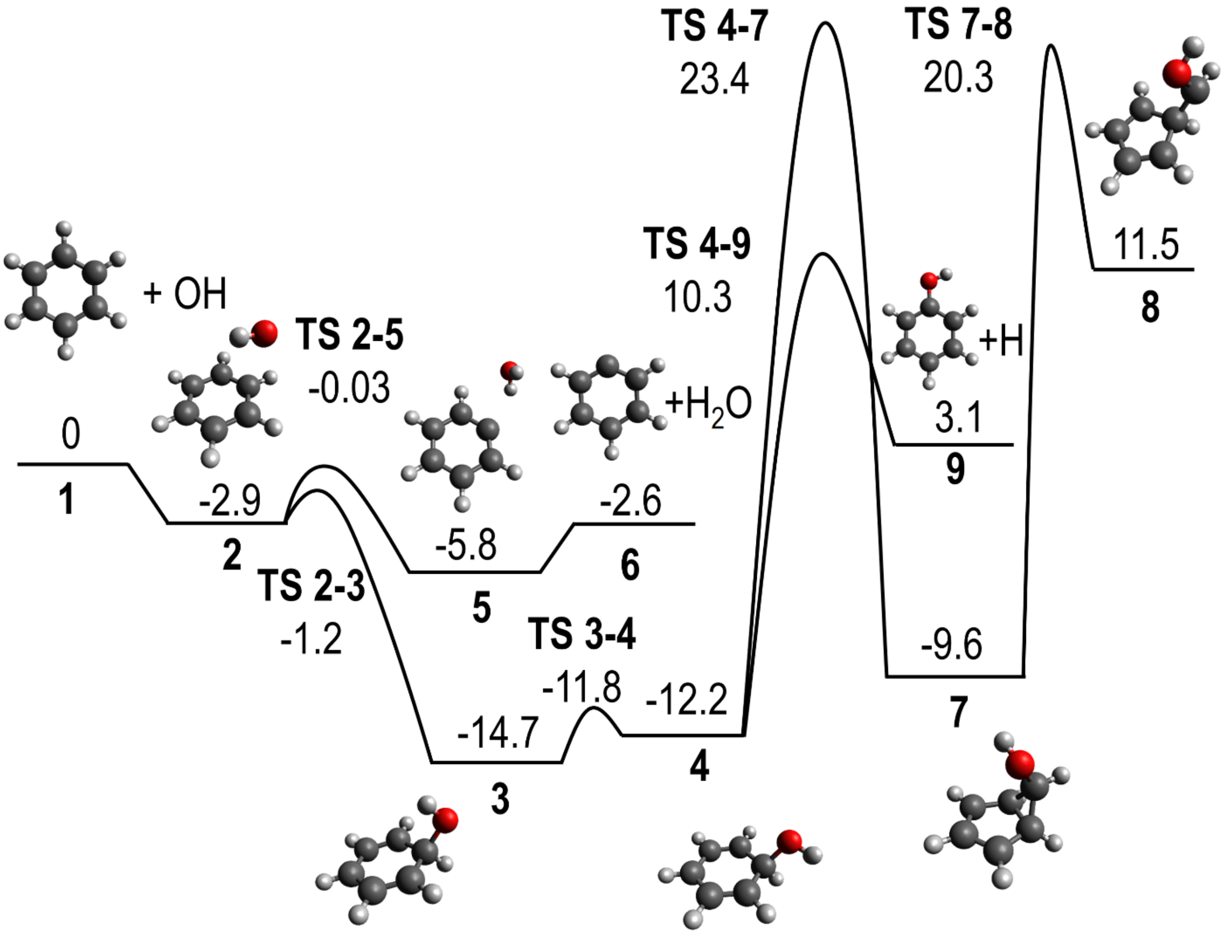


Figure 4.1. Potential energy surface for the reaction of benzene with OH at the B3LYP/6-311G(d,p) level of theory, including ZPE. Energies are in kcal/mol at 0 K relative to the reactants, **1**.

4.1.2 Benzene-phenol Complex

The influence of interacting PAH layers on oxidation was investigated by a benzene-phenol complex used to model interacting layers of soot; OH attaching to one layer may react with another layer. The PES of this system was calculated with the M06-2X density functional and 6-311G(d,p) basis set. B3LYP was not used in this case because it is unable to account for medium-range interactions [42] such as those in the benzene-phenol complex.

The computed PES is shown in Figure 4.2. No pathways were identified for the removal of CO. The single transition state that was identified had a nearly 100 kcal/mol barrier, indicating that continuing along that pathway was unlikely.

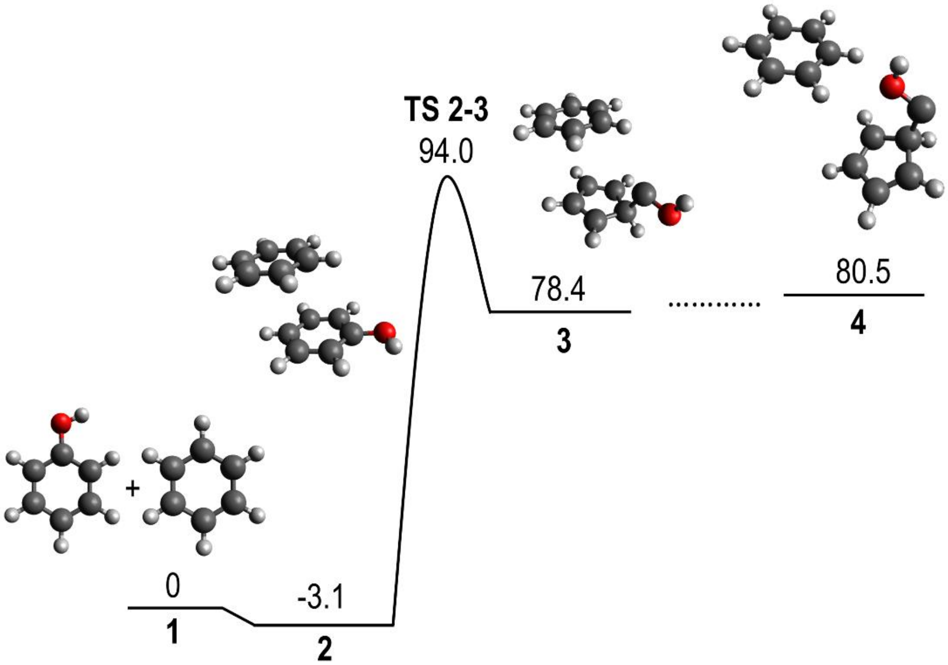


Figure 4.2. Potential energy surface for the reaction of benzene with phenol at the M06-2X/6-311G(d,p) level of theory, including ZPE. Energies are in kcal/mol at 0 K relative to the reactants, **1**.

4.1.3 OH + $C_{surface}$●

A phenanthrene radical was selected as the prototype for the $C_{surface}$● soot surface site. The adduct and initial wells of the singlet PES for the phenanthrene radical reacting with OH are shown in Figure 4.3. The PES shows the formation of five oxyradicals: **8**, **7**, **5**, **6**, and **4** associated with channels I–V shown in Figure 4.4−Figure 4.8, respectively. The formation of the first four oxyradicals, **8**, **7**, **5**, and **6**, was facilitated by H-atom migration, while the formation of **4** was enabled by H-atom elimination. Each of these five oxyradicals, as shown in Figure 4.4−Figure 4.8, can continue to isomerize, eventually eliminating CO.

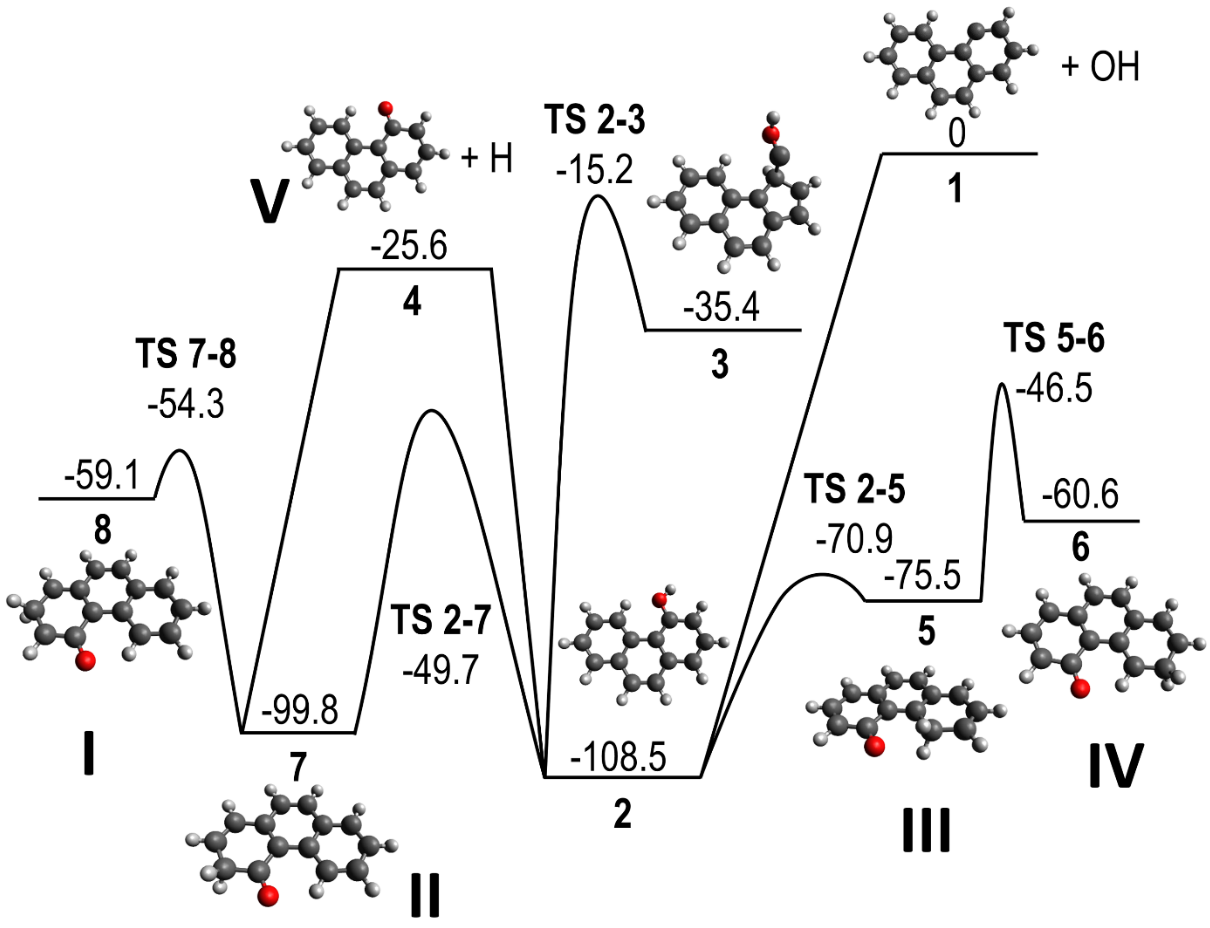


Figure 4.3. The initial wells of the PES for the reaction of a phenanthrene radical with OH. The bond dissociation energy for **2**→**4** and **2**→**1** were calculated at the CBS-QB3 level of theory, the remaining energies were found at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **1**.

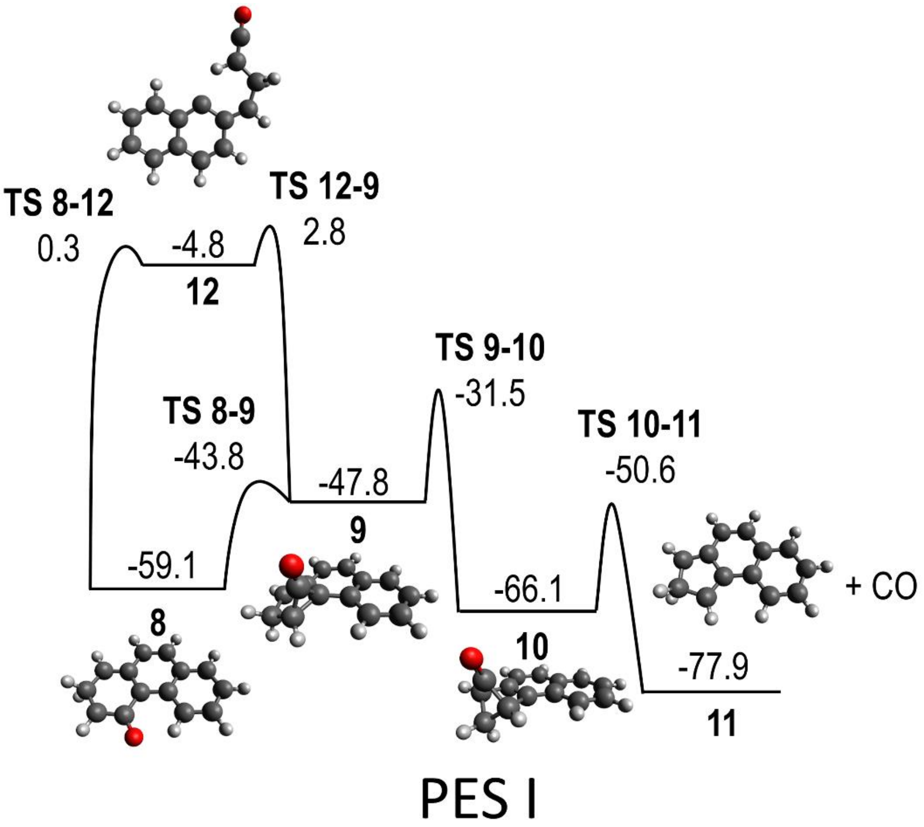


Figure 4.4. PES I for the reaction of a phenanthrene radical with OH at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **1** in Figure 4.3.

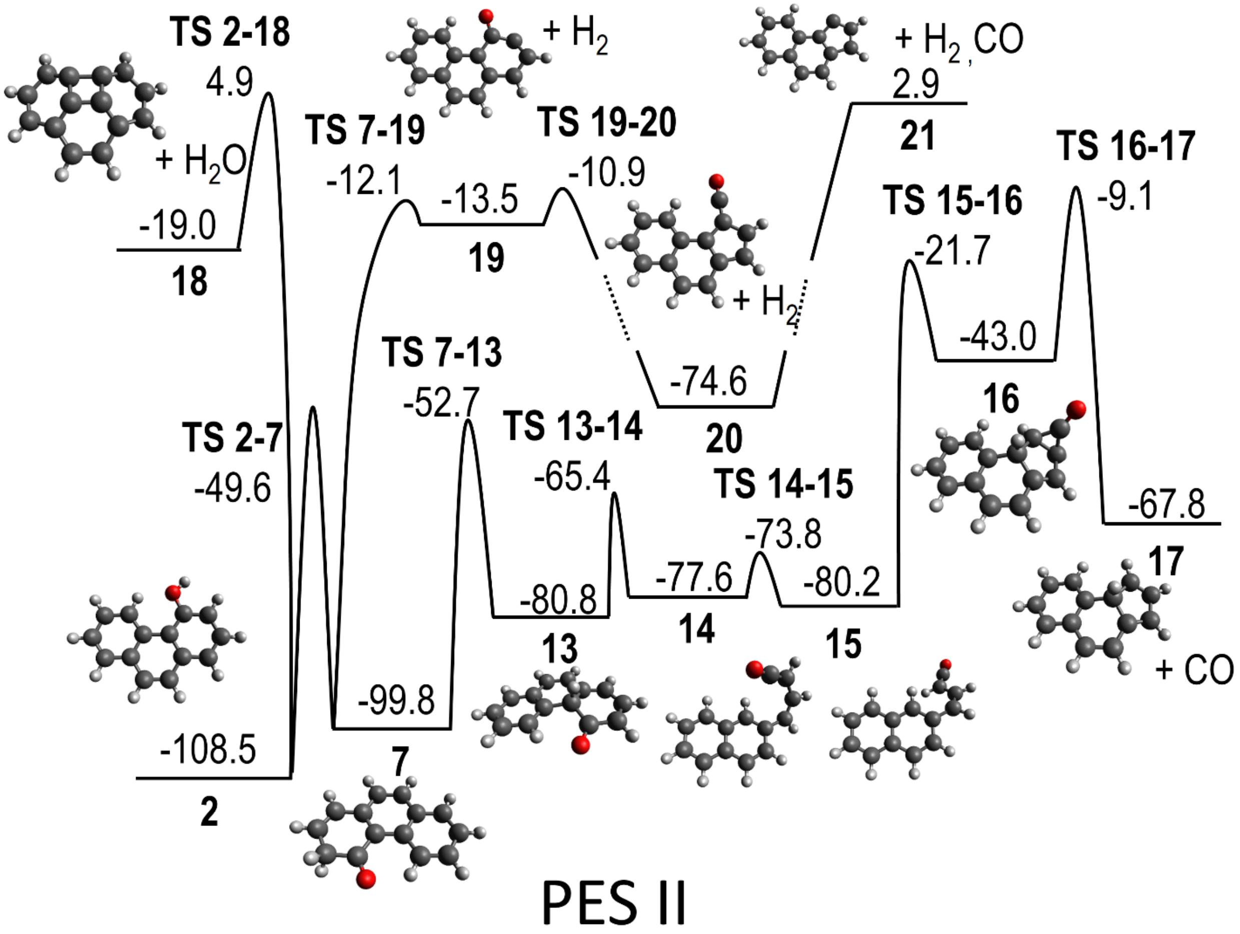


Figure 4.5. PES II for the reaction of a phenanthrene radical with OH at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **1** in Figure 4.3.

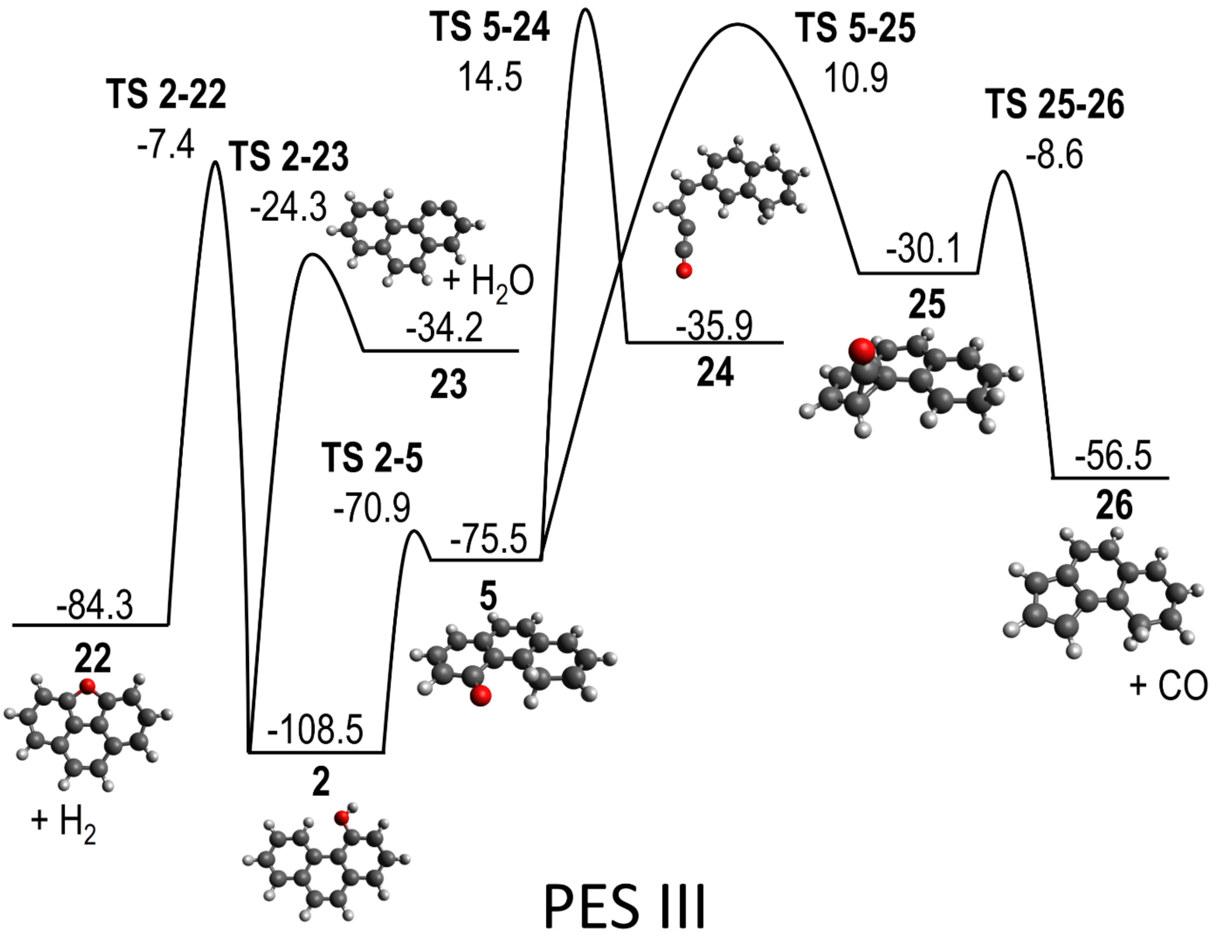


Figure 4.6. PES III for the reaction of a phenanthrene radical with OH at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **1** in Figure 4.3.

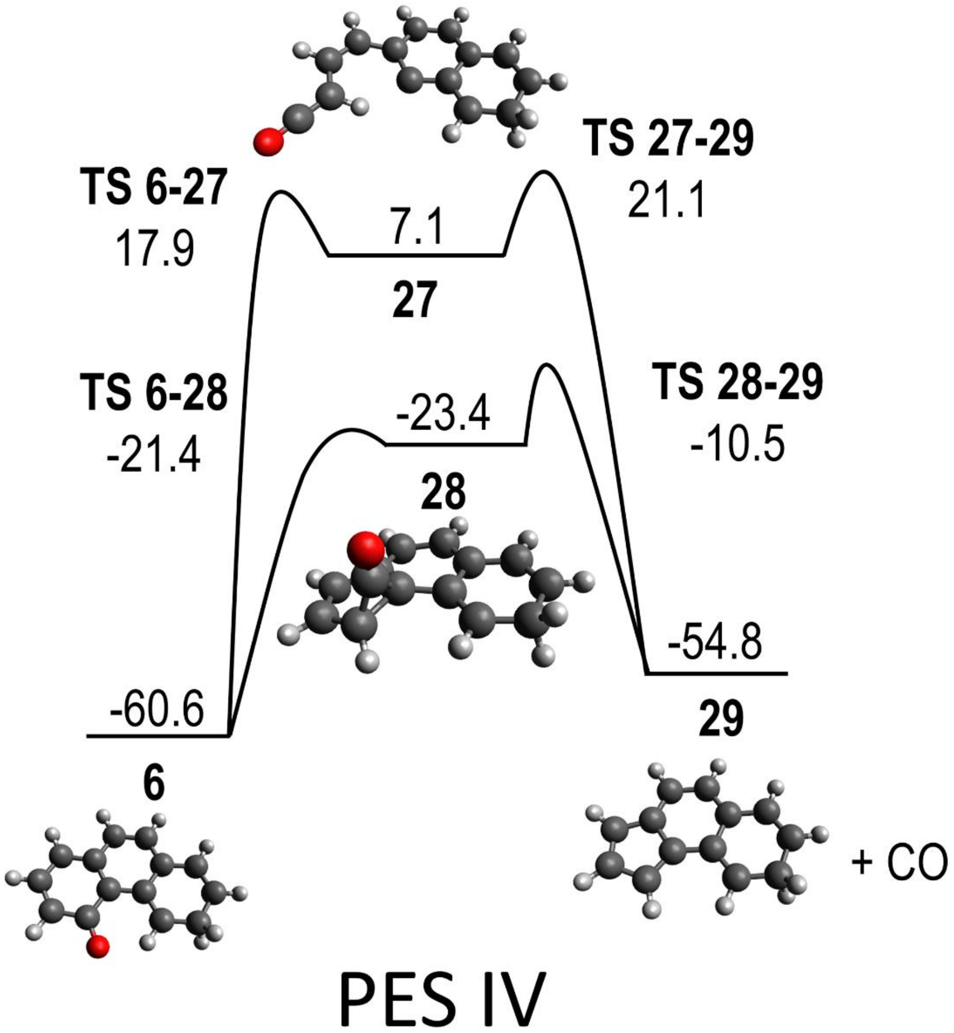


Figure 4.7. PES IV for the reaction of a phenanthrene radical with OH at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **1** in Figure 4.3.

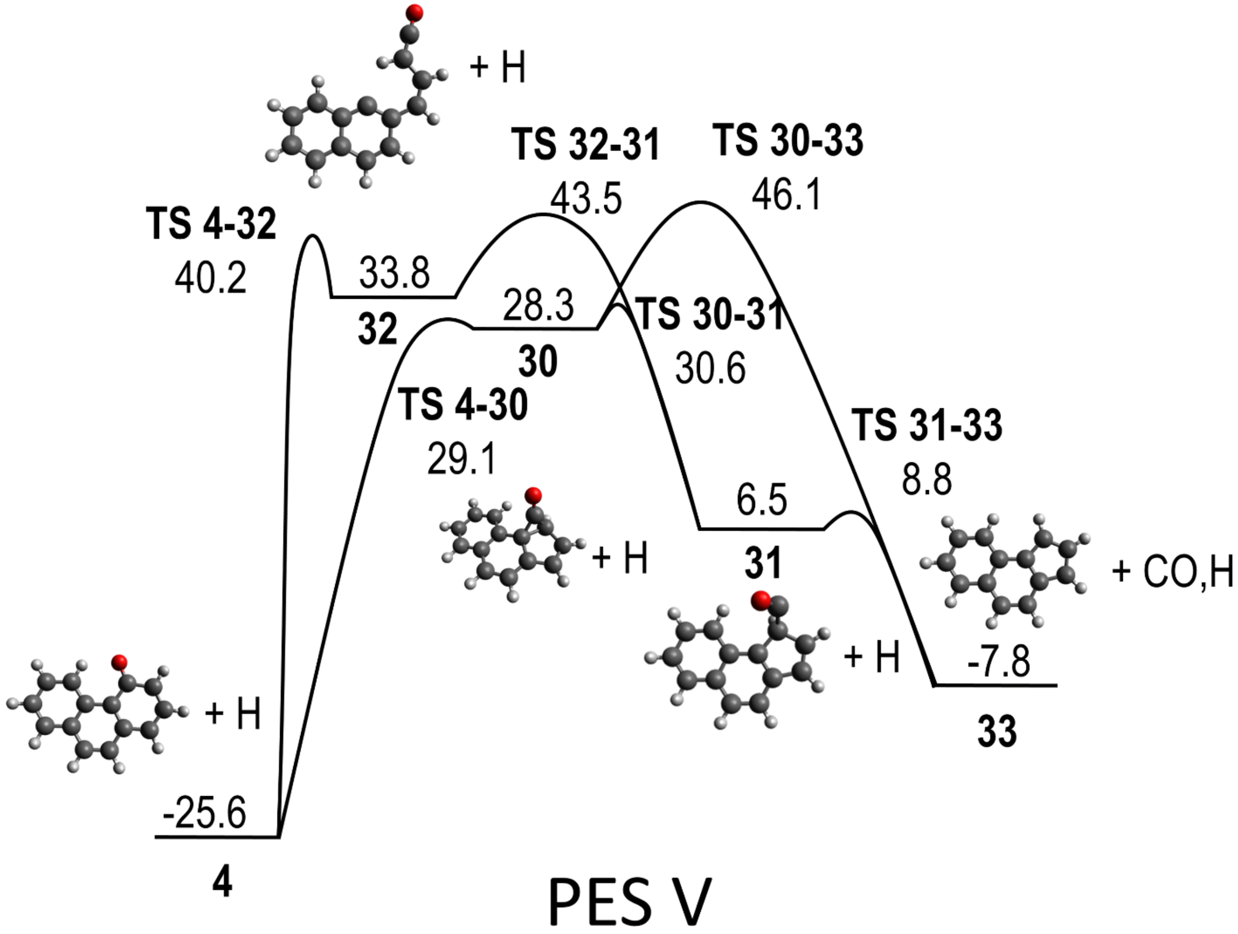


Figure 4.8. PES V for the reaction of a phenanthrene radical with OH at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **1** in Figure 4.3. Note that this PES is the same as phenanthrene oxyradical II, shown in Figure 3.2. The only difference is the inclusion of the + H and a shift in the zero point energy. The relative energies and barrier heights are identical.

The CBS-QB3 level of theory was used to calculate the bond dissociation energy (BDE) for the **2→4** and **2→1** reactions. This was done due to the importance of these two barrierless reactions to the overall system and because of B3LYP's known BDE underestimation [77]. The B3LYP/6-311G(d,p) dissociation energy for **2→1** was calculated to be 102.3 kcal/mol, while the CBS-QB3 value was 108.5 kcal/mol. The B3LYP/6-311G(d,p) dissociation energy for **2→4** was 75.5 kcal/mol while the CBS-QB3 value was 82.9 kcal/mol. In addition, **7**→**4** BDE was indirectly modified by the CBS-QB3 calculations. While the CBS-QB3 calculation was not performed for species **7**, by using the BDE of **2**→**4** and the relative energy between **2** and **7**, calculated at the B3LYP/6-311G(d,p) level of theory, the BDE for **7**→**4** was calculated to be 74.15 kcal/mol, while the B3LYP/6-311G(d,p) value was 66.68 kcal/mol. The energies shown in Figure 4.3 include the CBS-QB3 values for these reactions.

Pathways I–V are oxyradical decomposition pathways, similar in general features to each other and to those of the phenanthrene oxyradicals studied in Chapter 3; in fact, pathway V is the phenanthrene oxyradical II pathway, shown in Figure 3.2. Each of these pathways, however, has distinctive reactions and varying barrier heights. For instance, the barrier heights for the transition from oxyradical to cyclic intermediate for PES I, III, IV, and V were 15.3, 86.4, 39.2, and 54.7 kcal/mol, respectively. This wide range of barrier heights is related to the location of the hydrogen atom with respect to the chemisorbed oxygen atom. In all of these cases oxygen was located on the same site of the phenanthrene oxyradical; the relative location of the hydrogen atom was the primary cause for the differences between the five oxyradical decomposition pathways. The presence of oxyradicals in OH oxidation highlights the importance of oxyradicals in soot oxidation and support the notation that oxyradicals are key intermediates in soot oxidation.

4.2 Reaction Rate Coefficients

I first discuss the barrierless reaction channels, followed by the results of the overall kinetics.

4.2.1 Barrierless Reactions: *2→1, 2→4, 7→4, 20→21*

Reactions **2**→**1** and **20**→**21** were found to be well represented by a Morse Potential [61], while reactions **2**→**4** and **7**→**4** were best represented using a Varshni potential [62,63]. The Morse potential is of the following form

$$E(r) = D_e\left[1 - e^{-\alpha(r-R_e)}\right]^2 \tag{4.1}$$

And the Varshni potential is defined as

$$E(r) = D_e\left[1 - \left(\frac{R_e}{r}\right)e^{-\alpha(r^2-R_e{}^2)}\right]^2 \tag{4.2}$$

The calculated points from the potential energy scan and the fit, either Morse or Varshni, are presented below in Figure 4.9−Figure 4.12. Not the bond dissociation energy shown in these figures are larger than the values given in Figure 4.3. This is because the values in Figure 4.3 include ZPE while the values in Figure 4.9−Figure 4.12 do not include ZPE.

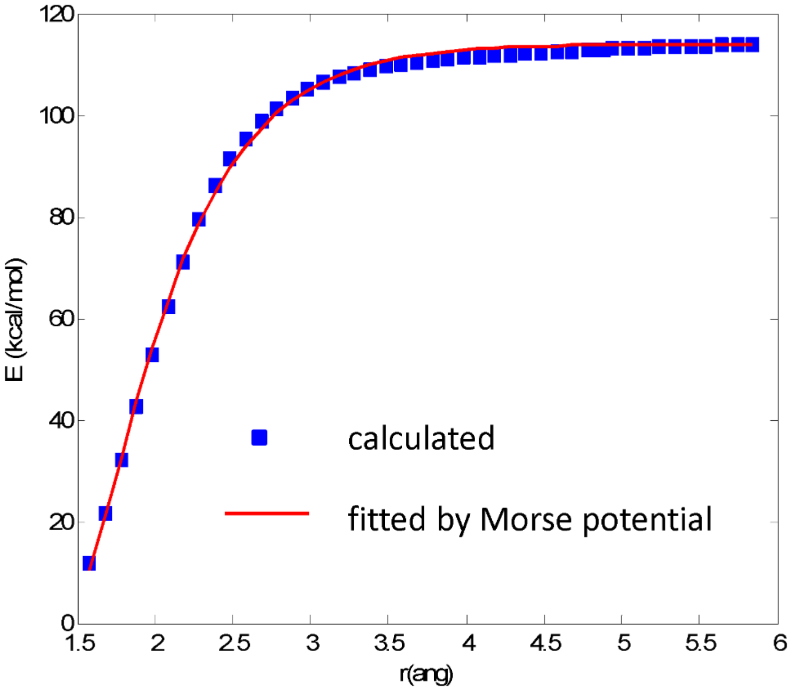


Figure 4.9. Calculated values and Morse potential for the **2→1** reaction. De = 114.05 kcal/mol, Re = 1.40 Å, and $\alpha = 2.02$ Å^{-1}.

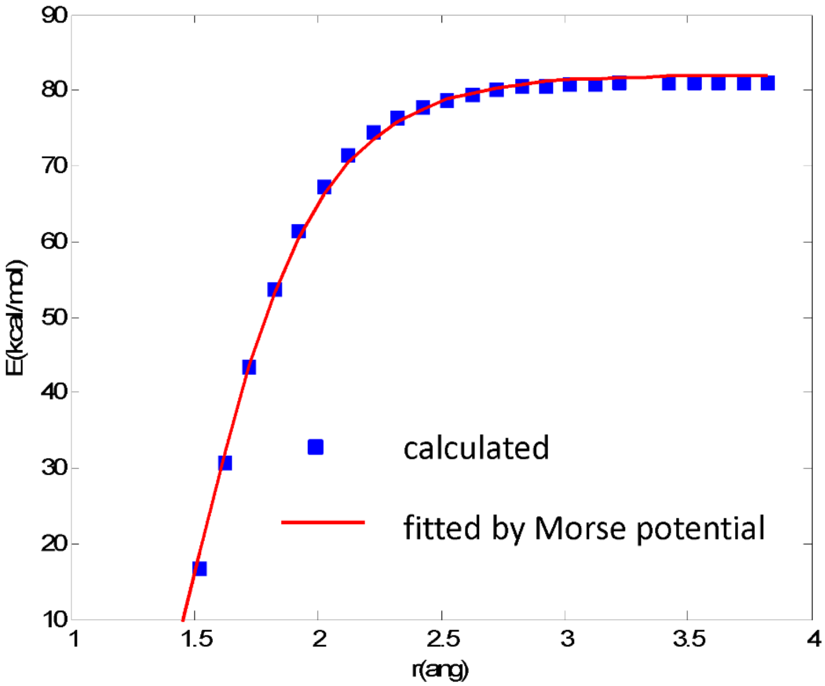


Figure 4.10. Calculated values and Morse potential for the **20→21** reaction. De = 82.0 kcal/mol, Re = 1.33 Å, and $\alpha = 3.265$ Å$^{-1.}$

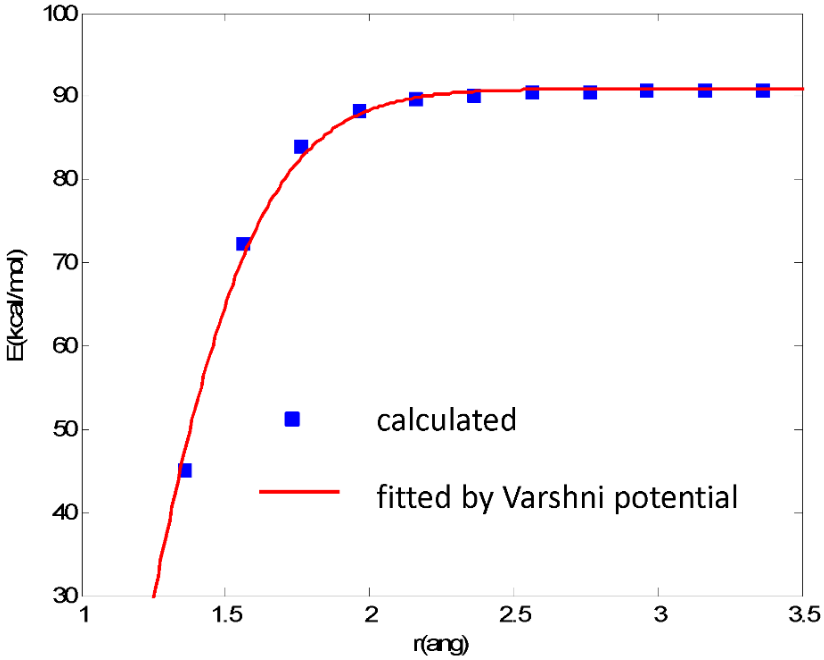


Figure 4.11. Calculated values and Varshni potential for the **2**→**4** reaction. De = 90.90 kcal/mol, Re = 1.02 Å, and α = 1.201 Å^{-2}.

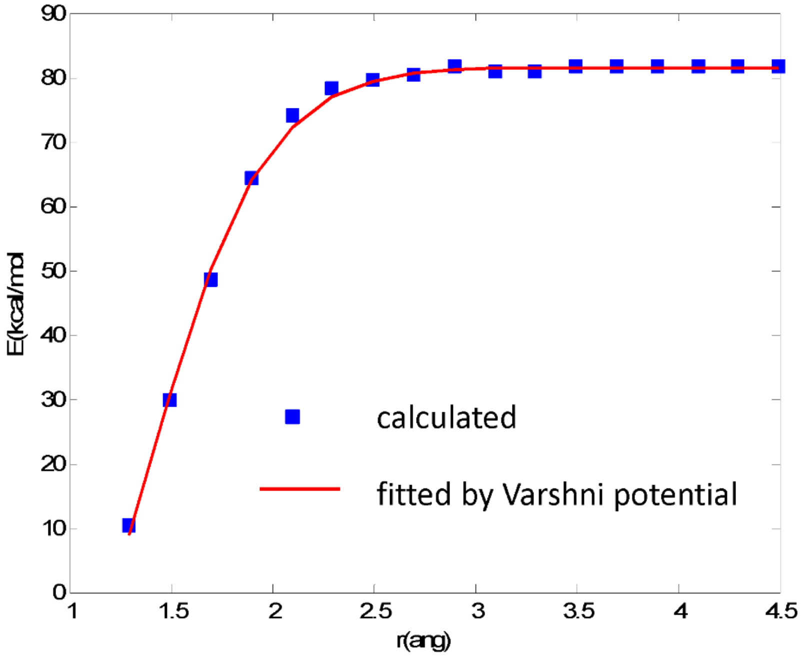


Figure 4.12. Calculated values and Varshni potential for the **7**→**4** reaction. De = 81.57 kcal/mol, Re = 1.142 Å, and α = 0.7225 Å^{-2}.

The reaction degeneracy for the barrierless reactions were assigned a value of 2 because the transition structures were optical isomers. The OH attack of the phenanthrene radical, **2→1**, was a very shallow attack, possibly indicating that the separation between the two transition structures is minor. If instead this reaction was modeled using a reaction degeneracy of 1, the chemical-activation results presented in this chapter would be modified by roughly a factor of 0.5. The potentials for reactions **2→1**, **2→4**, and **7→4** were scaled by the CBS-QB3 values.

4.2.2 VariFlex Minimum Bond Length Restriction

In applying VariFlex to this systems, I encountered a limitation in the program due to the large size of this system. As described in page 32 of the VariFlex manual, the reaction rate cannot be variationally calculated for bond lengths less than the distance from the center of mass for each fragment to the bonding point. For example, the reaction of **2** to **4** involved the breaking of the O-H bond. The distance from the center of mass of the phenanthrene oxyradical to the oxygen atom is 2.8 Å. Because of the restriction, VariFlex artificially restricts the minimum distance between the phenanthrene oxyradical and the H atom to 2.8 Å. If the true reaction rate minimum is found at bond lengths less than 2.8 Å, this restriction will lead to an over-estimate of the actual rate constant. In this system both of the H elimination pathways, **2** to **4** and **7** to **4**, suffered from this problem.

To understand and fix the issue, smaller structures were chosen as surrogate reactions to mimic the reactions involving the larger structures while avoiding this restriction. 2-propenol was selected for the **2** to **4** reaction and cyclohexadienone was selected for the **7** to **4** reaction. The BDEs, potentials, and symmetry for the surrogate reactions were modified to match the larger, original reactions. In this way, the bi-molecular rates of the surrogate reactions may match the rates of the original reactions. Figure 4.13 shows canonical reaction rates calculated for the **7** to **4** reactions as well as the respective surrogate reactions as a function of bond length. The surrogate reaction matches the original reaction quite well. This may not always be the case, but for these surrogates reactions it was the case. Furthermore the surrogate reaction shows how the original reaction does not extend far enough to capture the true variational minimum for the reaction. Reaction **2** to **4** showed similar characteristics.

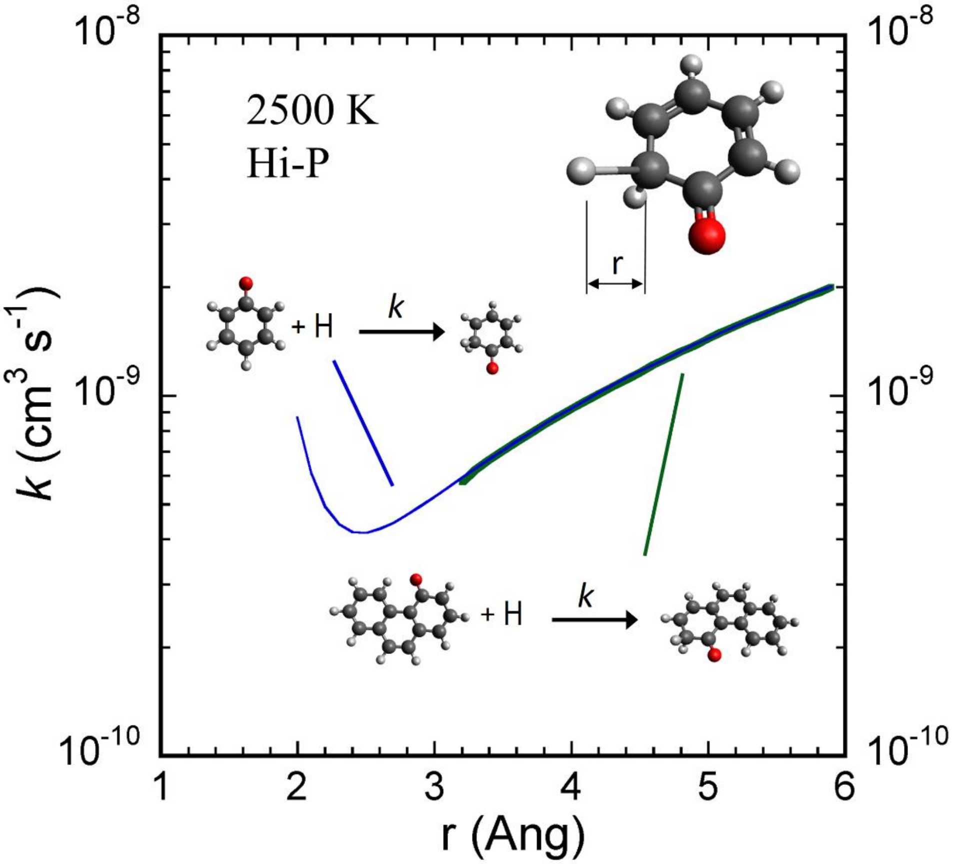


Figure 4.13. Canonical rate coefficient for the H addition reaction for both phenoxy and a phenanthrene radical as a function of bond length.

Next, to correct for the error, the microcanonical rates for the surrogate reactions were calculated for the full range and for the restricted range. The ratio needed to correct the restricted range values were then calculated. This correction factor was then applied to the microcanonical rates of the original system. The largest effect of this correction occurred at the high-pressure limit and 2500 K case. At these conditions the effect of the correction on the elementary reactions **7** to **4** and **2** to **4** was a factor of 0.6 and 0.7, respectively.

4.2.3 Master Equation Modeling Results

The species fractions resulting from the chemical-activation simulations of the combined system shown in Figure 4.3–Figure 4.8 are given in Table 4.1. The intermediates and products with species fractions less than 0.02 were assumed to be negligible and are not included in the table. The chemical-activation rate constants were calculated by multiplying the species fraction in Table 4.1 by the high-pressure rate of OH combining with a phenanthrene radical. Table 4.2 lists these high-pressure values for the three temperatures studied. The main products of the chemically-activated system were **11** (CO), **33** (H, CO), and **1** (reactants). In addition, at higher pressures and lower temperatures, species **2**, **7**, and **4** were collisionally stabilized and accumulated. Under these conditions chemical activation was not sufficient to drive the reaction completely to products.

Table 4.1. Species fractions resulting from the chemical-activation simulations of the system shown in Figure 4.3–Figure 4.8. Intermediate species indicate species that were collisionally stabilized and accumulated by the end of chemical activation.

	T = 1500 K				T = 2000 K				T = 2500 K			
	pressure (atm)				pressure (atm)				pressure (atm)			
	0.01	0.1	1	10	0.01	0.1	1	10	0.01	0.1	1	10
species #	intermediate species				intermediate species				intermediate species			
2	0.04	0.19	0.49	0.82	0.00	0.00	0.02	0.13	0.00	0.00	0.00	0.00
7	0.01	0.07	0.15	0.09	0.00	0.00	0.01	0.05	0.00	0.00	0.00	0.00
4	0.11	0.23	0.20	0.06	0.00	0.01	0.04	0.13	0.00	0.00	0.00	0.01
species #	product species fraction				product species fraction				product species fraction			
1	0.01	0.01	0.01	0.00	0.04	0.04	0.04	0.04	0.11	0.11	0.11	0.11
11	0.05	0.03	0.01	0.00	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01
33	0.78	0.46	0.12	0.01	0.91	0.91	0.85	0.60	0.85	0.85	0.85	0.84
Total	0.99	0.99	0.99	0.98	0.98	0.98	0.98	0.97	0.97	0.97	0.97	0.97

Table 4.2. High-pressure elementary reaction rates of OH attacking a phenanthrene radical.

T (K)	k_∞ (cm^3 mol^{-1} s^{-1})
1500	9.6×10^{13}
2000	1.1×10^{14}
2500	1.3×10^{14}

Including the reaction from **2** (or **7**) to **4** in the MultiWell simulation was a slight modification to the traditional MultiWell modeling. This is due to MultiWell modeling unimolecular reactions or dissociation reactions leading to a product. In this case of **2** (or **7**) reacting to **4**, however, it is a dissociation reaction leading to an intermediate that continues to decompose. The dissociating H-atom takes some of the internal energy of the system with it. The energy removed by the H-atom is ignored by MultiWell leading to a slight overestimation of the internal energy of **4**. This neglect is anticipated to have very little effect on the overall results because the amount of energy removed by a single H-atom is quite small compared to the overall internal energy of the 24-atom phenanthrene oxyradical.

The time required for the chemical-activation simulations to reach thermal equilibrium was roughly from 5×10^{-8} to 5×10^{-5} s, possibly exceeding the time scale of their collisions with surrounding flame species. In this way, hot intermediates could undergo immediate reactions, thereby increasing, for instance, the rate of growth by acetylene or the rate of oxidation by O_2 and OH. In addition, because of the relatively slow thermal decomposition of the intermediates, they may also react before reaching product. For this initial investigation, I assumed that such secondary reactions did not occur. However, this could be an area of future research. Representative plots of species fractions from MultiWell chemical-activation runs are included in Figure 4.14 and Figure 4.15. These figures were constructed by running several MultiWell simulations of different time lengths. This allowed the construction of the overall plot over a wide range of time.

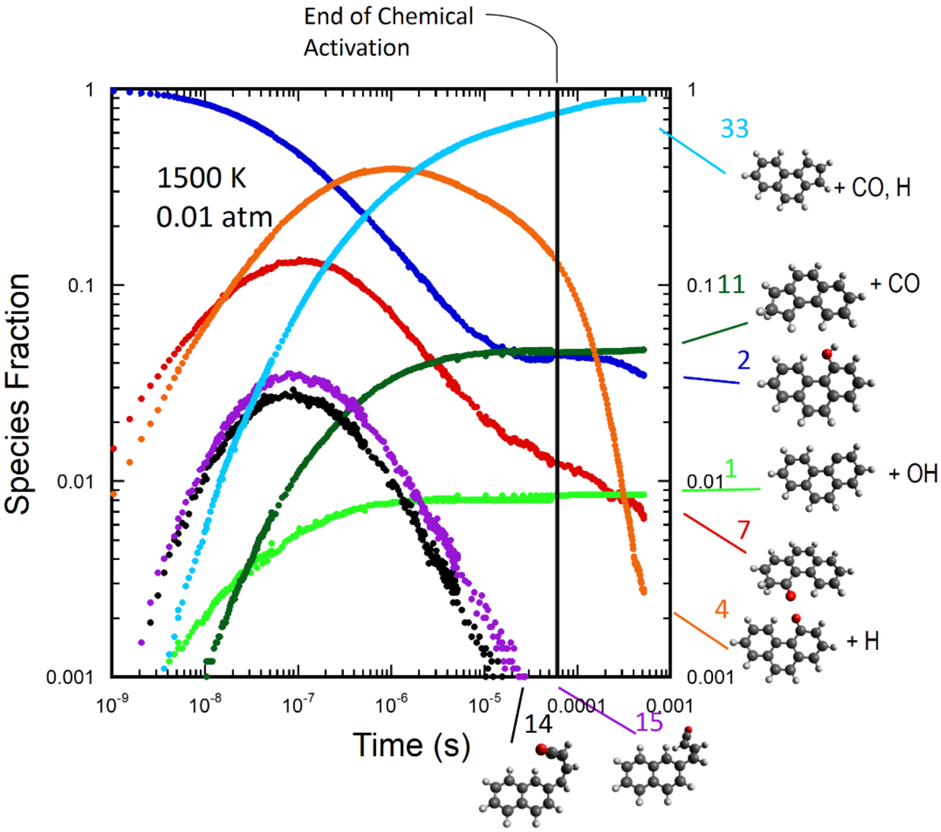


Figure 4.14. Representative species fraction plot from a MultiWell chemically-activated simulation, T = 1500 K, P = 0.01 atm.

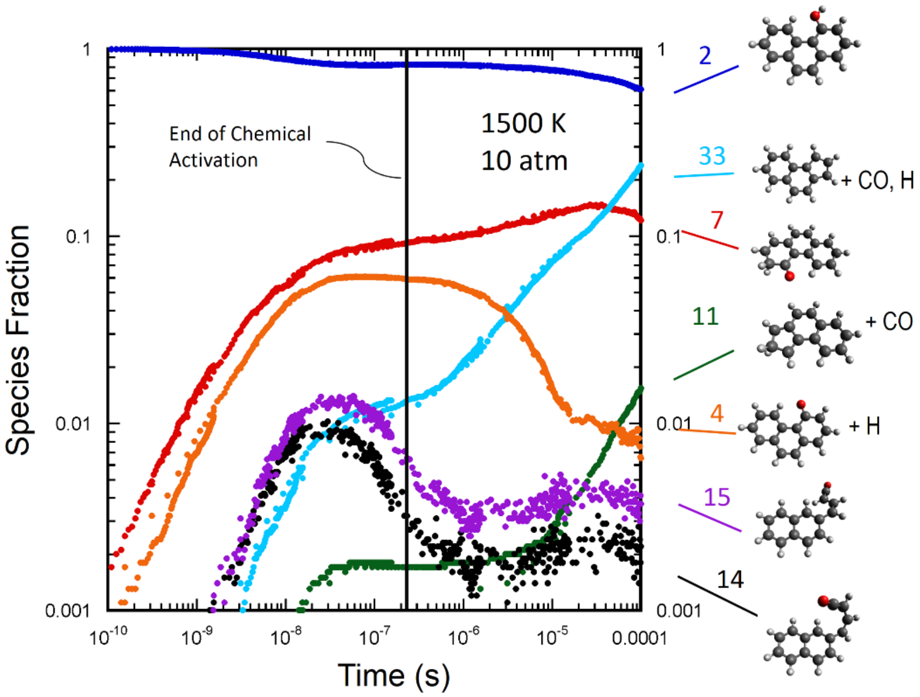


Figure 4.15. Representative species fraction plot from a MultiWell chemically-activated simulation, T = 1500 K, P = 10 atm.

When chemical activation was not sufficient to drive the reaction to products, the accumulating intermediates were modeled as distinct species undergoing thermal decomposition. These thermal-decomposition rate constants were computed in additional MultiWell thermal-decomposition simulations. The thermal product formation rates for **11**, **33**, and **1**, calculated from the thermal decomposition of species **2,** are shown in Table 4.3. Species **7** decomposition rates are not reported because species **7** and **2**, in the thermal decomposition simulation, are in quasi-equilibrium and decompose at the same rate. Thermal rates were only needed for conditions that led to accumulation of intermediate species in the chemical-activation simulations. For completeness, however, the thermal decomposition rates were calculated for all conditions. The thermal decomposition of species **4** was taken from Chapter 3.

Table 4.3. Product formation rates from the thermal decomposition of species **2**.

			s^{-1}	
T (K)	*P* (atm)	**1**	**11**	**33**
1500	0.01	-	68	560
	0.1	-	120	1.2×10^3
	1	-	160	1.9×10^3
	10	-	190	2.1×10^3
2000	0.01	35	970	1.2×10^4
	0.1	270	4.4×10^3	6.6×10^4
	1	1.8×10^3	1.5×10^4	2.7×10^5
	10	1.0×10^4	3.6×10^4	8.3×10^5
2500	0.01	6.8×10^2	1.3×10^3	3.1×10^4
	0.1	4.5×10^3	8.0×10^3	2.0×10^5
	1	2.8×10^4	4.2×10^4	1.2×10^6
	10	1.8×10^5	1.8×10^5	6.1×10^6

Thermal rate coefficients were used in conjunction with the chemical-activation rate coefficients to calculate the overall rate of CO expulsion from the reaction of OH with a phenanthrene radical. The reaction system used to calculate the overall reaction rate coefficients for a combined system of thermal and chemical-activation rates is shown in Figure 4.16.

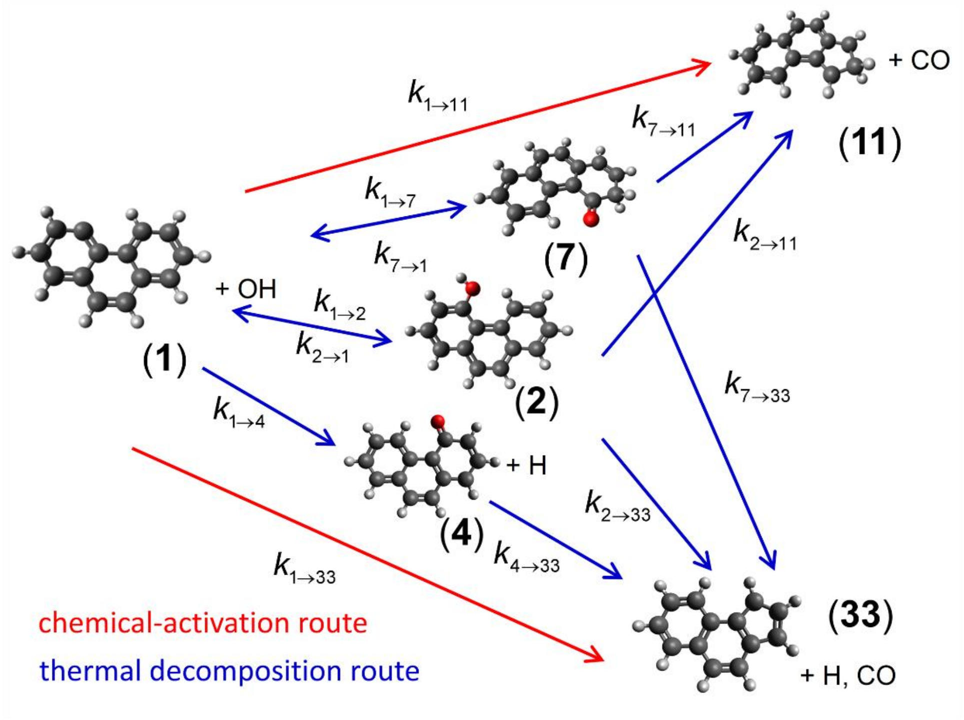


Figure 4.16. The reaction system illustrating the combined chemical activation and thermal decomposition required to calculate the overall oxidation of phenanthrene radicals by OH. The rates shown are not the elementary rates (except for $k_{1\to2}$ and $k_{2\to1}$), but rather are the chemical-activation and thermal decomposition rates calculated in MultiWell.

In this figure, the reactions starting from **1** are chemical activation, and those starting from **2**, **7**, and **4** are thermal decomposition. Based on the reaction system in Figure 4.16, the overall formation rate of CO is given by

$$\begin{aligned}\frac{d[\mathrm{CO}]}{dt} &= \frac{d[11]}{dt}+\frac{d[33]}{dt}\\ &= \left(k_{11}+k_{33}\right)[\mathrm{OH}][\text{Phenanthrene Radical}]\\ &= \quad k_{\mathrm{CO}} \quad [\mathrm{OH}][\text{Phenanthrene Radical}]\end{aligned} \tag{4.3}$$

The reaction rate coefficients k_{11} and k_{33} were derived by solving the set of differential equations defined by the kinetic system shown in Figure 4.16,

$$k_{11}(t) = k_{1\to11} + \frac{k_{1\to2}k_{2\to11}}{k_2}\left(1-e^{-k_2 t}\right) + \frac{k_{1\to7}k_{7\to11}}{k_7}\left(1-e^{-k_7 t}\right) \tag{4.4}$$

$$k_{33}(t) = k_{1\to33} + \frac{k_{1\to2}k_{2\to33}}{k_2}\left(1-e^{-k_2 t}\right) + \frac{k_{1\to7}k_{7\to33}}{k_7}\left(1-e^{-k_7 t}\right) + k_{1\to4}\left(1-e^{-k_{4\to33} t}\right) \tag{4.5}$$

$$k_2 = k_{2\to 1} + k_{2\to 11} + k_{2\to 33} \tag{4.6}$$

$$k_7 = k_{7\to 1} + k_{7\to 11} + k_{7\to 33} \tag{4.7}$$

When chemical activation carried the system to completion, e.g., at high temperatures and low pressures, k_{CO} was calculated as the sum of $k_{1\to 11}$ and $k_{1\to 33}$. At these conditions, $k_{1\to 2}$, $k_{1\to 7}$, and $k_{1\to 4}$ equal zero, and Equations 4.4 and 4.5 reduce to time-independent $k_{1\to 11}$ and $k_{1\to 33}$, respectively.

Conversely, when the accumulation of **2**, **7**, or **4** was significant, k_{CO} became time-dependent. This is seen in the time dependence of Equations 4.4 and 4.5. Figure 4.17 shows a representative plot of k_{CO} versus time for such a case. The initial value of k_{CO} (k^0_{CO}) is the sum of the chemical-activation rate constants, $k_{1\to 11}$ + $k_{1\to 33}$. k_{CO} then grows from this initial value and eventually reaches the steady-state value, k^∞_{CO}. I defined a “ramp-up” time as the time for k_{CO} to reach 90% of k^∞_{CO}. Table 4.4 lists the ramp-up times for the conditions studied. Strong temperature dependence, caused by the temperature dependence of the thermal rates, was observed.

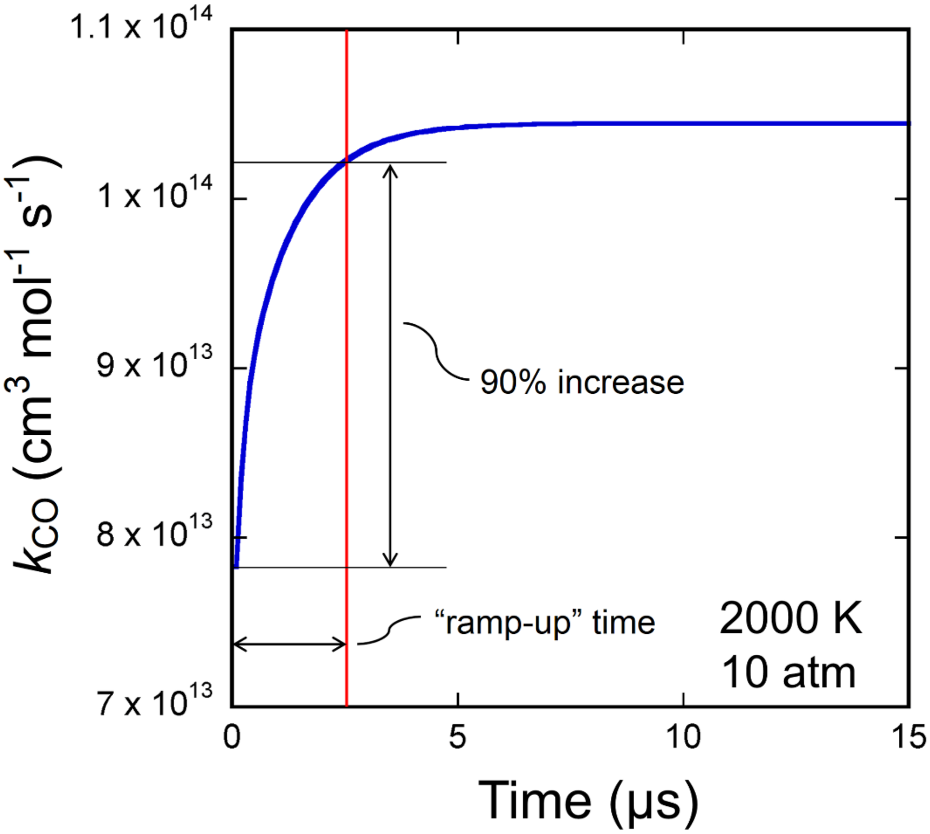


Figure 4.17. Representative plot of k_{CO}. The ramp-up time, defined as the time for k_{CO} to reach 90% of its final value, is shown.

Table 4.4. Ramp-up times of k_{CO}. Ramp-up time is defined as the time for k_{CO} to reach 90% of its final value.

	Ramp-up time (ms) Pressure (atm)			
T (K)	0.01	0.1	1	10
1500	1.8	1.2	1.0	1.0
2000	–	–	0.005	0.002
2500	–	–	–	–

The contributions of chemical activation and thermal decomposition to the total oxidation rate of phenanthrene radicals at 10 atm are shown in Figure 4.18. At 1500 K the oxidation occurred exclusively through thermal decomposition. At these conditions the collisional deactivation of the reacting species was faster than the chemical activation, which led to the accumulation of intermediates. These intermediates then decomposed thermally. At 2500 K, the opposite occurred. The chemical activation was sufficiently fast and all of the species reacted to products before any accumulation occurred. Similar trends were obtained for other pressures studied, with thermal decomposition contributing less at lower pressures.

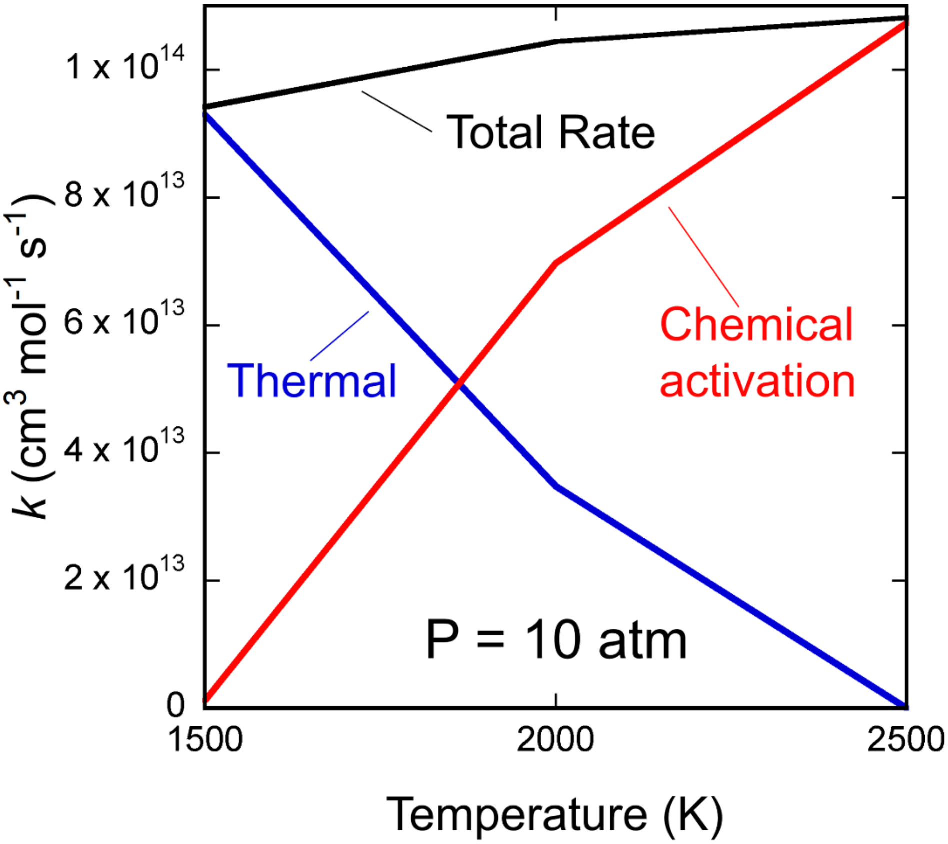


Figure 4.18. Representative plot showing contributions of the chemical activation and thermal decomposition to the overall oxidation rate.

The computed values of k_{CO}^{∞}, the overall steady-state oxidation rate of phenanthrene radicals by OH, were independent of pressure and only slightly temperature dependent. The k_{CO}^{∞} values at 1500, 2000, and 2500 K were 0.94, 1.05, and 1.09 $\times10^{14}$ cm^3 mol^{-1} s^{-1}, respectively. This insensitivity to pressure and temperature arises mainly due to two factors. First, the high-pressure rates for the initial elementary step of OH + phenanthrene radical (Table 4.2) change very little with temperature. Second, the reverse barrier, back to reactant **1**, is quite high, 108 kcal/mol. Because of this high barrier backward and multiple lower energy pathways forward, even as pressure changes, the rate back to reactant remained very low compared to the forward rates. This, in turn, leads to pressure insensitivity and contributes to temperature insensitivity. Note that the thermal rates, the ramp-up time, and the competition between the thermal and chemical-activation pathways were temperature and pressure dependent. The insensitivity of the overall computed here rate to temperature and pressure is in agreement with the experimental findings of Faeth and co-workers [35].

Applying collision theory [78] to the computed overall reaction rate, an η_{OH} value of 17% was obtained for the range of pressures and temperatures covered by the present study, which is close to the results of both Neoh et al.'s and Faeth and co-worker's. However, this comparison presumes that the creation of surface radical sites is not rate controlling. Such an assumption is reasonable, given the largely oxidative experimental environment created for the study of soot oxidation [28]. A fitting comparison requires modeling of the entire system, including formation of $C_{surface}\bullet$ sites and their disappearance due to various reactions. The detailed reaction kinetics obtained here is a step toward such future modeling, as the computed pathways are promisingly fast.

4.3 Phenol Decomposition PES Sensitivity Analysis

To understand the sensitivity of MultiWell calculations to PES results, the thermal decomposition of phenol was studied. As stated above, there is no elementary work on soot oxidation by OH to compare the dissertation results to. However, a reaction with similarities, phenol decomposition, has been studied experimentally [79,80] and theoretically at the G2M level of theory [81].

4.3.1 PES Results

Figure 4.19 contains the PES from my B3LYP/6-311G(d,p) calculations of the phenol system, as well as the G2M energy of Xu and Lin [81]. The energy calculated at the G2M level were generally within 2-4 kcal/mol of the B3LYP/6-311G(d,p) calculations. The largest deviation was in the BDE energy of the H atom elimination. This is to be expected, as noted in Section 4.1.3, because of B3LYP's known deficiencies in calculating BDE.

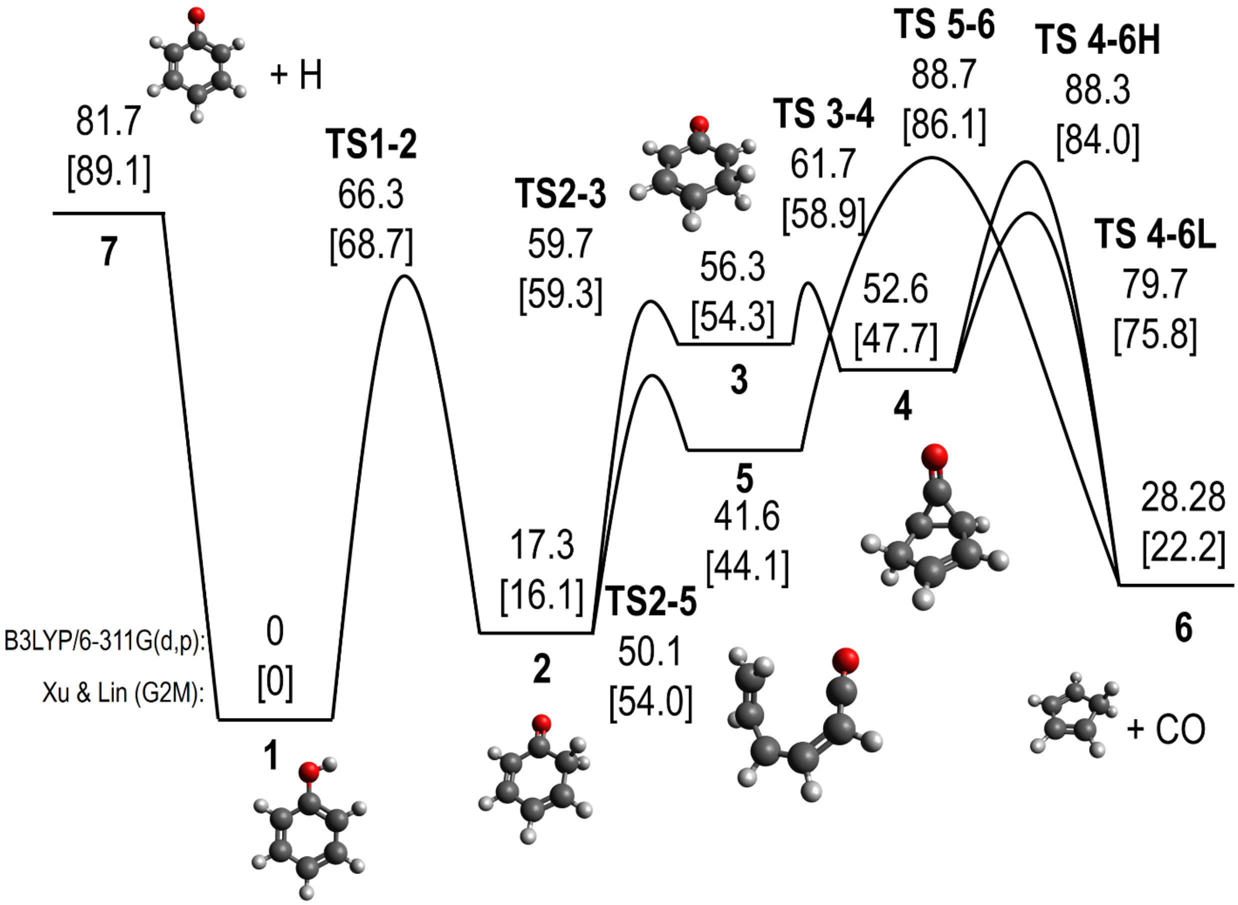


Figure 4.19. PES for the thermal decomposition of phenol. The unbracketed results were calculated here at the B3LYP/6-311G(d,p) level of theory. The bracketed results were taken from Xu and Lin [81] and were calculated at the G2M//B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **1**.

4.3.2 Reaction Rate Coefficients

Using MultiWell, the thermal decomposition rates of the system shown in Figure 4.19 were calculated using both the here calculated B3LYP energies and the G2M energies of Xu and Lin [81]. Because Xu and Lin performed their geometry optimization at the B3LYP/6-311G(d,p) level of theory, the same level of theory used here, the geometries, frequencies, and moments of inertia in the B3LYP and G2M calculations were the same. Only the G2M single point energy calculations were different. The H elimination channel was not included in the MultiWell calculations because Xu and Lin did not include it in their analysis of phenol decomposition. Additionally Scheer et al. [80] determined that the H-elimination pathway would not be significant, especially at lower temperatures. To compare to the experimental data of Horn et al. [79], calculations were carried out at intervals of 100 K between temperatures of 1500−2000 K and at 2.5 atm. In addition to using the constant $\langle \Delta E \rangle_{\text{down}}$ = 260 cm^{-1} value, the thermal decomposition rates were also calculated using the temperature dependent value of $\langle \Delta E \rangle_{\text{down}}$, calculated using Equation 2.1. The results of these calculations, as well as the results of both Xu and Lin and Horn et al., are shown in Figure 4.20.

The results show that the rates calculated using the B3LYP energies were 2.6 times slower at 1500 K and 1.6 times slower at 2000 K than the rates calculated with the G2M energies. The G2M rates were generally within a factor of 2 of the Horn data, while the B3LYP results were within a factor of 3−5. The difference between the two $\langle \Delta E \rangle_{\text{down}}$ approaches was minimal, with the maximum deviation occurring at 2000 K. In this case the temperature dependent $\langle \Delta E \rangle_{\text{down}}$ calculations were 1.7 times faster than the constant $\langle \Delta E \rangle_{\text{down}}$ calculations. This was the same for both the B3LYP and G2M calculations.

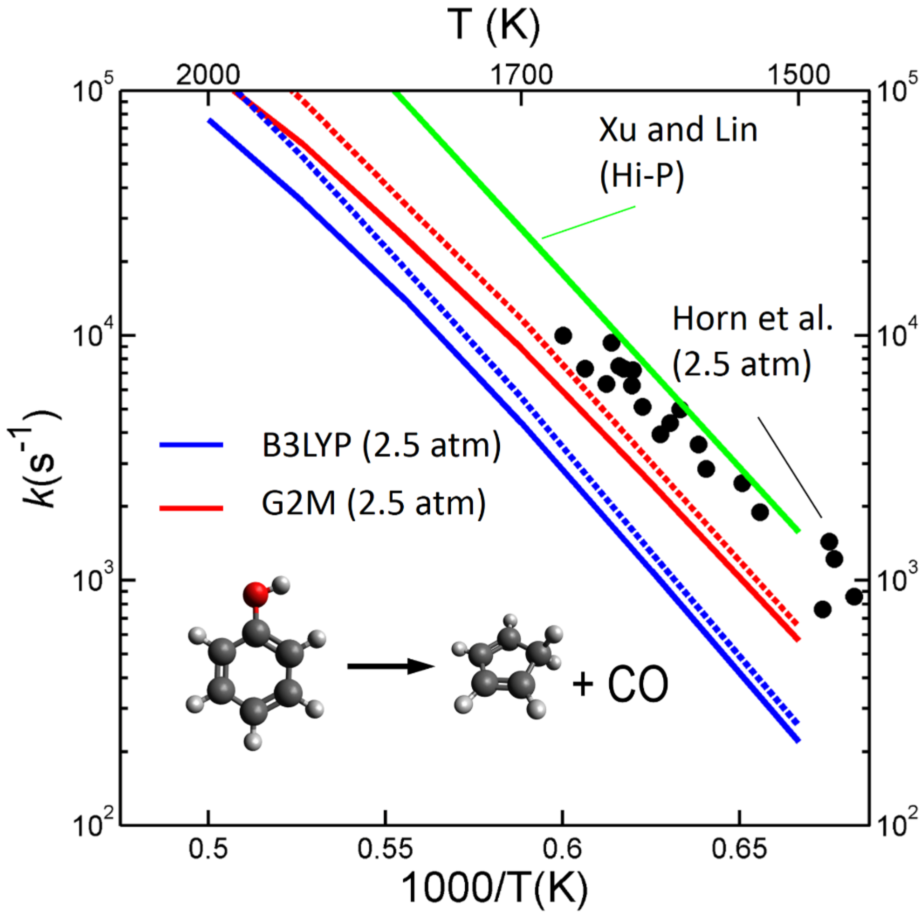


Figure 4.20. Thermal decomposition of phenol, calculated using the B3LYP results of the present work (blue) and the G2M results of Xu and Lin [81] (red). The solid lines were calculated with the constant $\langle \Delta E \rangle_{\mathrm{down}} = 260\ \mathrm{cm}^{-1}$, while the dashed lines were calculated using the temperature dependent $\langle \Delta E \rangle_{\mathrm{down}}$ values from Equation 2.1. The black circles are the experimental results of Horn et al. [79] and the green line is from Xu and Lin's theoretical study [81].

The Xu and Lin data was calculated using ChemRate [82], and they indicated that there calculations showed no pressure dependence. This is surprising given the known pressure dependence of the similarly structured PES of phenoxy decomposition [55,57]. Here the calculated rates were pressure dependent. The 1 atm values of the rate coefficient calculated using the B3LYP energies were 1.9×10^2 and $5.3 \times 10^4\ \mathrm{s}^{-1}$ for 1500 and 2000 K, respectively. Whereas the 2.5 atm results were 2.2×10^2 and $7.6 \times 10^4\ \mathrm{s}^{-1}$ for 1500 and 2000 K, respectively. The 1500 K results seemed to be approaching the high pressure limit, but likely not the 2000 K results. Because our focus in this section is on sensitivity, large temperature and pressure ranges were not calculated.

A sensitivity analysis was performed to observe how values from the PES shown in Figure 4.19 impact the MultiWell calculated thermal decomposition rate of phenol. The goal was to see what changes to the B3LYP energies were needed to match the decomposition rate found using the G2M energies. This simple sensitivity analysis was carried out by replacing a B3LYP energetic value with the corresponding G2M value. Because lower temperature simulations take longer to run than higher temperature simulations, all of these sensitivity calculations were performed at 2000 K and 2.5 atm. Table 4.5 contains the results of this analysis. The table indicates the species or transition state that was modified, and in all cases the modification was from the B3LYP value to the G2M value. All other values were maintained at the B3LYP energy.

Table 4.5. Results of sensitivity analysis of the thermal decomposition rate (*k*) of phenol to the PES energies. The first two rows contain rates calculated using the B3LYP and G2M energy values. The species numbers in the other rows indicate what B3LYP values on the PES shown in Figure 4.19 were replaced with the G2M value. For example in the third row, **4**, the B3LYP value of 52.6 kcal/mol was replaced by the G2M value of 47.7, while keeping all other energies at the B3LYP values.

Energy configuration	k (s^{-1})	k/k_{G2M}
B3LYP energies	7.6e4	0.6
G2M energies	1.2e5	1.0
4	8.9e4	0.7
TS4-6L	1.3e5	1.1
4 and **TS4-6L**	1.3e5	1.1
TS3-4	7.9e4	0.7
3 and **TS3-4**	8.0e4	0.7
2 and **TS2-3**	7.6e4	0.6
TS1-2	7.4e4	0.6

Table 4.5 shows that there are a number of changes that can be made to the energies that translate into meaningful changes in the phenol decomposition rate. For example lowering **TS4-6L** from the B3LYP value of 79.7 kcal/mol to the G2M value of 75.8 kcal/mol increased the B3LYP rate to essentially match the G2M rate. In this case the barrier height (**4-6L**) decreased from 27.1 kcal/mol to 23.2 kcal/mol, a substantial decrease which led to a nearly factor of 2 increase in the decomposition rate. If instead the energy of species **4** and **TS4-6L** are modified from their B3LYP value to match the G2M value, the end result is nearly the same, a nearly factor of two increase in the decomposition rate. However, the reasoning changes. In this second example, the barrier height **4-6L** actually increases, from 27.1 to 28.1 kcal/mol. In addition, the reverse barrier from **4** back to **3** also increases going from 9.1 to 14.0 kcal/mol. In this case the increase in rate is due to the fact that the reverse barrier is substantially higher, allowing for the forward reaction out of **4** to be more competitive.

As the above demonstrates, and is clear from transition state theory, the barrier heights, both reverse and forward, play significant roles in determining rates. From this kinetic perspective, it may be more useful to present the PES in Figure 4.19 in a different way, labeling barrier heights rather than energies of intermediates and transition structures. This alternative emphasis is shown in Figure 4.21. In this arrangement different trends are more easily observed than in Figure 4.19. For example it is clear that the reverse barriers for each step along the **1** to **2** to **3** to **4** pathway are larger for the G2M energies compared to the B3LYP energies. This would suggest that as the reacting specie moves from well to well on this path, the B3LYP energies, compared to the G2M energies, would promote more species to react backwards, while the G2M energies would promote more species reacting forward. Another example of the increased clarity is seen examining the branching ratio out of **3**. In the B3LYP case, the forward barrier is 2.0 kcal/mol higher than the reverse. In the G2M case, on the other hand, the forward barrier was 0.4 kcal/mol less than the reverse. Again this indicates that the G2M energies are more favorable to the forward progress of the reaction, while the B3LYP energies are less so.

Using Figure 4.21 as the basis, further sensitivity analysis was performed. In this case the B3LYP barriers, rather than individual wells or transition structure energies, were changed to match the G2M barriers. This is a more consistent approach than replacing a single stationary point, as was just presented above. For example when the energy of **4** was changed to match the G2M energy, the reverse barrier from **4** to **3** was then calculated using a mixture of G2M (for **4**) and B3LYP (for **TS3-4**) energies. This mixed methods barrier height than become 14.0 kcal/mol, substantially higher than either the B3LYP barrier height of 9.1 kcal/mol or the G2M height of 11.2 kcal/mol. In this alternative approach of changing barriers, a more consistent handling of relative energies is encouraged. The sensitivity results are shown in Table 4.6.

Table 4.6. Results of sensitivity analysis of the thermal decomposition (*k*) of phenol to the PES energies. The first two rows contain the rates calculated using the B3LYP and G2M energy values. The species numbers in the other rows indicate what B3LYP barrier heights on the PES shown in Figure 4.21 were replaced with the G2M heights. For example in the third row, **2** to **1**, the B3LYP barrier height of 49.0 kcal/mol was replaced by the G2M value of 52.6, while keeping all other barrier heights at the B3LYP values.

Energy configuration	k (s^{-1})	k/k_{G2M}
B3LYP energies	7.6e4	0.6
G2M energies	1.2e5	1.0
2 to **1**	1.4e5	1.2
3 to **2**	9.7e4	0.8
4 to **3**	1.0e5	0.8
1 to **2**	5.2e4	0.4

The results in Table 4.6 again show multiple variations that lead to closer matching between the B3LYP and G2M results. The reverse barrier **2** to **1** was modified to match G2M results, while leaving all other barriers the same. The results show a large increase in the rate constant and essentially match the G2M calculated rate. Similarly the reverse barrier from well **3** to **2** was also modified to match the 5.0 kcal/mol value of the G2M results. Again the results more closely matched the G2M calculated rate constants. Finally, varying the reverse barrier of **4** to **3** also yielded increases in the decomposition rate. In these three cases, it was an increase in the reverse barrier that led to faster overall rates.

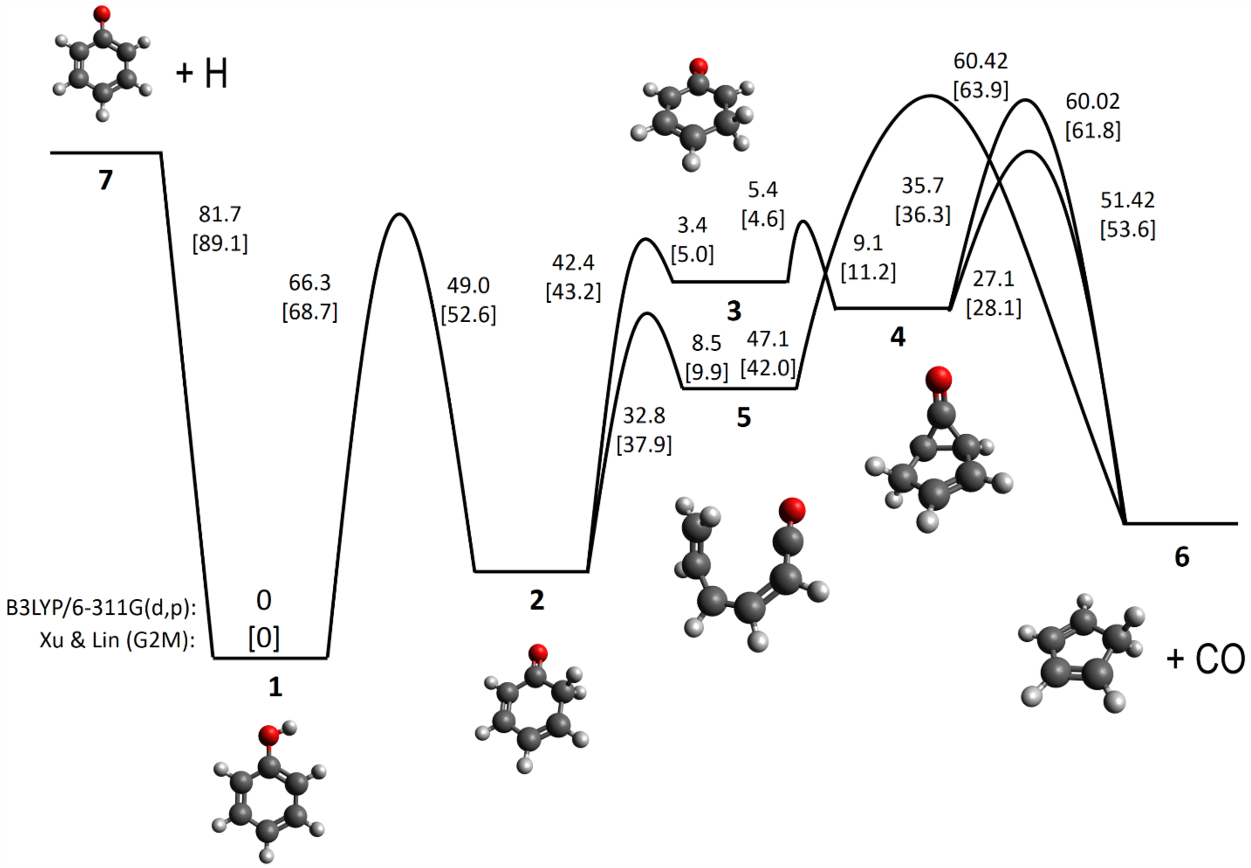


Figure 4.21. PES, showing barrier heights, for the thermal decomposition of phenol. The un-bracketed results were calculated here at the B3LYP/6-311G(d,p) level of theory. The bracketed results were taken from Xu and Lin [81] and were calculated at the G2M//B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol. This PES is identical to Figure 4.19, the only difference is the labeling focuses on barrier heights rather than the energy at each stationary point.

The factors affecting the thermal decomposition rate of phenol were more clearly seen when barrier heights were the parameters varied, rather than individual energies of wells or transition structures. The barrier height sensitivity analysis indicates that the difference between the rates calculated using the B3LYP energy compared to the G2M energy was primarily related to the higher barriers for the reverse reaction along the G2M decomposition pathway. In some cases, including the initial barrier, the B3LYP forward barrier height was lower than the G2M heights, but in all cases the G2M reverse barriers were higher. These higher reverse barriers allowed for the more rapid overall decomposition rate calculated with the G2M energies.

4.4 Summary

The energetics of three different PAH edge sites reacting with OH were computed to explore pathways leading to CO expulsion. Two reaction systems, OH + benzene and a benzene-phenol complex, did not show viable pathways to rapid CO expulsion. The third one, OH reacting with a phenanthrene radical was the most promising of the three PAH edge sites studied, containing multiple pathways for CO elimination.

The kinetics of the OH + phenanthrene radical reaction were studied by calculating both the chemical-activation and thermal-decomposition reaction rates. Chemical activation, at lower temperatures and higher pressures, was not sufficient to drive the reaction completely to products. The reaction progress was impeded by the rapid de-energizing of intermediate species. In such cases, the rates were calculated by chemical activation followed by thermal decomposition of the de-energized intermediate species. This led to a time dependence of the overall rate coefficients for CO formation. After an initial ramp-up time, the rate coefficient reached a steady-state value.

The computed overall oxidation rate of phenanthrene radicals by OH was found to be insensitive to pressure and temperature and was approximately 1×10^{14} cm^3 mol^{-1} s^{-1}.

The two principal processes involved in phenanthrene radical oxidation by OH were H atom migration/elimination followed by oxyradical decomposition. H atom migration/elimination made possible the relatively rapid rearrangement of the PAH edge, forming kinetically favorable oxyradicals which then decomposed. These same two processes would be expected to be present in soot surface oxidation by OH.

Chapter 5

Triplet Surface Results

The main results of this dissertation, presented above in Chapter 4, are based on the calculation of the OH + phenanthrene radical on the *singlet* surface. However, the same reaction can occur on the *triplet* surface. Although the relevance of the triplet surface is suspected to be less than the singlet surface, as discussed in Section 5.3, it is still included here for completeness and comparison. The triplet surface results, calculated in the same way as the singlet results of Chapter 4, are presented in this chapter.

5.1 PES Results

The adduct and initial wells of the triplet PES (t-PES) for the phenanthrene radical reacting with OH are shown in Figure 5.1. The PES shows the formation of five oxyradicals: **t-7**, **t-6**, **t-3**, **t-5**, and **t-4** associated with channels t-I through t-V shown in, respectively, Figure 5.2−Figure 5.6. The general structure and form of the t-PES surface are the same as the singlet. The formation of the first four oxyradicals, **t-7**, **t-6**, **t-3**, and **t-5**, was facilitated by H-atom migration, while the formation of **4** was enabled by H-atom elimination, just as in the singlet results.

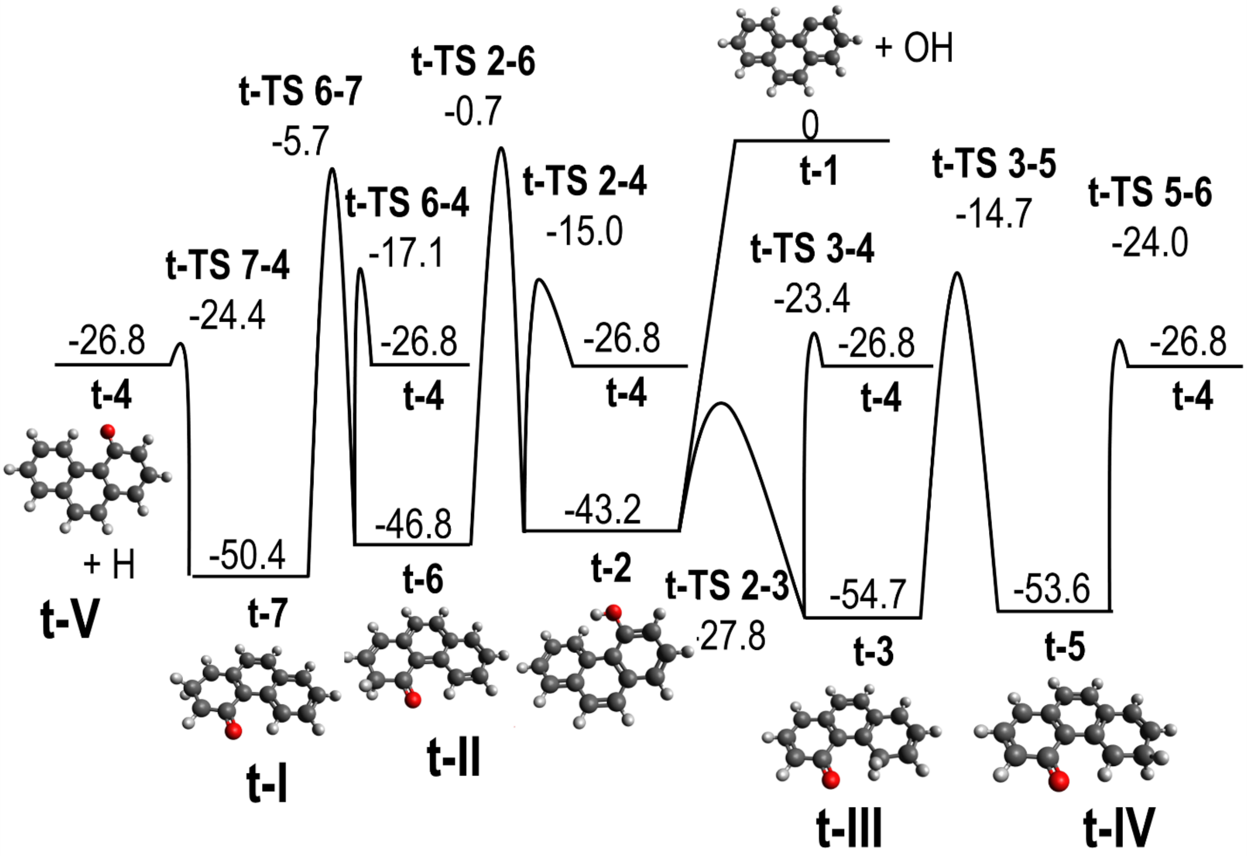


Figure 5.1. The initial wells of the PES for the reaction of a phenanthrene radical with OH on the triplet surface at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **t-1**.

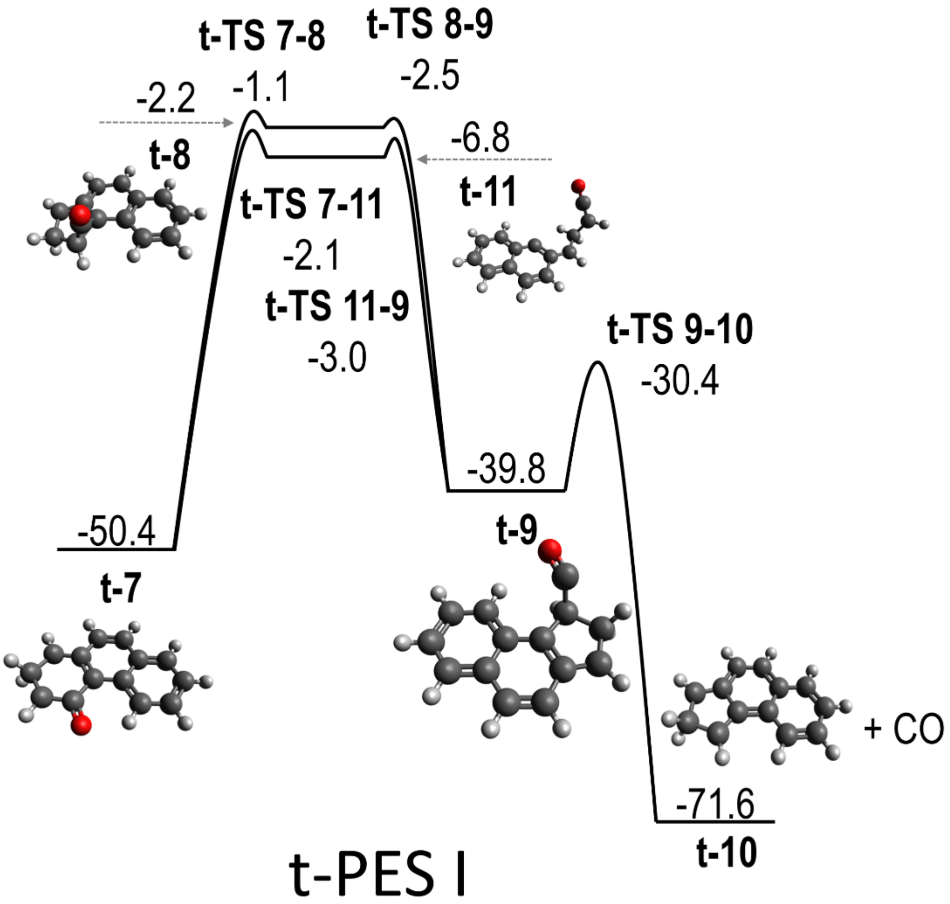


Figure 5.2. t-PES I for the reaction of a phenanthrene radical with OH on the triplet surface at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **t-1** in Figure 5.1.

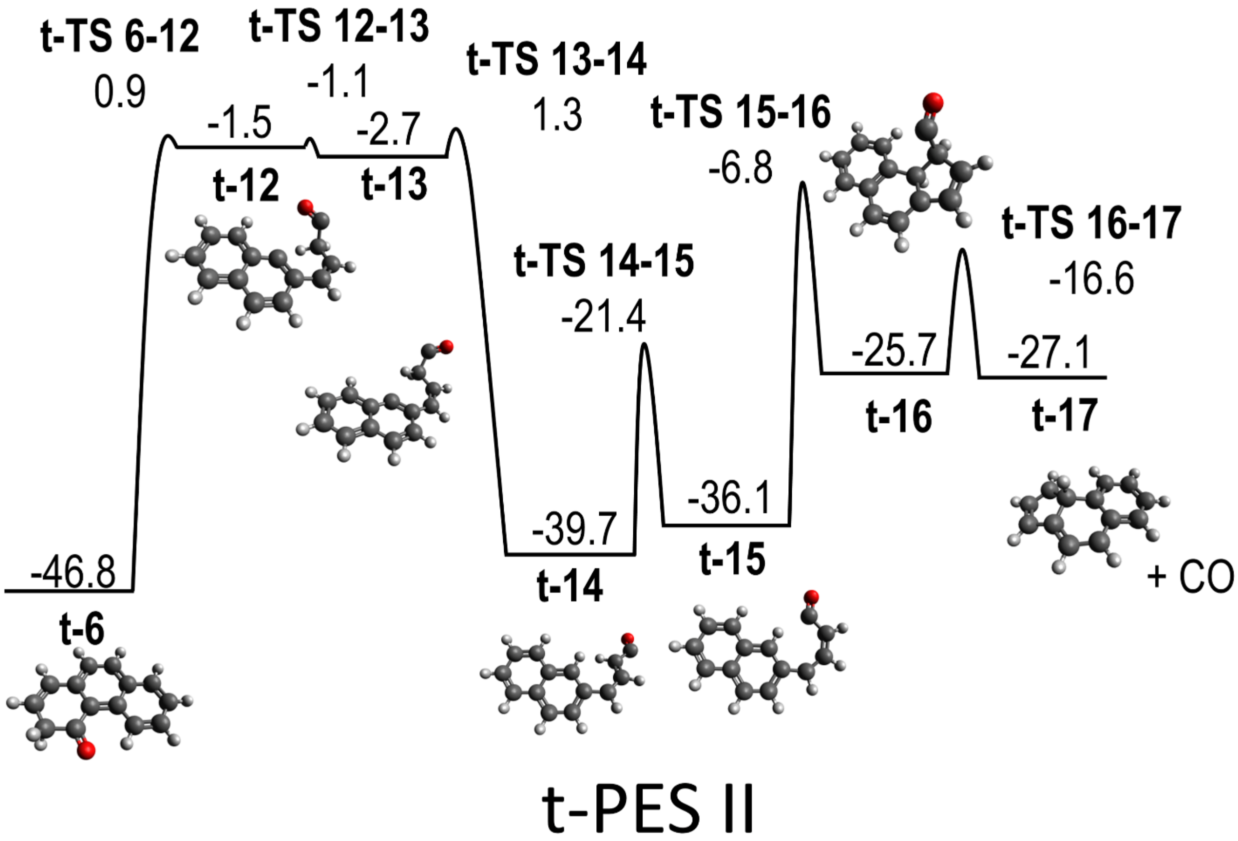


Figure 5.3. t-PES II for the reaction of a phenanthrene radical with OH on the triplet surface at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **t-1** in Figure 5.1.

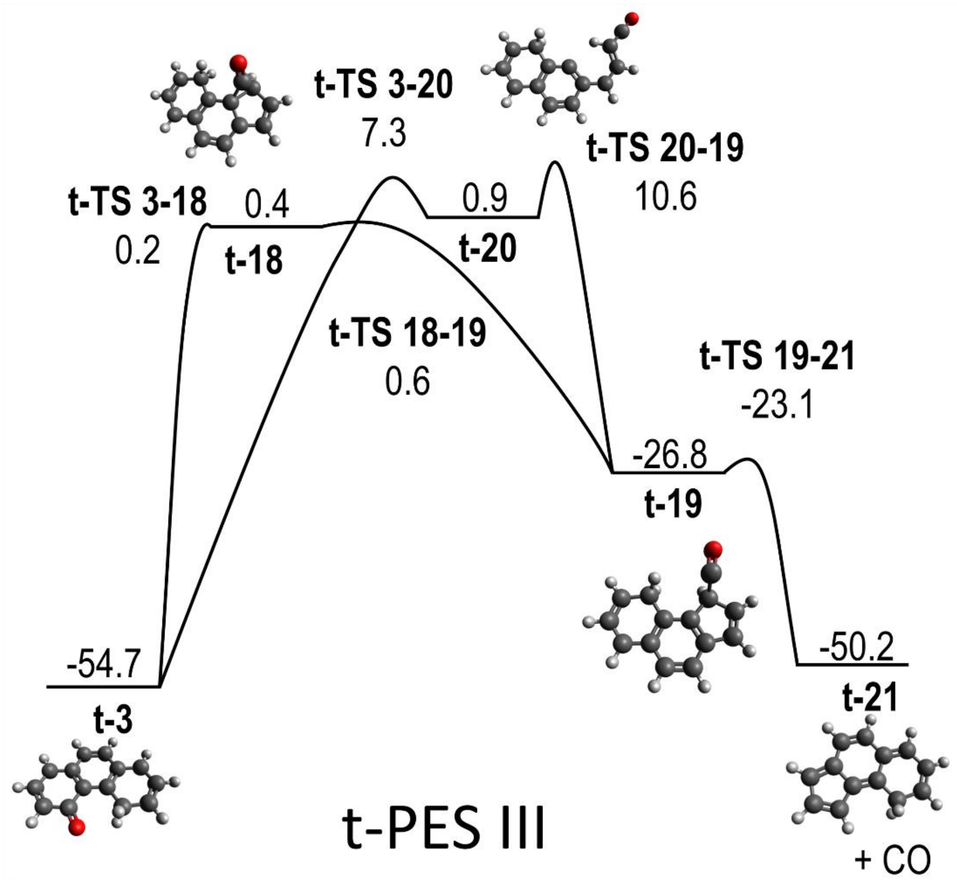


Figure 5.4. t-PES III for the reaction of a phenanthrene radical with OH on the triplet surface at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **t-1** in Figure 5.1.

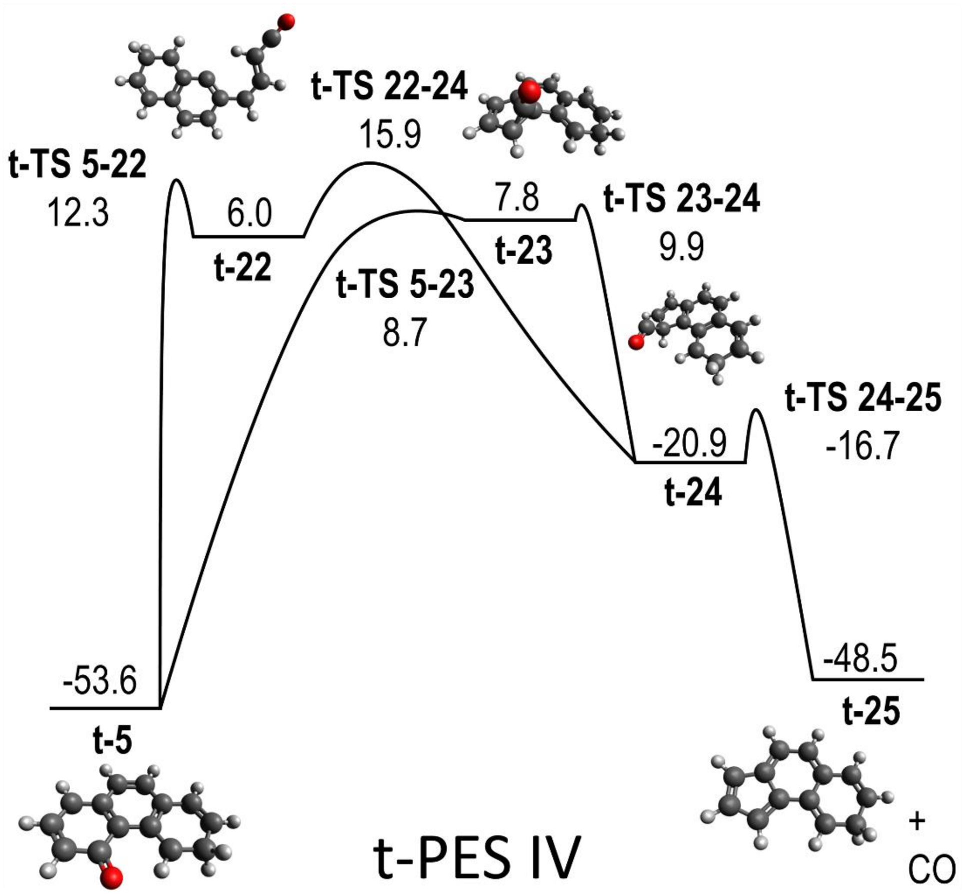


Figure 5.5. t-PES IV for the reaction of a phenanthrene radical with OH on the triplet surface at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **t-1** in Figure 5.1.

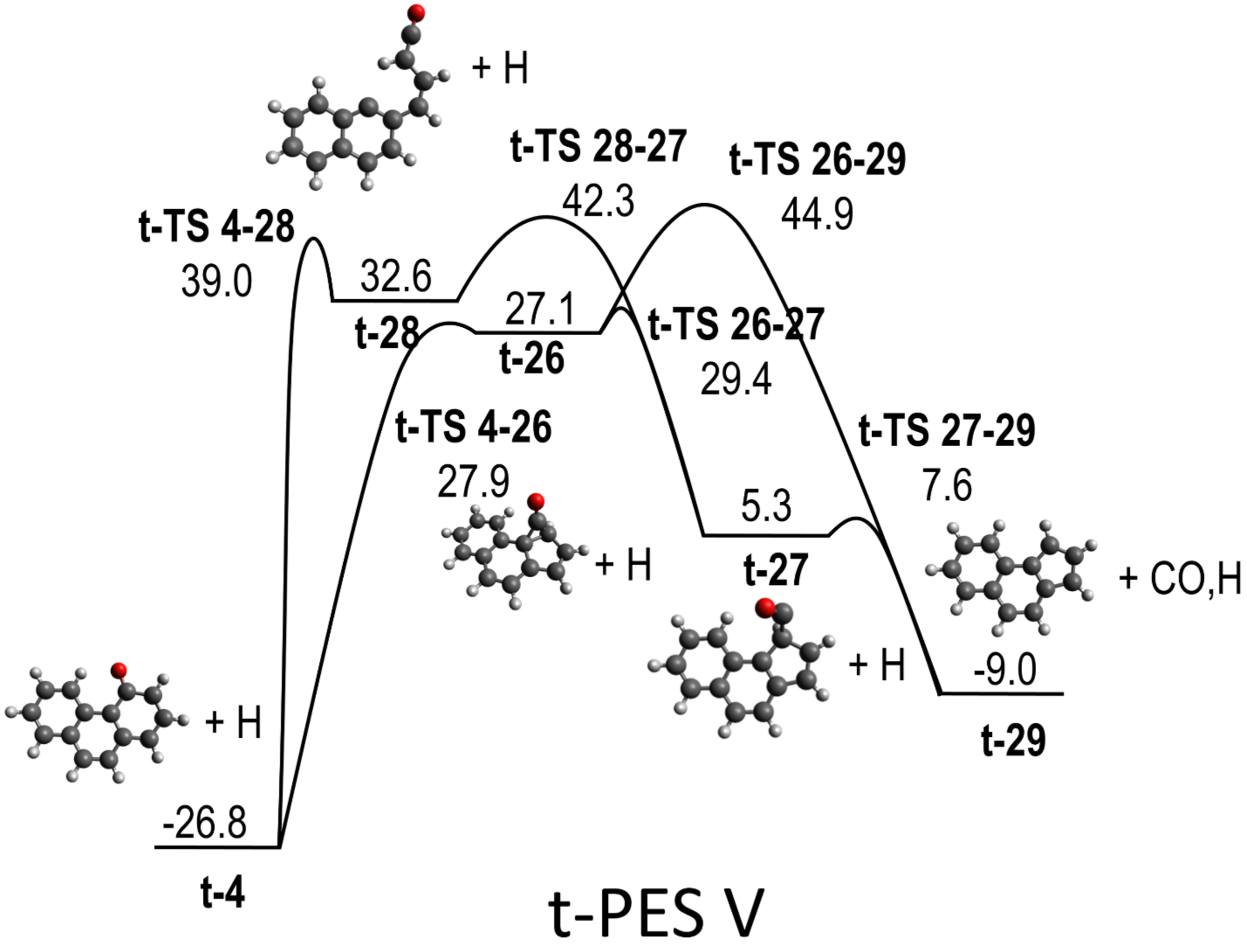


Figure 5.6. t-PES V for the reaction of a phenanthrene radical with OH at the B3LYP/6-311G(d,p) level of theory. Energies, which include ZPE, are in kcal/mol at 0 K relative to the reactants, **t-1** in Figure 5.1. Note that this is the same PES (with the zero point of energy shifted) as shown in Figure 3.2 and Figure 4.8.

The primary difference between the triplet and the singlet results was that the triplet energies were substantially higher in potential energy than the singlet energies. For example, the depth of the initial adduct (at the B3LYP/6-311G(d,p) level of theory) on the singlet surface, **2**, was 102.3 kcal/mol, while the triplet was 43.2 kcal/mol. In addition to these energetic differences, there are a number of pathway differences between the two surfaces. The most significant may be that on the triplet surface there were distinct transition structures for H-atom dissociation, i.e. **t-TS7-4**, **t-TS6-4**, **t-TS3-4**, and **t-TS5-4**, while the singlet surface reactions for H-atom dissociation were barrierless.

5.2 Reaction Rate Coefficients

5.2.1 Barrierless reaction: 2→1

Compared to the singlet surface result, only one barrierless reaction was found on the triplet surface. The points found on the potential energy surface scan are shown in Figure 5.7. Compared to the barrierless reactions on the singlet surface, this barrierless reaction was not well defined by either a Morse or Varshni potential. Instead, each point is read into VariFlex and VariFlex extrapolates between the points.

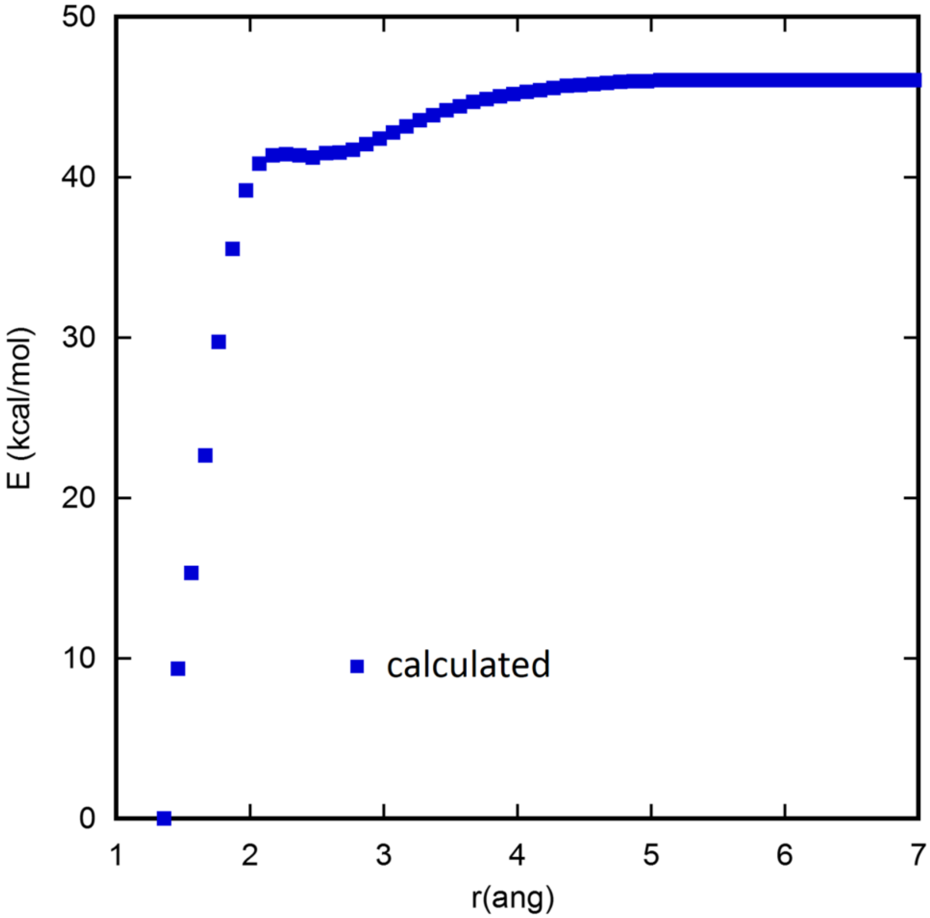


Figure 5.7. Results of potential energy surface scan for the initial OH attack on a phenanthrene radical (**t-1→t-2**).

The reaction path degeneracy, just as in the singlet case, was increased by a factor of two because the transition structure was an optical isomer.

5.2.2 Master Equation Modeling

The species fractions resulting from the chemical-activation simulations of the combined system shown in Figure 5.1–Figure 5.6 are given in Table 5.1. The chemical-activation rate constants were calculated by multiplying the species fraction in Table 5.1 by the high-pressure rate of OH combining with a phenanthrene radical. Table 5.2 lists these high-pressure triplet surface values for the three temperatures studied. The main products of the chemically-activated system were **t-29** (H,CO) and **1** (reactants). In addition, at higher pressures and lower temperatures, species **t-4** was collisionally stabilized and accumulated.

Table 5.1. Species fractions resulting from the chemical-activation simulations of the system shown in Figure 5.1–Figure 5.6.

	T = 1500 K				T = 2000 K				T = 2500 K			
	pressure (atm)				pressure (atm)				pressure (atm)			
species #	0.01	0.1	1	10	0.01	0.1	1	10	0.01	0.1	1	10
t-1	0.12	0.12	0.12	0.11	0.32	0.32	0.32	0.32	0.49	0.49	0.49	0.49
t-21	-	-	-	-	-	-	-	-	0.01	0.01	0.01	0.01
t-29	0.64	0.39	0.16	0.04	0.68	0.66	0.60	0.44	0.50	0.50	0.50	0.48
t-4	0.24	0.49	0.72	0.85	0.00	0.02	0.08	0.23	-	-	-	0.02
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99	1.00	1.00	1.00	1.00

Table 5.2. High-pressure elementary reaction rates of OH attacking a phenanthrene radical on the triplet surface.

T (K)	k_∞ (cm^3 mol^{-1} s^{-1})
1500	1.6×10^{13}
2000	2.4×10^{13}
2500	3.2×10^{13}

As was done on the singlet surface, thermal rate coefficients were used in conjunction with the chemical-activation rate coefficients to calculate the overall rate of CO expulsion from the reaction of OH with a phenanthrene radical on the triplet surface. The reaction system used to calculate the overall reaction rate coefficients for a combined system of thermal and chemical-activation rates is shown in Figure 5.8. The triplet reaction system was simpler than the singlet system. In the singlet system there was the accumulation of three intermediates, while the triplet system contained only one, **t-4**. Furthermore, no additional thermal decomposition rates needed to be calculated because the thermal decomposition of **t-4** was calculated in Chapter 3 as phenanthrene II oxyradical.

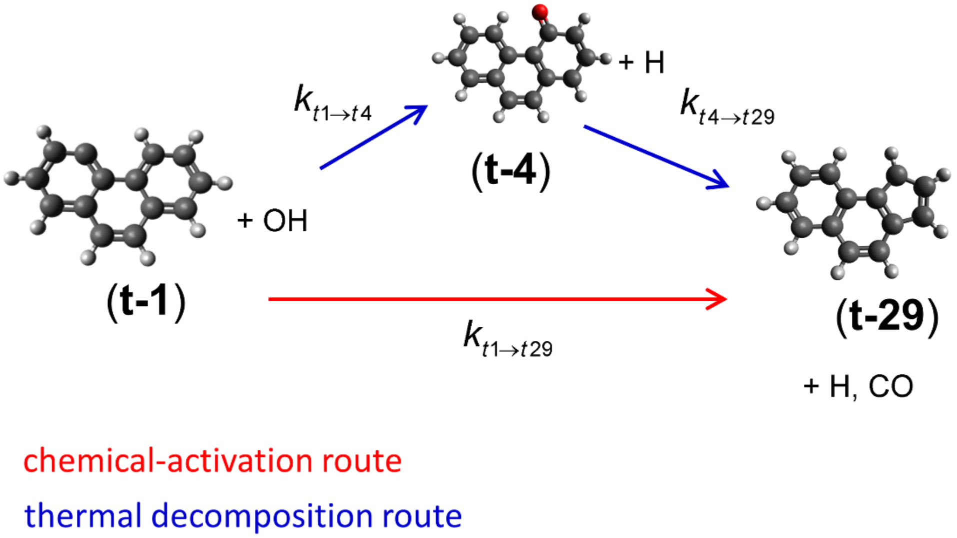


Figure 5.8. The reaction system illustrating the combined chemical activation and thermal decomposition required to calculate the overall oxidation of phenanthrene radicals by OH on the triplet surface.

Based on the reaction system shown in Figure 5.8, and following the same approach presented in Chapter 4, the rate constant for the formation of **t-29**, the overall triplet rate, is given as

$$k_{co,triplet} = k_{t29}\left(t\right) = k_{t1\rightarrow t29} + k_{t1\rightarrow t4}\left(1 - e^{-k_{t4\rightarrow t29}t}\right) \tag{5.1}$$

Again, just as in the case of the singlet, the triplet surface results were time dependent, and the ramp up times (defined in Figure 4.17) for the triplet system are presented in Table 5.3. The ramp up times were faster for the triplet results vs the singlet results. This is due to slower thermal decomposition of species **2** and **7** on the singlet surface versus species **t-4**.

Table 5.3. Ramp-up times of $k_{\text{CO,triplet}}$. Ramp-up time is defined as the time for $k_{\text{CO,triplet}}$ to reach 90% of its final value.

	Ramp-up time, triplet, (μs)			
	Pressure (atm)			
T (K)	0.01	0.1	1	10
1500	190	55	20	14
2000	45	7	1.4	0.36
2500	–	–	–	–

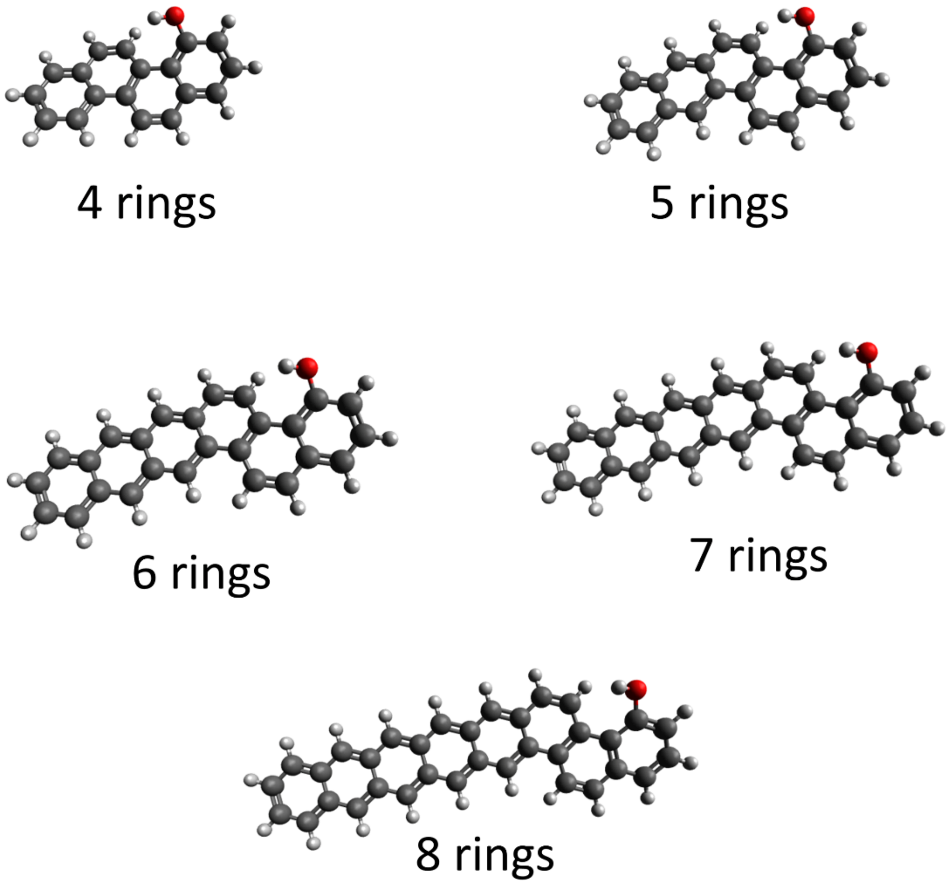
The overall rate, $k^{\infty}_{\text{CO,triplet}}$, which is found as t→∞, was calculated for the triplet reaction. Again, as was found for the singlet case, $k^{\infty}_{\text{CO,triplet}}$ is independent of pressure, and only slightly dependent on temperature. The values for 1500, 2000, and 2500 K were found to be, 1.4, 1.6, and 1.6 ×10^{13} cm^3 mol^{-1} s^{-1}, respectively. The triplet rates are roughly a factor of 6 times slower than the singlet rates

5.3 Combining Triplet and Singlet Rates

The dynamic calculations needed to determine the initial branching into the singlet or triplet surface of the OH attacking a phenanthrene radical are beyond the scope of this dissertation. Such a calculation could start with identifying the conical intersection between the two surfaces, an expensive calculation. Furthermore, there may be many such intersections because many of the geometries on the singlet and triplet surface are similar. However, finding the conical intersections would provide no insight into the triplet/singlet branching ratio. No simple theory, similar to Transition State Theory, exist to calculate the branching ratio from a conical intersection. Rather, trajectory simulation must be performed [83]. Often, due to the greater stability of the singlet surface, the triplet reactions are ignored. For example, to my knowledge, the reaction of an H-atom with a $C_{surface}$● site is always treated as a singlet surface reaction [84] even though benzene and naphthalene, for example, have stable structure on the triplet surface.

For studies where the triplet surface results were accounted for, the overall rate was often just calculated as the addition of the triplet and singlet results. Tranter et al. [85] studied the self-reaction of phenyl radicals, including the abstraction reaction forming benzene and benzyne. This reaction takes place on both the singlet and triplet surface, and they calculated the reaction rate on both surfaces. When they included these reactions into their overall mechanism for modeling the formation of benzynes they added together the contributions of the singlet and triplet state, stating, “For the purposes of modeling, the assumption has been made that the triplet benzynes will convert rapidly to the singlet state”. A similar rationale could be used here to combine the triplet and singlet results.

A final, most relevant point about singlet and triplet, is as follows. It has been shown that as PAH’s grow larger, the singlet−triplet energy gap shrinks [86,87]. This would suggest that the triplet surface calculation of OH attacking a $C_{surface}$● site would possibly converge, or become similar to the singlet results as the substrate size increased. To test this, I carried out BDE calculations for OH reacting with increasingly sized $C_{surface}$● PAHs. The calculations were performed at the B3LYP/6-311G(d,p) level of theory and included ZPE. The structures used are shown in Figure 5.9.


4 rings

5 rings

6 rings

7 rings

8 rings

Figure 5.9. Structures used in calculating BDE of OH with the radical PAH.

The results of the triplet and singlet BDE are shown in Table 5.4. The table shows that the singlet and triplet results approach one another as the size of the PAH grows. Significantly, the singlet results stay nearly constant, and it is the triplet results that approach the singlet results. Based on this analysis, which indicates that the triplet surface energies approach the singlet surface energies, I recommend the use of the singlet surface results as a prototype reaction of OH reacting with a $C_{surface}$● site. The triplet surface results were still included in this dissertation for completeness, but do not appear to be as significant to oxidation by OH of larger PAHs and soot as the singlet surface results.

Table 5.4. BDE energy for OH + PAH radical. Geometries are shown in Figure 5.9.

	BDE (kcal/mol)	
# of rings	singlet	triplet
4	99.9	48.9
5	99.7	58.9
6	99.7	71.6
7	99.7	81.3
8	99.6	88.5

5.4 Summary

The energetics of the OH + phenanthrene radical reaction, on the triplet surface were performed. Similar to the singlet results, the main pathways were enabled by H-atom migration and elimination. The triplet surface results were energetically less stable then the similar geometry on the singlet surface. In some cases, the triplet geometries were 60 kcal/mol higher in potential energy then the singlet geometry.

The kinetics of the OH + phenanthrene radical reaction were studied and compared to the singlet results. The triplet pathways followed similar trends as the singlet pathways, namely chemical activation driving most of the reaction to product at higher temperatures and lower pressures, while accumulation of intermediates occurred at lower temperatures and higher pressures. In the triplet system only one intermediate accumulated, compared to the three of the singlet system. The computed overall oxidation rate of phenanthrene radicals by OH was found to be insensitive to pressure and temperature and was approximately 1.6×10^{13} cm^3 mol^{-1} s^{-1}.

A recommendation to use the singlet results is given based on examples in the literature, the energetic stability of the singlet surface, and the approach of the triplet surface energies to the singlet surface energies as the substrate size increases.

Chapter 6

Summary and Future Work

6.1 Summary

In this dissertation, for the first time, an analysis on elementary pathways and mechanisms for the oxidation of PAHs by OH were presented. These results have immediate impact on the soot community by replacing the current empirical handling of soot oxidation by OH with detailed results based on these PAH prototype reactions of a soot edge.

Chapter 3 discusses the initial work completed on armchair edge oxyradical decomposition. Oxyradicals are presumed to be key intermediates in oxidation pathways of soot. Because of this, the initial focus of the dissertation was in understanding how oxyradicals decompose. It was shown how armchair oxyradicals decompose similarly to zigzag edge oxyradicals, and how size affects decomposition rates. These results were subsequently used in calculating oxidation by OH in Chapters 4 and 5.

Building on these results, in Chapter 4 a number of different PAH edge types were investigated and it was determined that oxidation of soot by OH will most likely occur on a C_{surface}● site. Furthermore, the detailed pathways and reaction rates for the reaction of OH with a phenanthrene radical were identified, the phenanthrene radical being a prototype of a C_{surface}● site. The OH oxidation pathways were composed of multiple oxyradicals, supporting the notion in Chapter 3 that oxyradicals are important. The overall rate for OH with a phenanthrene radical was found to be independent of pressure and temperature, approximately 1×10^{14} cm^3 mol^{-1} s^{-1}. Chapter 5 studied the same reaction (OH + a phenanthrene radical), but on the triplet surface. I recommend the use of the singlet results based on examples in the literature, the energetic stability of the singlet surface, and the approach of the triplet surface energies to the singlet surface energies as substrate size increases.

6.2 Future Work

Much of the work presented here was performed using phenanthrene or a phenanthrene radical as a prototype for a soot surface edge. An open questions, addressed in part in Chapter 3, is how rates calculated on small prototype reactions, e.g. phenanthrene, change as larger substrates sizes are used. This area could be further explored for OH oxidation of soot by calculating OH oxidation on a larger system such as the benzoperylene used in the armchair oxyradical study. The focus of this future work should be on understanding how rates calculated on these relatively small PAHs translate to larger structures, just as was done with oxyradical decomposition. A related question is at what size PAH a reaction reaches the high pressure limit.

It would be beneficial to look at the reaction of OH with a zigzag edge site. Although previous work indicates such reactions are unlikely [47], study on corner zigzag sites might introduce different chemistry.

As mentioned in Section 4.2.3, secondary reactions with either hot or cold intermediates from the OH + phenanthrene radical reaction path are likely due to the long lived nature of some of the intermediates. Studying the reactions of these intermediates with O, OH, or H would indicate if these reactions do occur and at what rate. Furthermore, due to the long lived nature of these intermediates, I would expect to find oxyradicals and C-OH sites on soot edges.

As computational power increases, examining the PES of the systems studied at higher levels of theory would hone the results presented here to a greater degree of accuracy.

Finally, the rates found for OH oxidation can be immediately incorporated into KMC modeling; providing a detailed description into how OH oxidizes soot. This modeling would allow for a more in-depth comparison to experiments of soot oxidation by OH.

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Appendix A

Oxyradical Decomposition Details

A.1 Hi-Pressure limit rate calculations

The derivation of the overall, high pressure decomposition rates of the oxyradicals from Chapter 3 are presented here. The high-pressure rates for each elementary step along the five oxyradical pathways were calculated in MultiWell. These elementary rate coefficients are presented below in Table A.1−Table A.5. In order to transform these rates to a single overall rate, i.e. oxyradical→attached 5-member ring+CO, the standard steady state approximation for intermediates was used. This was done for each of the five oxyradical systems (shown in Figure 3.1−Figure 3.5). The derived steady-state expressions for the high-pressure-limit rate coefficients, k_∞ (in s^{-1}), of each of the five oxyradicals are presented below:

R3.1:

$$\begin{aligned} num = {} & k_{1\to6}k_{6\to7}((k_{2\to1}+k_{2\to7})((k_{3\to2}+k_{3\to4}+k_{3\to5})k_{5\to1}+(k_{3\to2}+k_{3\to4})k_{5\to3})k_{7\to4}+ \\ & k_{2\to3}(k_{3\to5}k_{5\to1}k_{7\to4}+k_{3\to4}(k_{5\to1}+k_{5\to3})(k_{7\to2}+k_{7\to4})))+k_{1\to5}k_{5\to3}((k_{6\to1}+ \\ & k_{6\to7})((k_{2\to1}+k_{2\to3})k_{3\to4}k_{7\to2}+(k_{2\to7}k_{3\to2}+(k_{2\to1}+k_{2\to3}+k_{2\to7})k_{3\to4})k_{7\to4})+ \\ & (k_{2\to1}+k_{2\to3}+k_{2\to7})k_{3\to4}k_{6\to1}k_{7\to6})+k_{1\to2}(k_{2\to7}((k_{3\to2}+k_{3\to4}+k_{3\to5})k_{5\to1}+ \\ & (k_{3\to2}+k_{3\to4})k_{5\to3})(k_{6\to1}+k_{6\to7})k_{7\to4}+k_{2\to3}k_{3\to4}(k_{5\to1}+k_{5\to3})((k_{6\to1}+k_{6\to7})(k_{7\to2}+k_{7\to4})+ \\ & k_{6\to1}k_{7\to6})) \end{aligned}$$

$$\begin{aligned} den = {} & k_{2\to7}((k_{3\to2}+k_{3\to4}+k_{3\to5})k_{5\to1}+(k_{3\to2}+k_{3\to4})k_{5\to3})((k_{6\to1}+k_{6\to7})k_{7\to4}+k_{6\to1}k_{7\to6})+ \\ & k_{2\to3}((k_{3\to4}+k_{3\to5})k_{5\to1}+k_{3\to4}k_{5\to3})((k_{6\to1}+k_{6\to7})(k_{7\to2}+k_{7\to4})+k_{6\to1}k_{7\to6})+ \\ & k_{2\to1}((k_{3\to2}+k_{3\to4}+k_{3\to5})k_{5\to1}+(k_{3\to2}+k_{3\to4})k_{5\to3})((k_{6\to1}+k_{6\to7})(k_{7\to2}+k_{7\to4})+k_{6\to1}k_{7\to6}) \end{aligned}$$

$$k_\infty = \frac{num}{den}$$

R3.2 and R3.4:

$$\begin{aligned} num = {} & k_{1\to5}\left(\left(k_{2\to1}+k_{2\to3}\right)k_{3\to4}+k_{2\to4}\left(k_{3\to2}+k_{3\to4}\right)\right)k_{5\to3}+ \\ & k_{1\to2}\left(k_{2\to3}k_{3\to4}\left(k_{5\to1}+k_{5\to3}\right)+k_{2\to4}\left(k_{3\to5}k_{5\to1}+k_{3\to2}\left(k_{5\to1}+k_{5\to3}\right)+k_{3\to4}\left(k_{5\to1}+k_{5\to3}\right)\right)\right) \end{aligned}$$

$$\begin{aligned} den = {} & k_{2\to3}\left(k_{3\to5}k_{5\to1}+k_{3\to4}\left(k_{5\to1}+k_{5\to3}\right)\right)+k_{2\to1}\left(k_{3\to5}k_{5\to1}+k_{3\to2}\left(k_{5\to1}+k_{5\to3}\right)+k_{3\to4}\left(k_{5\to1}+k_{5\to3}\right)\right)+ \\ & k_{2\to4}\left(k_{3\to5}k_{5\to1}+k_{3\to2}\left(k_{5\to1}+k_{5\to3}\right)+k_{3\to4}\left(k_{5\to1}+k_{5\to3}\right)\right) \end{aligned}$$

$$k_\infty = \frac{num}{den}$$

R3.3:

$$num = k_{3\to4}\left(k_{1\to5}\left(k_{2\to1}+k_{2\to3}\right)k_{5\to8}k_{8\to3}+k_{1\to2}k_{2\to3}\left(k_{5\to8}k_{8\to3}+k_{5\to1}\left(k_{8\to3}+k_{8\to5}\right)\right)\right)$$

$$\begin{aligned} den = {} & k_{2\to3}\left(k_{3\to8}k_{5\to1}k_{8\to5}+k_{3\to4}\left(k_{5\to8}k_{8\to3}+k_{5\to1}\left(k_{8\to3}+k_{8\to5}\right)\right)\right)+ \\ & k_{2\to1}\left(k_{3\to8}k_{5\to1}k_{8\to5}+k_{3\to2}\left(k_{5\to8}k_{8\to3}+k_{5\to1}\left(k_{8\to3}+k_{8\to5}\right)\right)+k_{3\to4}\left(k_{5\to8}k_{8\to3}+k_{5\to1}\left(k_{8\to3}+k_{8\to5}\right)\right)\right) \end{aligned}$$

$$k_\infty = \frac{num}{den}$$

R3.5:

$$k_\infty = \frac{k_{3\to4}\left(k_{1\to5}k_{5\to3}+k_{1\to3}\left(k_{5\to1}+k_{5\to3}\right)\right)}{k_{3\to5}k_{5\to1}+k_{3\to1}\left(k_{5\to1}+k_{5\to3}\right)+k_{3\to4}\left(k_{5\to1}+k_{5\to3}\right)}$$

Table A.1. High pressure rate coefficients (in s^{-1}) of the elementary steps for the decomposition of phenanthrene oxyradical I

T(K)	$k_{1\to2}$	$k_{1\to5}$	$k_{1\to6}$	$k_{2\to1}$	$k_{2\to3}$	$k_{2\to7}$	$k_{5\to1}$	$k_{5\to3}$
1500	7.9E+06	5.0E+05	1.3E+04	6.2E+12	2.9E+12	6.5E+11	1.6E+12	5.9E+11
1600	2.2E+07	2.0E+06	8.0E+04	6.3E+12	3.2E+12	8.2E+11	1.6E+12	6.1E+11
1700	5.3E+07	7.0E+06	3.8E+05	6.5E+12	3.5E+12	9.9E+11	1.6E+12	6.3E+11
1800	1.2E+08	2.1E+07	1.6E+06	6.6E+12	3.7E+12	1.2E+12	1.5E+12	6.5E+11
1900	2.4E+08	5.7E+07	5.4E+06	6.7E+12	4.0E+12	1.4E+12	1.5E+12	6.7E+11
2000	4.5E+08	1.4E+08	1.7E+07	6.8E+12	4.2E+12	1.6E+12	1.5E+12	6.9E+11
2100	8.0E+08	3.1E+08	4.6E+07	6.9E+12	4.5E+12	1.8E+12	1.5E+12	7.1E+11
2200	1.4E+09	6.4E+08	1.2E+08	6.9E+12	4.7E+12	2.0E+12	1.5E+12	7.3E+11
2300	2.2E+09	1.2E+09	2.7E+08	7.0E+12	4.9E+12	2.2E+12	1.5E+12	7.4E+11
2400	3.4E+09	2.3E+09	5.9E+08	7.1E+12	5.1E+12	2.5E+12	1.5E+12	7.6E+11
2500	5.0E+09	4.0E+09	1.2E+09	7.1E+12	5.3E+12	2.7E+12	1.5E+12	7.7E+11
T(K)	$k_{6\to1}$	$k_{6\to7}$	$k_{3\to2}$	$k_{3\to4}$	$k_{3\to5}$	$k_{7\to2}$	$k_{7\to6}$	$k_{7\to4}$
1500	2.6E+12	5.2E+11	5.6E+09	3.7E+13	2.7E+08	4.0E+10	1.2E+08	4.0E+13
1600	2.9E+12	5.7E+11	8.4E+09	3.8E+13	5.9E+08	5.2E+10	2.7E+08	4.1E+13
1700	3.1E+12	6.2E+11	1.2E+10	3.9E+13	1.2E+09	6.5E+10	5.7E+08	4.1E+13
1800	3.4E+12	6.6E+11	1.7E+10	4.0E+13	2.3E+09	8.0E+10	1.1E+09	4.2E+13
1900	3.6E+12	7.1E+11	2.3E+10	4.0E+13	4.0E+09	9.7E+10	2.0E+09	4.2E+13
2000	3.9E+12	7.5E+11	3.0E+10	4.1E+13	6.6E+09	1.1E+11	3.4E+09	4.2E+13
2100	4.1E+12	7.9E+11	3.8E+10	4.1E+13	1.1E+10	1.3E+11	5.5E+09	4.2E+13
2200	4.3E+12	8.3E+11	4.7E+10	4.2E+13	1.6E+10	1.5E+11	8.6E+09	4.3E+13
2300	4.5E+12	8.6E+11	5.8E+10	4.2E+13	2.3E+10	1.8E+11	1.3E+10	4.3E+13
2400	4.7E+12	9.0E+11	6.9E+10	4.3E+13	3.3E+10	2.0E+11	1.9E+10	4.3E+13
2500	4.9E+12	9.3E+11	8.2E+10	4.3E+13	4.6E+10	2.2E+11	2.6E+10	4.3E+13

Table A.2. High pressure rate coefficients (in s^{-1}) of the elementary steps for the decomposition of phenanthrene oxyradical II.

T(K)	$k_{1\to2}$	$k_{1\to5}$	$k_{2\to1}$	$k_{2\to3}$	$k_{5\to1}$	$k_{5\to3}$
1500	4.0E+05	6.8E+05	4.4E+12	3.5E+12	6.7E+11	6.7E+10
1600	1.3E+06	2.9E+06	4.5E+12	3.7E+12	7.7E+11	8.4E+10
1700	3.7E+06	1.1E+07	4.6E+12	3.9E+12	8.8E+11	1.0E+11
1800	9.3E+06	3.3E+07	4.7E+12	4.1E+12	9.9E+11	1.3E+11
1900	2.1E+07	9.2E+07	4.7E+12	4.3E+12	1.1E+12	1.5E+11
2000	4.5E+07	2.3E+08	4.8E+12	4.4E+12	1.2E+12	1.7E+11
2100	8.9E+07	5.3E+08	4.9E+12	4.6E+12	1.3E+12	2.0E+11
2200	1.6E+08	1.1E+09	4.9E+12	4.7E+12	1.4E+12	2.3E+11
2300	2.9E+08	2.3E+09	5.0E+12	4.9E+12	1.5E+12	2.6E+11

2400	4.8E+08	4.3E+09	5.0E+12	5.0E+12	1.7E+12	2.9E+11
2500	7.8E+08	7.7E+09	5.1E+12	5.1E+12	1.8E+12	3.2E+11

T(K)	$k_{3\to2}$	$k_{3\to4}$	$k_{3\to5}$	$k_{2\to4}$
1500	4.8E+08	1.3E+13	1.0E+08	6.0E+10
1600	8.3E+08	1.4E+13	2.4E+08	8.9E+10
1700	1.4E+09	1.5E+13	5.3E+08	1.3E+11
1800	2.1E+09	1.6E+13	1.1E+09	1.7E+11
1900	3.1E+09	1.7E+13	2.0E+09	2.3E+11
2000	4.3E+09	1.8E+13	3.4E+09	2.9E+11
2100	6.0E+09	1.9E+13	5.7E+09	3.7E+11
2200	8.0E+09	2.0E+13	9.1E+09	4.5E+11
2300	1.0E+10	2.1E+13	1.4E+10	5.4E+11
2400	1.3E+10	2.2E+13	2.1E+10	6.4E+11
2500	1.7E+10	2.2E+13	3.0E+10	7.5E+11

Table A.3. High pressure rate coefficients (in s^{-1}) of the elementary steps for the decomposition of phenanthrene oxyradical III.

T(K)	$k_{1\to2}$	$k_{1\to5}$	$k_{2\to1}$	$k_{2\to3}$	$k_{3\to2}$	$k_{3\to4}$
1500	2.6E+05	4.8E+05	2.6E+12	3.9E+12	8.1E+07	9.4E+12
1600	8.6E+05	1.8E+06	2.6E+12	4.0E+12	1.6E+08	1.1E+13
1700	2.5E+06	5.9E+06	2.6E+12	4.0E+12	3.0E+08	1.2E+13
1800	6.3E+06	1.7E+07	2.6E+12	4.0E+12	5.3E+08	1.3E+13
1900	1.4E+07	4.2E+07	2.6E+12	4.0E+12	8.7E+08	1.4E+13
2000	3.1E+07	9.8E+07	2.6E+12	4.0E+12	1.4E+09	1.5E+13
2100	6.1E+07	2.1E+08	2.6E+12	4.1E+12	2.1E+09	1.6E+13
2200	1.1E+08	4.2E+08	2.6E+12	4.1E+12	3.0E+09	1.7E+13
2300	2.0E+08	7.8E+08	2.6E+12	4.1E+12	4.2E+09	1.8E+13
2400	3.4E+08	1.4E+09	2.6E+12	4.1E+12	5.7E+09	1.9E+13
2500	5.4E+08	2.4E+09	2.6E+12	4.1E+12	7.7E+09	2.0E+13

T(K)	$k_{3\to8}$	$k_{5\to1}$	$k_{5\to8}$	$k_{8\to5}$	$k_{8\to3}$
1500	1.1E+08	7.8E+11	8.3E+11	4.7E+11	5.0E+11
1600	2.7E+08	7.9E+11	8.7E+11	5.0E+11	5.5E+11
1700	5.8E+08	8.0E+11	9.1E+11	5.3E+11	5.9E+11
1800	1.2E+09	8.1E+11	9.4E+11	5.6E+11	6.3E+11
1900	2.1E+09	8.2E+11	9.7E+11	5.9E+11	6.6E+11
2000	3.7E+09	8.3E+11	1.0E+12	6.2E+11	7.0E+11
2100	6.2E+09	8.4E+11	1.0E+12	6.4E+11	7.3E+11
2200	9.8E+09	8.4E+11	1.1E+12	6.7E+11	7.6E+11
2300	1.5E+10	8.5E+11	1.1E+12	6.9E+11	7.9E+11
2400	2.2E+10	8.6E+11	1.1E+12	7.1E+11	8.2E+11

2500	3.1E+10	8.6E+11	1.1E+12	7.3E+11	8.5E+11

Table A.4. High pressure rate coefficients (in s^{-1}) of the elementary steps for the decomposition of benzoperylene oxyradical.

T(K)	$k_{1\to2}$	$k_{1\to5}$	$k_{2\to1}$	$k_{2\to3}$	$k_{2\to4}$
1500	3.0E+04	3.5E+03	4.7E+12	2.6E+12	2.4E+11
1600	1.1E+05	1.9E+04	4.7E+12	2.9E+12	3.1E+11
1700	3.7E+05	8.8E+04	4.7E+12	3.2E+12	3.8E+11
1800	1.1E+06	3.4E+05	4.7E+12	3.6E+12	4.6E+11
1900	2.7E+06	1.1E+06	4.8E+12	3.9E+12	5.4E+11
2000	6.2E+06	3.4E+06	4.8E+12	4.2E+12	6.2E+11
2100	1.3E+07	9.0E+06	4.8E+12	4.4E+12	7.1E+11
2200	2.6E+07	2.2E+07	4.8E+12	4.7E+12	8.1E+11
2300	5.0E+07	5.0E+07	4.8E+12	5.0E+12	9.0E+11
2400	1.6E+08	1.9E+08	9.8E+12	1.1E+13	2.0E+12
2500	2.7E+08	3.7E+08	9.5E+12	1.1E+13	2.1E+12
T(K)	$k_{3\to2}$	$k_{3\to4}$	$k_{3\to5}$	$k_{5\to1}$	$k_{5\to3}$
1500	5.5E+09	1.3E+13	2.9E+08	6.4E+11	1.6E+11
1600	8.5E+09	1.3E+13	6.2E+08	7.5E+11	2.0E+11
1700	1.2E+10	1.4E+13	1.2E+09	8.7E+11	2.4E+11
1800	1.7E+10	1.5E+13	2.2E+09	9.8E+11	2.9E+11
1900	2.3E+10	1.5E+13	3.8E+09	1.1E+12	3.4E+11
2000	3.1E+10	1.6E+13	6.1E+09	1.2E+12	3.9E+11
2100	4.0E+10	1.6E+13	9.5E+09	1.3E+12	4.4E+11
2200	5.0E+10	1.7E+13	1.4E+10	1.5E+12	4.9E+11
2300	6.1E+10	1.7E+13	2.0E+10	1.6E+12	5.4E+11
2400	1.5E+11	3.5E+13	5.5E+10	3.4E+12	1.2E+12
2500	1.7E+11	3.5E+13	7.3E+10	3.5E+12	1.3E+12

Table A.5. High pressure rate coefficients (in s^{-1}) of the elementary steps for the decomposition of the extended-armchair oxyradical.

T(K)	$k_{1\to3}$	$k_{1\to5}$	$k_{3\to1}$	$k_{3\to4}$	$k_{3\to5}$	$k_{5\to1}$	$k_{5\to3}$
1500	7.2E+03	1.9E+04	2.7E+09	1.3E+13	3.1E+09	1.1E+12	4.7E+11
1600	2.8E+04	8.3E+04	4.3E+09	1.4E+13	5.6E+09	1.2E+12	5.1E+11
1700	9.6E+04	3.0E+05	6.5E+09	1.6E+13	9.6E+09	1.2E+12	5.5E+11
1800	2.8E+05	9.4E+05	9.5E+09	1.7E+13	1.5E+10	1.2E+12	5.9E+11
1900	7.5E+05	2.6E+06	1.3E+10	1.8E+13	2.4E+10	1.2E+12	6.2E+11
2000	1.8E+06	6.6E+06	1.8E+10	1.9E+13	3.5E+10	1.2E+12	6.5E+11

2100	3.9E+06	1.5E+07	2.4E+10	2.0E+13	4.9E+10	1.3E+12	6.8E+11
2200	8.1E+06	3.2E+07	3.1E+10	2.1E+13	6.8E+10	1.3E+12	7.1E+11
2300	1.6E+07	6.4E+07	3.9E+10	2.3E+13	9.1E+10	1.3E+12	7.4E+11
2400	2.8E+07	1.2E+08	4.8E+10	2.4E+13	1.2E+11	1.3E+12	7.6E+11
2500	4.9E+07	2.2E+08	5.8E+10	2.4E+13	1.5E+11	1.3E+12	7.9E+11

A.2 Details of PES

Table A.6. For all optimized structures in Chapter 3 the following are reported: total energies, zero-point energies, expectation values of S^2 operator (projected values are in parentheses), vibrational frequencies, rotational constants, and input parameters for the unsymmetrical hindered rotor implementation in MultiWell. All calculations were carried out at the B3LYP/6-311G(d,p) level of theory.

Species (Stationary point)	Total Energy (hartrees)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm^{-1})	Rotational constants (GHz)
Phenanthrene I (**1**)	-614.26654	0.184762	0.79(0.75)	71.83 99.36 162.72 203.06 234.92 278.88 387.09 397.24 410.03 423.60 463.58 503.93 514.94 536.47 540.97 629.87 638.50 706.93 715.13 725.06 759.37 777.71 793.21 816.79 847.32 874.09 883.45 887.13 901.84 962.30 974.68 996.59 999.37 1009.10 1059.05 1112.00 1151.39 1169.08 1184.01 1219.40 1240.86 1254.13 1268.78 1303.63 1312.44 1359.47 1391.59 1433.04 1443.24 1459.71 1495.56 1509.54 1536.39 1569.32 1605.82 1628.17 1649.09 3158.11 3162.55 3164.93 3174.32 3180.75 3188.18 3196.09 3196.68 3209.70	1.3130 0.4484 0.3343
Phenanthrene I (**2**)	-614.19262	0.182287	0.78(0.75)	72.70 82.30 141.61 178.12 243.89 249.71 326.41 417.18 422.69 446.96 483.86 500.69 516.22 526.34 558.17 620.70 629.54 665.57 669.90 737.84 748.22 756.60 768.74 795.75 824.52 857.86 867.46 873.13 916.91 954.28 974.57 977.14 989.59 991.75 1019.70 1047.23 1062.63 1093.99 1162.05 1176.50 1177.89 1198.61 1225.99 1235.56 1249.10 1292.62 1341.97 1368.87 1403.71 1419.28 1462.30 1472.53 1546.08 1572.41	1.2105 0.4825 0.3707

				1616.93 1640.57 1919.64 3126.01 3135.47 3158.66 3161.90 3167.56 3180.26 3182.34 3190.71 3218.63	
Phenanthrene I (**3**) Note: Same structure as Phenanthrene II 3	-614.21516	0.183246	0.75(0.75)	41.32* 83.41 111.04 151.47 201.91 238.22 264.51 331.64 418.08 430.52 457.29 471.29 516.18 523.01 553.73 591.38 655.83 678.54 693.93 715.96 759.13 760.60 773.10 818.60 844.74 857.73 874.72 900.29 955.02 959.79 970.92 974.79 993.32 1003.11 1047.08 1056.62 1117.68 1151.41 1168.44 1177.67 1183.58 1211.11 1237.55 1246.87 1288.42 1358.95 1378.50 1396.05 1410.03 1468.43 1487.46 1552.77 1586.56 1620.32 1638.02 1664.08 1914.82 3016.88 3159.08 3162.27 3170.37 3180.05 3184.63 3195.82 3199.08 3229.95	1.0233 0.5813 0.3973
	*Vibration replaced by unsymmetrical hindered rotor (hrd 8 8 1)			'Vhrd2' 1 0.1 260.43 -61.81 172.20 -45.22 -16.43 -1.63 6.30 -4.39	'Ihrd1' 1 0.1 11.44 1.83 2.79 6.38 1.46 1.54 0.94 0.43
Phenanthrene I (**4**) Note: Same structure as Phenanthrene II 4	-500.88710	0.173399	0.77(0.75)	113.80 138.85 236.84 240.37 278.51 424.38 426.95 457.51 501.09 518.28 535.81 549.80 584.74 684.74 689.62 716.38 734.30 753.20 773.37 813.38 836.40 849.17 872.66 873.43 890.94 927.76 954.41 964.26 991.50 998.57 1041.35 1063.36 1091.64 1161.74 1174.11 1184.17 1210.74 1239.61 1280.47 1287.98 1347.94 1374.25 1383.83 1424.01 1467.45 1474.55 1487.62 1554.34 1590.62 1605.24 1658.53 3158.02 3160.86 3165.76 3177.68 3179.19 3188.89 3205.07 3211.91 3231.50	1.8559 0.6744 0.4947
CO	-113.34624	0.005057		2219.82	0

					58.0386 58.0386
Phenanthrene I (**5**)	-614.15921	0.179149	0.76(0.75)	39.39* 70.08 92.98 137.66 156.68 202.23 229.42 297.60 305.15 360.19 421.80 448.18 462.21 490.38 502.92 539.29 547.27 571.74 597.49 629.75 645.01 698.50 713.62 741.55 753.98 798.03 810.17 837.24 854.32 875.25 892.25 958.03 966.31 994.37 1001.50 1058.72 1065.70 1147.47 1171.39 1183.26 1199.49 1213.31 1239.66 1276.66 1293.74 1359.45 1384.57 1390.71 1452.71 1457.20 1496.05 1543.78 1584.21 1626.94 1648.13 1662.34 2197.42 3011.33 3015.68 3159.43 3161.77 3173.05 3179.64 3187.44 3209.09 3244.32	0.8476 0.5738 0.3460
	*Vibration replaced by unsymmetrical hindered rotor (hrd 15 14 1)		'Vhrd2' 1 0 603.00 -397.44 -6.044 -185.20 156.18 -89.74 -6.74 11.89 19.89 -15.10 14.34 -7.54 4.23 0.27 -2.87	'Ihrd1' 1 0 32.51 3.26 -3.34 -5.51 8.22 -6.19 3.75 3.22 2.77 -1.30 1.50 0.55 0.33 -0.14	
Phenanthrene I (**6**)	-614.14029	0.179423	0.78(0.75)	26.17 70.73 83.20 109.19 178.29 208.21 243.72 300.87 336.39 362.63 413.86 439.29 493.72 504.12 514.40 523.08 544.80 573.31 587.37 625.77 646.26 685.14 712.56 751.38 776.79 781.91 788.19 800.78 876.23 887.74 891.33 952.32 973.48 988.07 1004.54 1069.88 1079.11 1119.75 1133.69 1179.52 1184.36 1217.06 1236.88 1244.85 1296.74 1335.45 1352.82 1406.16 1446.03 1483.35 1507.68 1547.49 1591.14 1619.50 1649.39 1662.45 2201.09 3090.61 3152.70 3157.80 3159.27 3169.13 3176.81 3180.92 3191.40 3258.77	1.8033 0.3009 0.2598

Phenanthrene I (**7**)	-614.19420	0.182238	0.76(0.75)	29.72* 77.42 98.25 147.12 176.86 248.68 280.64 304.31 379.43 418.56 451.05 465.03 524.41 533.27 552.83 613.99 615.76 681.19 685.71 714.69 738.17 757.63 762.52 801.75 817.02 847.64 868.05 881.37 888.48 946.56 956.33 985.13 986.33 994.83 1034.19 1063.04 1105.49 1120.35 1163.74 1184.74 1192.14 1209.10 1229.32 1244.49 1273.85 1315.15 1334.51 1380.74 1427.28 1485.04 1504.08 1566.65 1592.12 1624.20 1646.27 1677.46 1907.63 2984.25 3158.10 3161.53 3169.48 3180.10 3181.15 3191.66 3224.39 3230.24	1.3157 0.4082 0.3227
	*Vibration replaced by unsymmetrical hindered rotor (hrd 4 4 1)			'Vhrd2' 1 0 224.74 -161.79 -90.40 39.97	'Ihrd1' 1 0 12.22 2.98 -1.21 -7.10
Phenanthrene I (**TS 1-2**)	-614.18589	0.181397	0.77(0.75)	83.21 91.20 161.92 190.91 250.36 278.87 368.72 408.53 412.22 426.47 488.11 509.07 519.44 540.84 568.12 634.42 657.60 678.12 714.18 733.15 753.99 763.93 795.87 824.55 838.37 875.82 876.88 889.95 946.66 958.58 972.37 993.82 1009.14 1050.06 1062.87 1087.79 1116.68 1165.45 1179.85 1194.49 1224.03 1230.42 1247.48 1298.63 1302.80 1354.23 1379.16 1403.63 1422.00 1469.14 1470.45 1549.49 1576.99 1621.22 1645.07 1851.98 3128.39 3130.85 3160.59 3164.16 3170.56 3181.97 3182.77 3192.45 3192.99	1.2294 0.4709 0.3541
Phenanthrene I (**TS 1-5**)	-614.15608	0.179026	0.76(0.75)	60.24 85.85 130.64 157.44 186.64 228.48 246.74 307.01 361.19 418.44 430.38 460.07 494.94 511.68 540.04 541.51 556.93 589.26 616.82 665.65 696.32 713.29 762.79 766.21 811.55 828.34 837.69 869.21 882.94 890.09 965.37 974.91 977.60 999.61 1047.78 1073.41	1.0332 0.4938 0.3518

				1130.45 1168.93 1172.42 1198.04 1208.29 1238.50 1275.83 1290.35 1343.32 1377.24 1392.33 1421.50 1456.76 1494.93 1540.42 1589.09 1628.62 1648.35 1663.67 2213.82 3018.81 3151.01 3158.51 3160.69 3169.62 3177.19 3185.16 3197.28 3225.36	
Phenanthrene I (**TS 1-6**)	-614.12792	0.178704	0.79(0.75)	10.58 63.11 112.40 122.13 194.75 254.53 293.62 326.04 365.50 405.80 413.58 454.52 501.93 513.20 521.15 539.49 560.88 582.56 656.00 674.02 696.02 701.36 753.05 757.70 781.65 783.92 801.66 852.64 885.10 887.84 952.88 983.33 984.80 993.70 1033.12 1072.40 1122.09 1138.00 1167.44 1185.14 1217.21 1229.13 1241.94 1299.07 1336.11 1372.01 1383.75 1435.96 1481.36 1509.49 1553.51 1596.51 1620.83 1650.45 1674.05 2208.38 3126.95 3131.87 3155.99 3160.20 3169.66 3175.97 3183.26 3192.58 3236.11	1.4309 0.3607 0.3012
Phenanthrene I (**TS 2-3**)	-614.18065	0.181419	0.78(0.75)	74.07 90.72 135.38 202.93 249.91 259.28 341.45 392.92 417.22 436.50 446.73 483.60 521.14 537.09 559.83 626.02 673.43 683.12 734.02 748.95 762.86 777.10 795.33 818.32 833.81 862.37 876.38 893.93 958.49 977.71 990.99 993.92 1007.48 1047.85 1052.46 1094.21 1105.32 1167.11 1178.40 1180.95 1223.10 1234.66 1241.85 1288.42 1350.28 1358.11 1375.70 1412.95 1418.98 1476.08 1479.57 1552.80 1587.52 1626.22 1652.53 1898.30 3001.32 3159.41 3162.45 3167.70 3179.57 3182.80 3190.73 3202.98 3220.34	1.1171 0.5152 0.3746
Phenanthrene I (**TS 2-7**)	-614.17130	0.181178	0.78(0.75)	74.92 80.99 146.57 166.82 248.67 258.21 312.05 361.59 417.28 429.31 449.31 460.66 519.87 533.20 565.79 616.22 686.38 686.73 713.80 756.45 761.69 793.17	1.2965 0.4381 0.3489

				803.42 817.78 828.83 847.47 879.74 884.84 955.25 981.58 982.26 991.44 993.28 1014.97 1056.64 1110.82 1123.83 1166.66 1181.86 1205.67 1216.35 1225.71 1234.51 1272.86 1320.01 1348.59 1382.74 1418.39 1447.35 1478.11 1494.98 1572.94 1577.61 1641.75 1643.36 1903.12 2986.85 3159.00 3161.99 3168.37 3180.06 3182.99 3191.16 3225.19 3228.10	
Phenanthrene I (**TS 5-3**)	-614.15185	0.179092	0.77(0.75)	53.00 76.63 121.00 141.96 209.27 242.59 269.43 323.93 400.15 423.77 426.72 440.41 507.76 512.23 533.73 546.35 585.00 613.70 629.75 673.92 707.38 723.03 762.57 766.36 809.78 837.09 854.74 877.88 890.83 905.83 963.27 975.90 991.81 996.41 1046.36 1056.96 1106.97 1170.24 1178.92 1183.75 1203.11 1236.87 1265.48 1297.48 1320.40 1366.80 1388.07 1402.40 1461.07 1492.40 1544.62 1581.84 1619.45 1641.84 1661.36 2159.27 3068.81 3113.98 3158.84 3161.18 3170.00 3177.47 3185.30 3195.72 3201.04	0.9498 0.5495 0.3644
Phenanthrene I (**TS 6-7**)	-614.12827	0.178734	0.78(0.75)	39.23 76.79 112.94 125.84 212.72 252.95 256.83 341.65 383.37 407.40 413.16 467.53 510.18 515.09 535.64 542.11 592.24 609.13 652.74 676.34 692.75 712.34 749.62 761.79 783.04 801.67 825.05 843.98 887.09 891.23 954.87 984.61 993.28 1008.26 1026.08 1069.99 1113.12 1123.79 1167.15 1184.08 1212.37 1235.02 1239.74 1298.38 1321.51 1335.82 1369.23 1434.40 1482.84 1505.63 1541.52 1593.35 1620.84 1648.59 1669.44 2158.31 3075.09 3155.90 3159.51 3168.24 3175.85 3180.08 3180.34 3190.45 3205.01	1.5317 0.3464 0.2904

Phenanthrene I (**TS 3-4**) Note: Same structure as Phenanthrene II TS 3-4	-614.20939	0.181146	0.76(0.75)	56.90* 69.77 109.52 151.35 162.31 241.32 259.45 295.39 390.49 432.26 436.11 468.14 510.16 521.52 557.80 604.07 628.35 683.04 689.01 744.36 754.05 760.41 803.92 833.52 852.32 875.04 882.84 928.93 957.76 968.65 980.17 984.53 992.47 1024.50 1045.17 1064.46 1111.75 1165.79 1179.98 1183.50 1234.53 1243.03 1272.41 1290.61 1354.31 1377.51 1392.23 1420.67 1465.68 1484.88 1536.75 1557.83 1599.32 1619.82 1659.82 2000.87 3158.54 3161.67 3166.17 3176.51 3179.03 3179.67 3189.28 3203.26 3228.31	1.0835 0.5257 0.4056
	*Vibration replaced by unsymmetrical hindered rotor (hrd 5 5 1)			'Vhrd2' 1 0 419.23 258.67 -89.68 73.16 22.37	'Ihrd1' 1 0 12.47 0.13 -1.27 6.88 0.21
Phenanthrene I (**TS 7-4**)	-614.18983	0.180147	0.76(0.75)	25.98* 57.97 98.61 123.43 187.67 250.44 274.76 289.94 342.78 418.27 438.49 458.08 520.30 526.96 552.61 565.54 607.61 686.10 697.08 718.65 754.76 759.48 791.61 812.22 835.54 849.81 876.96 886.57 950.33 954.99 973.23 982.59 991.87 993.11 1010.30 1061.99 1112.53 1161.81 1184.31 1206.09 1220.79 1231.78 1279.03 1284.79 1326.79 1336.58 1377.37 1426.12 1480.86 1499.64 1534.30 1585.29 1597.15 1641.52 1647.86 1965.67 3154.34 3158.19 3161.16 3168.82 3179.50 3180.28 3191.18 3225.89 3229.23	1.3060 0.3979 0.3213
	*Vibration replaced by unsymmetrical hindered rotor (hrd 5 5 1)			'Vhrd2' 1 0 606.04 410.20 -176.84 32.12 15.87	'Ihrd1' 1 0 11.07 0.48 -3.69 5.53 1.19

Phenanthrene II

Species (Stationary point)	Total Energy (hartrees)	ZPE (unscaled) (hartrees)	$<S^2>$	Frequencies (unscaled) (cm^{-1})	Rotational constants (GHz)
Phenanthrene II (**1**)	-614.26807	0.185077	0.78(0.75)	61.69 97.58 164.30 220.69 247.05 270.96 359.83 399.71 411.61 460.85 492.25 516.24 530.43 543.99 551.27 566.99 644.72 678.91 704.41 717.86 759.24 777.77 811.17 821.24 846.16 847.78 888.32 902.19 974.52 982.58 988.22 991.01 1021.78 1037.46 1064.01 1102.35 1150.76 1168.65 1176.16 1188.70 1224.24 1234.95 1250.76 1302.73 1341.73 1372.80 1387.96 1407.97 1452.06 1460.46 1489.61 1533.86 1547.03 1563.06 1580.74 1638.98 1649.70 3159.49 3161.79 3166.96 3172.04 3178.86 3182.36 3187.09 3198.78 3252.03	1.2109 0.5321 0.3696
Phenanthrene II (**2**)	-614.17928	0.182000	0.79(0.75)	69.05 93.10 143.38 183.28 211.65 254.96 302.73 386.50 421.56 428.22 482.59 505.29 512.71 546.14 582.57 588.21 651.38 683.30 698.29 720.45 746.87 751.95 789.46 792.76 805.26 851.48 883.02 906.20 918.00 929.11 939.93 950.41 985.14 986.89 1030.07 1036.82 1065.79 1099.46 1121.85 1151.17 1183.33 1216.70 1228.34 1240.31 1286.54 1307.84 1323.18 1349.84 1390.13 1413.39 1462.77 1508.55 1530.07 1546.14 1597.17 1633.90 1909.04 3106.39 3159.06 3161.49 3163.63 3176.87 3181.31 3191.20 3197.16 3217.49	1.1347 0.5604 0.4284

Phenanthrene II (**3**) Note: Same structure as Phenanthrene I 3	-614.21516	0.183246	0.75(0.75)	41.32* 83.41 111.04 151.47 201.91 238.22 264.51 331.64 418.08 430.52 457.29 471.29 516.18 523.01 553.73 591.38 655.83 678.54 693.93 715.96 759.13 760.60 773.10 818.60 844.74 857.73 874.72 900.29 955.02 959.79 970.92 974.79 993.32 1003.11 1047.08 1056.62 1117.68 1151.41 1168.44 1177.67 1183.58 1211.11 1237.55 1246.87 1288.42 1358.95 1378.50 1396.05 1410.03 1468.43 1487.46 1552.77 1586.56 1620.32 1638.02 1664.08 1914.82 3016.88 3159.08 3162.27 3170.37 3180.05 3184.63 3195.82 3199.08 3229.95	1.0233 0.5813 0.3973
	*Vibration replaced by unsymmetrical hindered rotor (hrd 8 8 1)			'Vhrd2' 1 0.1 260.44 -61.81 172.20 -45.22 -16.43 -1.63 6.30 -4.39	'Ihrd1' 1 0.1 11.44 1.83 2.79 6.38 1.46 1.54 0.94 0.43
Phenanthrene II (**4**) Note: Same structure as Phenanthrene I 4	-500.88710	0.173399	0.77(0.75)	113.80 138.85 236.84 240.37 278.51 424.38 426.95 457.51 501.09 518.28 535.81 549.80 584.74 684.74 689.62 716.38 734.30 753.20 773.37 813.38 836.40 849.17 872.66 873.43 890.94 927.76 954.41 964.26 991.50 998.57 1041.35 1063.36 1091.64 1161.74 1174.11 1184.17 1210.74 1239.61 1280.47 1287.98 1347.94 1374.25 1383.83 1424.01 1467.45 1474.55 1487.62 1554.34 1590.62 1605.24 1658.53 3158.02 3160.86 3165.76 3177.68 3179.19 3188.89 3205.07 3211.91 3231.50	1.8559 0.6744 0.4947
Phenanthrene II (**5**)	-614.16980	0.181372	0.76(0.75)	33.91* 57.78 87.92 98.81 173.34 185.39 225.56 241.44 384.39 392.31 426.79 434.52 500.44 518.60 522.69 542.19 595.42 620.77 635.73 681.31 690.25 734.39 743.10 763.63 776.75 780.40 829.48 874.31 920.13 954.88 959.45 966.06 971.51 995.56 1039.33 1073.23	1.2244 0.3134 0.2495

				1138.31 1142.90 1162.42 1173.99 1198.73 1236.71 1264.42 1276.25 1346.01 1353.19 1362.43 1395.45 1443.64 1473.12 1495.83 1517.82 1577.65 1621.48 1647.13 1673.57 2206.03 3123.92 3150.25 3153.75 3158.73 3168.55 3171.60 3174.78 3181.28 3191.18	
	*Vibration replaced by unsymmetrical hindered rotor (hrd 10 14 1)		'Vhrd2' 1 0 1231.25 -591.66 -496.19 -257.36 162.02 -50.89 8.83 -0.70 -3.99 -1.11	'Ihrd1' 1 0 109.14 -27.72 -14.14 5.15 2.53 -0.07 -3.11 2.03 -0.45 -0.76 0.05 0.91 -0.98 0.02	
Phenanthrene II (**TS 1-2**)	-614.17737	0.181338	0.78(0.75)	88.37 98.53 157.85 195.79 246.70 259.44 332.36 415.32 420.42 466.82 487.61 508.41 539.89 546.91 581.25 643.06 668.98 684.21 712.79 739.73 756.24 775.15 792.49 806.94 865.11 877.78 883.12 913.11 945.01 955.67 976.56 988.68 1007.39 1020.63 1049.55 1064.46 1113.03 1126.99 1154.88 1183.78 1221.57 1239.87 1252.81 1285.28 1302.99 1331.35 1352.45 1401.13 1429.70 1460.66 1513.79 1527.32 1563.90 1597.16 1635.91 1865.98 3112.27 3160.88 3163.09 3171.38 3181.15 3182.37 3190.18 3193.03 3210.92	1.1287 0.5671 0.4160
Phenanthrene II (**TS 1-5**)	-614.15886	0.180607	0.76(0.75)	28.84* 59.07 89.61 158.45 185.27 209.07 255.73 356.53 395.52 423.95 435.36 474.43 502.53 517.28 538.39 547.00 615.93 627.20 667.40 685.56 732.59 762.84 773.45 777.65 795.13 829.93 877.00 920.28 951.78 957.16 969.68 995.43 997.86 1005.13 1039.27 1131.77 1140.60 1167.07 1172.42 1201.65 1231.40 1237.50 1267.60 1348.71 1364.35 1379.41 1394.04 1423.96 1447.03 1492.55 1520.22 1578.47 1629.06 1650.93 1680.60 2211.55 3124.74 3146.07 3148.03 3152.39 3158.13 3169.78 3174.47 3182.05 3192.67	1.0571 0.4073 0.3075

	*Vibration replaced by unsymmetrical hindered rotor (hrd 6 13 1)			'Vhrd2' 1 0 1542.46 -460.01 -931.49 -146.94 -0.95 1.71	'Ihrd1' 1 0 122.70 -18.25 -10.63 0.31 -1.57 2.68 -4.33 2.63 -0.10 0.81 0.15 -0.89 0.36
Phenanthrene II (**TS 2-3**)	-614.17483	0.181279	0.78(0.75)	85.46 96.02 144.63 191.26 226.81 268.99 339.41 403.44 423.42 433.77 455.26 482.36 518.54 542.25 579.00 600.01 668.22 678.84 730.63 739.90 759.11 792.67 808.38 812.28 840.23 878.59 910.44 933.96 950.18 954.23 972.73 982.83 988.33 1042.66 1054.83 1086.33 1116.29 1143.06 1160.93 1182.43 1216.03 1232.42 1246.91 1290.13 1320.97 1350.19 1375.78 1392.87 1447.50 1469.06 1527.71 1540.30 1571.19 1595.83 1642.64 1905.80 3006.62 3159.47 3163.31 3166.95 3177.78 3180.66 3191.10 3198.62 3223.80	1.1037 0.5753 0.4210
Phenanthrene II (**TS 2-4**)	-614.14915	0.180213	0.77(0.75)	74.35 90.95 118.09 164.90 232.47 256.15 281.34 391.12 409.15 416.91 485.95 502.05 518.51 538.30 576.48 598.97 603.97 680.32 697.06 724.04 752.86 757.56 784.56 791.08 819.35 859.07 863.72 892.96 905.73 940.75 952.32 962.25 989.72 1036.05 1057.59 1070.92 1092.58 1132.66 1151.66 1180.90 1222.09 1229.51 1241.79 1263.23 1296.49 1331.88 1356.43 1418.80 1427.10 1468.85 1482.61 1529.06 1549.47 1607.82 1636.01 1993.44 3158.18 3159.86 3166.63 3176.37 3181.08 3190.76 3203.43 3219.59 3238.61	1.1612 0.5268 0.4562
Phenanthrene II (**TS 5-3**)	-614.15328	0.180235	0.77(0.75)	40.17* 73.39 111.40 152.63 199.66 208.06 256.27 366.67 395.38 421.83 436.22 449.84 500.02 516.79 539.17 588.54 612.39 645.40 663.15 686.37 726.63 761.41 772.55 788.45 803.51 829.98 877.24 918.17 956.27 958.93 967.06 976.04 995.44 1005.53 1040.02 1099.75	0.9889 0.4681 0.3270

				1137.87 1167.31 1174.57 1177.23 1223.11 1234.37 1264.39 1301.64 1345.33 1364.75 1389.76 1397.88 1451.42 1487.11 1528.62 1576.49 1613.93 1646.99 1665.84 2151.65 3102.45 3150.84 3155.32 3165.79 3168.08 3172.35 3177.85 3188.92 3191.95	
	*Vibration replaced by unsymmetrical hindered rotor (hrd 8 5 1)			'Vhrd2' 1 0 2861.70 -602.04 -1403.91 -311.57 -176.91 -131.96 -118.01 -81.97	'Ihrd1' 1 0 137.36 7.02 -1.34 15.43 5.63
Phenanthrene II (**TS 3-4**) Note: Same structure as Phenanthrene I TS 3-4	-614.20939	0.181146	0.76(0.75)	56.90* 69.77 109.52 151.35 162.31 241.32 259.45 295.39 390.49 432.26 436.11 468.14 510.16 521.52 557.80 604.07 628.35 683.04 689.01 744.36 754.05 760.41 803.92 833.52 852.32 875.04 882.84 928.93 957.76 968.65 980.17 984.53 992.47 1024.50 1045.17 1064.46 1111.75 1165.79 1179.98 1183.50 1234.53 1243.03 1272.41 1290.61 1354.31 1377.51 1392.23 1420.67 1465.68 1484.88 1536.75 1557.83 1599.32 1619.82 1659.82 2000.87 3158.54 3161.67 3166.17 3176.51 3179.03 3179.67 3189.28 3203.26 3228.31	1.0835 0.5257 0.4056
	*Vibration replaced by unsymmetrical hindered rotor (hrd 5 5 1)			'Vhrd2' 1 0 419.23 258.67 -89.68 73.16 22.37	'Ihrd1' 1 0 12.47 0.13 -1.27 6.88 0.21

Phenanthrene III

Species (Stationary point)	Total Energy (hartrees)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm^{-1})	Rotational constants (GHz)

Phenanthrene III (**1**)	-614.27310	0.185187	0.78(0.75)	68.88 95.15 142.64 229.10 242.62 285.65 330.23 398.72 424.22 426.19 445.50 496.55 502.91 560.64 611.82 630.12 657.62 665.96 719.79 734.55 751.32 783.22 794.38 796.99 850.59 879.34 893.31 893.96 956.69 977.55 992.33 1013.57 1014.72 1059.46 1063.15 1102.86 1131.66 1160.65 1180.67 1185.59 1207.17 1253.77 1297.29 1297.47 1323.68 1344.34 1357.69 1417.87 1454.97 1480.25 1501.44 1524.95 1557.74 1571.49 1607.38 1621.61 1645.43 3167.32 3168.44 3176.04 3182.09 3185.22 3190.09 3194.74 3200.95 3207.44	1.1155 0.5296 0.3591
Phenanthrene III (**2**)	-614.18158	0.181781	0.78(0.75)	68.38 96.69 100.29 168.76 198.12 273.40 292.42 343.95 406.89 438.94 444.77 485.15 508.00 520.19 560.25 611.09 621.41 656.93 700.93 725.76 730.91 751.42 773.84 784.06 812.67 850.23 879.72 922.81 935.36 949.68 965.10 966.77 989.65 1009.99 1020.58 1047.49 1056.61 1113.41 1136.49 1165.41 1173.59 1183.47 1214.85 1233.45 1294.95 1323.93 1332.20 1349.83 1405.56 1435.09 1489.58 1495.00 1537.64 1586.30 1607.83 1634.09 1889.33 3097.19 3163.00 3165.34 3167.17 3172.98 3182.33 3185.23 3192.50 3195.91	1.1282 0.5365 0.3962
Phenanthrene III (**3**)	-614.23332	0.18372	0.75(0.75)	40.95* 92.39 113.54 143.10 163.72 211.26 285.84 340.17 419.40 424.41 443.62 449.88 516.01 537.63 574.07 634.29 646.20 653.59 721.73 750.23 752.79 768.13 794.89 802.17 868.58 881.32 894.68 905.28 951.25 952.36 991.34 993.21 1024.28 1046.49 1054.22 1117.38 1128.80 1155.03 1165.56 1180.26 1183.17 1197.33 1210.81 1247.09 1321.29 1322.03 1334.82 1379.02 1475.54 1482.75 1508.49 1510.78 1620.63 1625.51	0.9813 0.5591 0.3683

				1644.50 1648.87 1917.34 3002.53 3163.06 3164.28 3170.87 3174.39 3180.03 3184.43 3190.41 3193.61	
	*Vibration replaced by unsymmetrical hindered rotor (hrd 5 5 1)			'Vhrd2' 1 0 163.40 -5.19 163.92 -13.36 9.11	'Ihrd1' 1 0 12.92 -1.45 -1.57 7.27 -1.2738
Phenanthrene III (**4**)	-500.90229	0.174408	0.77(0.75)	107.89 135.17 217.67 281.52 305.41 417.67 427.61 440.27 499.59 543.48 545.06 571.45 629.65 656.44 711.85 736.38 752.48 753.80 784.71 793.71 853.50 874.92 880.26 885.99 944.01 944.46 979.16 981.45 1006.46 1036.86 1041.57 1111.24 1116.79 1150.35 1177.48 1179.50 1210.42 1237.15 1269.46 1319.39 1329.18 1358.47 1388.17 1462.49 1468.20 1501.32 1501.88 1601.52 1604.12 1611.37 1623.54 3159.82 3160.78 3165.40 3166.89 3176.31 3176.96 3188.80 3189.42 3209.22	2.2804 0.5858 0.4661
Phenanthrene III (**5**)	-614.17298	0.181473	0.76(0.75)	31.92 51.23 79.64 100.64 150.67 195.86 248.35 289.09 329.87 410.92 424.86 453.43 462.48 512.08 541.92 563.50 608.97 620.14 633.59 674.33 709.20 733.44 746.18 767.91 771.18 854.00 860.45 881.00 946.54 955.62 986.59 987.00 989.00 1021.92 1051.58 1070.73 1116.78 1127.29 1142.31 1175.27 1187.48 1201.87 1236.36 1281.36 1302.08 1317.05 1326.76 1425.60 1436.80 1470.46 1490.97 1520.78 1567.25 1605.07 1630.63 1637.04 2204.16 3152.42 3158.25 3160.42 3164.77 3169.28 3175.58 3178.31 3187.43 3191.69	1.0464 0.4960 0.3691

Phenanthrene III **(8)**	-614.17500	0.181508	0.76(0.75)	30.19 59.73 81.06 88.49 131.07 201.10 253.69 298.41 318.83 407.92 425.32 462.07 481.34 518.44 536.20 563.46 607.19 619.46 636.63 667.97 707.02 744.59 759.87 768.36 775.71 845.80 856.53 879.49 944.83 957.65 985.70 987.06 987.45 1022.29 1053.46 1075.93 1109.10 1124.76 1138.00 1175.95 1188.63 1205.35 1238.57 1281.10 1311.43 1314.32 1325.57 1414.99 1433.71 1468.42 1483.68 1525.50 1566.42 1602.50 1631.15 1639.30 2203.96 3154.49 3158.23 3164.21 3169.28 3169.99 3174.46 3179.56 3187.46 3192.46	0.8485 0.5338 0.3377
Phenanthrene III **(TS 1-2)**	-614.18156	0.181524	0.78(0.75)	95.66 100.41 158.11 190.96 262.76 277.98 331.39 405.38 431.37 439.52 484.43 507.91 520.84 562.33 601.68 622.40 658.83 701.05 728.93 731.12 756.99 775.23 783.52 815.36 851.46 880.41 924.16 929.44 948.29 964.13 966.16 989.10 1014.18 1022.67 1048.00 1058.56 1113.41 1138.12 1167.37 1173.64 1183.67 1216.19 1238.77 1295.18 1324.26 1332.77 1349.47 1408.92 1435.47 1490.67 1494.75 1537.83 1586.21 1608.11 1633.89 1882.22 3101.36 3163.55 3165.42 3167.92 3172.93 3182.21 3186.25 3192.50 3195.97	1.1244 0.5368 0.3946
Phenanthrene III **(TS 1-5)**	-614.17171	0.181328	0.76(0.75)	37.74 93.22 103.42 173.79 200.79 250.20 291.67 332.92 410.60 436.62 441.64 458.87 505.76 519.76 565.40 612.06 616.18 636.75 656.00 695.82 730.06 741.97 767.56 772.39 843.64 854.08 880.57 944.96 956.18 982.60 986.03 987.44 1022.44 1054.07 1071.44 1117.82 1125.32 1146.88 1176.48 1191.12 1206.99 1238.57 1288.90 1301.52 1321.72 1339.42 1429.99 1440.95 1475.43 1497.53 1520.53 1563.72 1600.45 1637.99	0.9656 0.5199 0.3473

				1639.13 2163.13 3121.51 3160.55 3162.76 3170.02 3173.24 3180.34 3182.62 3190.08 3194.34	
Phenanthrene III (**TS 5-8**)	-614.16954	0.181222	0.76(0.75)	45.46 77.62 86.90 122.10 195.45 261.06 296.13 325.54 392.13 421.21 457.63 481.98 505.75 531.40 565.21 584.34 620.70 628.54 674.61 705.61 733.43 745.10 772.42 784.22 853.70 857.41 897.27 943.29 968.35 980.05 984.18 997.91 1024.27 1056.21 1072.45 1107.37 1119.94 1138.75 1177.16 1187.00 1194.15 1242.52 1279.34 1299.36 1310.54 1328.82 1390.78 1435.86 1467.88 1485.92 1514.35 1572.12 1603.13 1631.31 1635.29 2213.60 3155.69 3162.88 3164.66 3165.54 3171.86 3175.70 3185.37 3187.08 3193.63	0.8879 0.5100 0.3559
Phenanthrene III (**TS 2-3**)	-614.18101	0.181345	0.78(0.75)	90.50 112.89 116.94 172.94 217.84 276.00 348.39 386.98 417.61 450.22 478.22 496.91 511.66 551.66 595.50 627.77 641.22 702.22 711.75 726.37 746.73 772.84 782.25 825.92 851.25 880.60 927.29 938.40 954.84 967.50 992.26 1008.79 1016.79 1029.05 1047.82 1069.57 1115.14 1138.72 1168.02 1177.59 1184.49 1219.78 1233.14 1302.64 1329.69 1332.62 1352.55 1418.85 1453.94 1491.44 1497.11 1543.94 1591.42 1610.00 1637.71 1883.91 3048.31 3163.55 3165.55 3168.22 3173.15 3182.63 3184.33 3192.60 3194.95	1.1191 0.5397 0.3939
Phenanthrene III (**TS 8-3**)	-614.16857	0.18079	0.77(0.75)	40.59 79.63 100.34 105.81 206.62 244.80 275.72 368.89 395.44 407.00 438.78 461.61 488.44 516.59 568.54 577.42 626.70 649.87 687.55 713.76 730.36 752.23 774.47 790.58 850.47 863.43 892.33 938.92 957.21 972.39 984.11 993.33 1024.48 1054.45 1064.54 1076.85 1118.85 1135.80 1177.98 1186.09 1187.05 1247.03	0.8496 0.5380 0.3395

				1289.43 1318.02 1319.41 1332.86 1343.41 1441.45 1469.64 1491.60 1509.61 1585.05 1605.81 1626.56 1637.71 2168.60 3128.62 3144.85 3156.44 3163.69 3165.34 3173.11 3181.89 3184.71 3192.79	
Phenanthrene III (**TS 3-4**)	-614.22483	0.181328	0.76(0.75)	39.09* 85.02 101.02 114.66 149.16 213.00 286.44 316.70 363.17 422.22 431.49 451.17 510.95 568.20 575.45 578.31 634.69 657.87 743.79 754.82 756.47 775.58 794.14 846.96 865.59 876.41 885.67 945.28 949.18 969.10 987.14 989.72 1021.11 1043.66 1049.89 1118.74 1126.31 1156.28 1180.89 1183.61 1218.01 1226.66 1238.61 1320.48 1330.70 1348.66 1382.29 1470.35 1483.34 1503.97 1506.54 1614.23 1618.96 1634.98 1641.54 1987.51 3142.72 3161.83 3163.28 3168.33 3171.80 3178.25 3180.81 3189.87 3191.08	0.9484 0.5483 0.3671
	*Vibration replaced by unsymmetrical hindered rotor (hrd 5 5 1)			'Vhrd2' 1 0 323.14 226.23 -30.68 68.92 -0.14	'Ihrd1' 1 0 13.44 -0.09 -0.86 5.34 -0.46

Benzoperylene

Species (Stationary point)	Total Energy (hartrees)	ZPE (unscaled) (hartrees)	$<S^2>$	Frequencies (unscaled) (cm^{-1})	Rotational constants (GHz)
Benzoperylene (**1**)	-920.44927	0.257458	0.79(0.75)	44.63 73.12 116.91 135.00 192.25 242.38 279.79 289.41 292.87 329.50 335.28 375.43 394.99 427.49 447.11 454.42 474.76 486.26 520.65 525.63 542.90 544.73 557.41 573.85 613.86 645.71 645.77 678.36 691.85 714.17 744.16 762.46 765.88 769.51 780.26 792.64	0.3767 0.3231 0.1739

				807.30 815.95 841.72 854.41 871.48 874.63 941.63 949.54 962.66 972.86 982.71 985.29 997.98 1013.13 1017.61 1087.45 1130.62 1150.37 1159.71 1167.61 1174.51 1209.45 1220.94 1233.74 1242.22 1252.38 1262.07 1265.16 1330.76 1344.05 1349.13 1378.81 1390.69 1415.01 1426.83 1438.63 1456.93 1461.02 1474.07 1510.26 1523.59 1534.27 1558.88 1581.97 1600.91 1617.20 1632.61 1646.22 1654.30 3156.94 3160.80 3161.94 3163.56 3164.27 3178.45 3179.69 3181.23 3182.35 3196.89 3252.37	
Benzoperylene (**2**)	-920.34778	0.254206	0.78(0.75)	57.44 85.20 98.79 120.34 186.38 214.80 228.39 251.80 278.22 301.52 327.31 362.86 391.06 406.67 450.58 461.21 474.01 490.81 502.51 531.90 539.89 543.22 562.48 591.72 598.41 615.49 638.80 667.36 672.60 690.38 717.14 734.50 746.66 765.87 776.14 779.61 804.13 831.03 840.45 849.92 856.66 868.52 898.98 913.56 932.42 958.16 966.05 968.95 976.26 984.82 987.99 1008.20 1053.96 1079.99 1125.84 1141.60 1164.11 1171.02 1189.89 1198.05 1214.25 1216.46 1228.29 1236.96 1258.08 1279.92 1319.90 1345.50 1367.70 1392.95 1408.60 1411.50 1423.28 1445.63 1457.31 1481.99 1512.80 1522.48 1544.27 1585.69 1616.03 1627.85 1635.16 1652.94 1901.75 3112.26 3158.25 3159.88 3162.36 3162.59 3169.80 3176.11 3178.34 3182.82 3187.73 3213.62	0.3763 0.3332 0.1888
Benzoperylene (**3**)	-920.37088	0.255164	0.75(0.75)	32.25* 52.88 95.39 100.92 136.10 204.42 231.81 258.57 280.61 294.57 316.79 359.95 380.83 393.27 419.84 449.25 454.65 478.82 484.58 501.77 526.11 544.03 548.05 571.82 590.01 623.96 636.28 642.85 678.17	0.3695 0.3325 0.1854

				708.29 726.01 745.88 747.79 771.35 775.79 808.92 811.81 824.13 838.24 846.72 860.29 866.00 905.28 913.73 943.66 959.33 975.57 980.63 989.74 991.10 1009.43 1059.07 1085.79 1125.52 1139.56 1160.00 1163.73 1174.51 1196.25 1213.19 1224.93 1235.73 1239.99 1256.98 1276.47 1326.73 1343.55 1368.15 1403.32 1409.47 1417.86 1421.43 1452.79 1459.67 1501.85 1527.61 1538.31 1550.98 1580.63 1599.66 1624.27 1633.71 1647.53 1677.66 1884.36 3028.19 3158.01 3158.93 3160.23 3164.30 3175.38 3177.04 3178.44 3182.74 3190.88 3220.58	
	*Vibration replaced by unsymmetrical hindered rotor (hrd 3 3 1)			'Vhrd2' 1 0 416.11 -107.40 -325.05	'Ihrd1' 1 0 10.61 0.23 -0.43
Benzoperylene (**4**)	-807.06489	0.246506	0.79(0.75)	91.14 102.94 132.23 207.98 241.68 275.86 288.49 316.87 336.48 379.50 402.97 422.35 461.55 474.78 485.71 499.03 517.85 543.45 573.72 583.51 593.01 614.63 635.14 665.83 671.86 705.13 708.93 738.12 745.49 768.10 771.00 805.89 808.45 814.28 835.49 855.99 856.47 892.39 900.12 903.90 944.80 953.91 966.34 974.62 981.77 1023.68 1059.66 1074.92 1086.39 1124.35 1152.25 1157.60 1163.81 1200.08 1207.78 1229.11 1238.78 1244.02 1252.64 1319.26 1322.91 1349.69 1365.84 1397.82 1410.29 1421.79 1435.41 1448.76 1455.06 1478.67 1493.23 1518.41 1529.71 1555.13 1581.92 1590.72 1612.43 1628.24 1668.76 3156.50 3157.83 3159.00 3163.43 3173.84 3174.65 3175.53 3176.47 3189.01 3204.61 3223.94	0.5065 0.3689 0.2134

Benzoperylene **(5)**	-920.33047	0.253222	0.77(0.75)	30.18 61.96 78.19 93.18 115.78 179.24 192.82 213.97 251.89 259.83 280.37 297.11 376.23 376.96 393.70 411.85 468.24 475.94 496.68 500.41 514.96 533.10 534.74 544.53 554.53 597.78 612.13 626.26 633.69 655.84 658.93 701.17 702.96 755.10 760.70 771.62 780.34 794.36 810.22 810.23 828.20 855.99 874.67 898.17 910.68 954.70 956.94 975.05 978.43 984.20 1016.95 1078.11 1085.62 1119.37 1140.00 1148.23 1167.37 1181.99 1199.73 1226.01 1230.67 1241.58 1249.27 1264.54 1309.37 1322.16 1334.14 1361.94 1393.97 1400.35 1415.82 1438.80 1445.44 1452.29 1469.83 1510.41 1535.04 1563.00 1575.83 1597.64 1617.18 1638.92 1650.06 1662.79 2198.46 3090.74 3155.16 3157.01 3159.32 3160.90 3163.72 3174.71 3176.15 3177.40 3178.38 3190.38	0.4200 0.2053 0.1379
Benzoperylene (**TS 1-2**)	-920.34731	0.253645	0.78(0.75)	66.19 91.79 108.70 141.29 189.84 215.98 256.44 282.17 295.03 312.97 341.13 390.67 394.72 435.51 451.81 473.38 488.61 492.96 524.53 533.18 541.91 554.31 585.24 592.60 615.71 644.46 656.91 666.47 684.82 717.02 724.45 749.44 765.66 775.37 779.59 803.08 830.85 839.51 849.26 857.74 872.23 905.38 914.82 945.57 958.75 960.50 968.96 976.58 984.89 991.43 1029.58 1056.41 1083.91 1127.92 1143.64 1165.93 1171.92 1191.65 1208.36 1219.99 1220.36 1236.31 1244.98 1259.73 1278.90 1320.10 1349.11 1368.29 1397.03 1410.15 1410.98 1424.31 1445.86 1455.54 1480.67 1513.82 1520.81 1545.47 1584.57 1612.96 1629.30 1635.16 1652.91 1872.38 3117.23 3158.70	0.3736 0.3346 0.1866

				3160.33 3163.50 3164.24 3173.67 3176.64 3178.67 3182.74 3188.89 3203.43	
Benzoperylene (**TS 1-5**)	-920.31806	0.252481	0.77(0.75)	29.55 65.27 92.64 104.17 120.26 186.65 224.34 251.72 261.78 276.32 305.39 357.14 379.72 391.98 412.12 432.94 471.84 478.43 506.60 513.19 526.90 530.26 542.69 555.71 573.02 597.68 616.21 633.69 639.44 689.37 696.82 706.09 748.79 759.89 773.90 776.51 786.81 807.22 813.27 827.53 845.01 864.75 897.60 911.69 954.89 957.22 978.54 987.82 989.87 1010.68 1028.88 1082.33 1118.80 1135.18 1146.30 1166.19 1168.91 1199.40 1221.72 1227.23 1244.15 1245.85 1265.88 1310.98 1325.83 1338.74 1377.28 1382.16 1402.00 1408.81 1435.47 1442.41 1453.19 1461.89 1511.78 1535.57 1564.00 1586.07 1599.93 1618.08 1635.42 1650.69 1669.80 2206.35 3126.62 3127.48 3156.98 3158.33 3160.32 3163.78 3175.71 3177.05 3178.10 3179.03 3193.71	0.3739 0.2645 0.1598
Benzoperylene (**TS 2-3**)	-920.33878	0.253177	0.78(0.75)	61.31 78.25 92.34 114.42 197.98 210.01 234.79 267.23 291.33 296.80 337.75 366.21 378.98 403.68 422.43 446.38 468.81 478.16 498.03 524.26 542.96 545.21 573.48 576.00 612.55 629.96 638.81 672.83 694.27 696.98 726.77 745.66 769.11 773.42 789.11 805.92 830.75 836.38 850.72 857.76 873.68 901.49 906.49 946.43 958.77 967.65 971.36 975.48 983.44 997.77 1055.32 1082.77 1094.54 1131.02 1149.08 1167.71 1171.20 1190.34 1198.93 1221.12 1222.64 1234.49 1244.36 1264.61 1308.97 1339.69 1343.26 1399.06 1406.57 1410.84 1419.03 1439.94 1451.93 1473.59 1490.05 1511.11 1535.15 1553.05 1578.37 1621.32	0.3702 0.3329 0.1856

				1628.43 1633.98 1654.22 1970.05 2961.27 3156.93 3158.52 3160.48 3161.92 3170.13 3174.64 3177.00 3182.30 3186.42 3225.35	
Benzoperylene (**TS 5-3**)	-920.31368	0.252239	0.78(0.75)	34.29 74.09 90.78 111.72 129.54 196.33 234.33 256.92 270.87 278.17 304.40 345.71 379.89 393.36 396.85 421.68 472.70 476.02 501.58 510.79 532.08 539.29 551.21 558.74 593.41 614.29 619.77 635.20 647.24 685.99 703.13 719.97 747.54 755.98 770.52 775.15 802.14 813.27 820.83 828.80 837.84 862.08 907.87 910.53 956.31 957.41 977.86 986.97 989.38 997.68 1026.20 1080.91 1107.02 1118.29 1143.86 1163.92 1169.57 1199.15 1209.77 1228.14 1240.98 1244.11 1265.75 1297.59 1308.62 1325.60 1352.25 1380.98 1404.58 1414.89 1429.45 1445.24 1457.79 1469.65 1510.25 1531.04 1552.05 1582.41 1601.97 1616.08 1625.29 1648.70 1666.78 2137.78 3075.06 3155.50 3156.78 3158.52 3161.78 3173.60 3174.41 3176.16 3176.94 3187.94 3188.32	0.3704 0.2747 0.1607
Benzoperylene (**TS 2-4**)	-920.32995	0.253377	0.78(0.75)	62.53 87.87 94.87 134.72 192.34 223.57 245.52 262.23 283.50 309.63 347.82 366.61 398.42 419.22 432.46 455.90 470.48 482.81 493.19 527.24 540.50 545.72 566.67 581.93 614.71 629.22 635.45 674.87 701.55 711.32 730.68 744.90 768.32 770.48 793.35 809.89 814.17 836.73 854.87 857.09 863.83 882.09 889.41 920.13 940.68 962.39 971.19 977.40 985.45 996.06 1041.29 1057.86 1081.88 1122.53 1141.44 1166.99 1172.40 1193.25 1200.28 1214.85 1232.68 1238.90 1256.48 1268.75 1302.78 1335.24 1350.12 1374.54 1392.43 1410.89 1413.84 1433.85 1448.25 1460.05	0.3807 0.3335 0.1953

				1478.39 1519.20 1524.21 1548.74 1600.26 1630.83 1635.87 1636.24 1659.28 1852.27 3157.98 3159.59 3162.06 3162.82 3170.53 3175.94 3177.90 3182.56 3187.58 3204.07 3219.89	
Benzoperylene (**TS 3-4**)	-920.36719	0.253029	0.79(0.75)	47.27* 69.64 89.69 109.91 126.53 177.88 208.78 254.32 280.26 292.69 311.59 346.42 384.33 395.44 410.29 429.93 476.04 477.23 495.21 502.60 535.59 544.79 567.68 581.21 585.56 621.10 637.00 654.06 676.05 708.80 726.37 746.29 754.93 767.10 774.23 808.11 809.30 823.37 834.75 853.32 859.75 889.73 901.46 944.00 954.89 956.96 976.21 980.13 985.06 1006.62 1061.11 1078.19 1085.53 1119.37 1152.44 1163.56 1173.31 1201.02 1221.53 1225.86 1239.63 1248.66 1255.81 1278.46 1326.25 1345.38 1368.88 1397.15 1404.63 1411.32 1419.24 1450.38 1453.49 1492.35 1495.79 1521.79 1540.28 1556.72 1584.54 1618.60 1628.64 1640.25 1665.33 1976.70 3156.84 3157.84 3159.16 3161.99 3166.91 3172.14 3174.35 3176.44 3179.77 3186.15 3222.59	0.3769 0.3146 0.1849
	*Vibration replaced by unsymmetrical hindered rotor (hrd 4 4 1)			'Vhrd2' 1 0 692.12 533.30 -127.09 -65.97	'Ihrd1' 1 0 11.08 0.00 0.28 0.02

Extended-armchair Structure

Species (Stationary point)	Total Energy (hartrees)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm^{-1})	Rotational constants (GHz)

Extended-armchair **(1)**	-1456.54065	0.38777	0.80(0.75)	21.21 36.73 56.69 86.87 109.10 136.88 168.36 177.51 194.28 199.92 218.65 255.72 273.78 292.66 297.18 305.49 320.14 344.79 355.48 367.12 370.10 391.29 395.79 442.39 446.28 446.92 466.74 480.98 493.53 510.80 525.24 529.00 529.59 538.26 542.04 545.82 556.62 572.04 583.18 594.65 598.32 618.70 619.78 628.26 638.82 657.47 662.03 703.69 708.89 712.87 730.69 740.15 749.24 760.58 769.57 772.92 775.88 777.00 788.50 797.06 804.62 814.96 836.05 840.85 860.01 881.77 883.84 892.98 902.66 913.66 918.28 942.15 957.95 978.30 980.56 982.92 988.61 1000.73 1013.24 1015.15 1024.63 1058.81 1082.43 1112.59 1116.48 1153.08 1164.78 1173.65 1181.29 1184.43 1202.59 1210.27 1213.76 1221.26 1243.06 1253.45 1261.44 1280.28 1293.21 1300.74 1305.23 1311.84 1322.05 1342.48 1353.25 1360.35 1367.65 1372.20 1399.48 1410.36 1411.51 1422.22 1433.67 1441.23 1445.88 1455.96 1466.24 1475.61 1483.94 1492.84 1506.21 1516.03 1525.84 1544.89 1557.08 1561.55 1598.84 1600.01 1608.33 1617.72 1629.76 1636.54 1645.45 1656.51 1668.75 3159.23 3160.02 3161.44 3163.00 3163.99 3164.69 3167.03 3179.49 3180.19 3180.73 3181.92 3183.72 3204.92 3220.81 3258.55	0.1958 0.0920 0.0626
Extended-armchair **(3)**	-1456.47008	0.38652	0.75(0.75)	33.59* 34.76 50.03 61.48 86.93 116.76 155.12 162.28 170.74 190.52 209.16 225.18 243.71 260.26 289.33 294.47 315.31 324.35 338.25 353.07 363.84 373.27 383.34 387.30 442.04 455.70 458.22 461.50 493.35 500.93 516.28 521.49 533.35 535.48 536.25 551.64 555.86 570.92 574.64 591.19 601.67 614.71 619.00 630.76 633.03 674.27 692.84 695.96 708.46 713.57	0.1816 0.0984 0.0644

				732.49 735.03 760.24 765.99 770.93 774.41 780.48 791.81 798.23 802.86 817.26 836.23 838.92 849.77 857.86 864.58 889.96 896.66 897.37 904.16 909.86 916.17 930.21 978.87 980.11 982.18 988.37 988.94 991.81 1006.06 1029.99 1051.47 1095.48 1100.30 1109.57 1125.22 1141.09 1150.82 1170.57 1171.79 1184.14 1189.39 1196.20 1208.29 1210.73 1226.17 1238.08 1253.38 1268.93 1279.77 1287.38 1318.46 1322.77 1327.23 1345.46 1358.20 1362.23 1392.60 1402.49 1411.72 1414.22 1425.01 1432.32 1440.77 1446.48 1454.16 1470.80 1472.21 1492.22 1513.65 1522.64 1533.58 1547.98 1581.23 1593.21 1599.25 1620.23 1623.51 1626.24 1635.29 1646.65 1647.67 1663.54 1691.06 1894.80 3030.39 3155.37 3156.21 3157.36 3158.37 3158.98 3162.62 3164.20 3171.58 3174.81 3176.02 3176.21 3178.65 3186.44 3192.55	
	*Vibration replaced by unsymmetrical hindered rotor (hrd 3 3 1)			'Vhrd2' 1 0 382.23 -170.61 280.86	'Ihrd1' 1 0 13.142 -0.087 0.266
Extended-armchair (**5**)	-1456.43164	0.38457	0.77(0.75)	21.03 38.16 46.73 58.04 81.70 103.76 137.89 145.17 160.32 179.40 200.15 213.31 251.24 265.20 276.14 280.28 306.29 325.20 337.83 346.57 362.93 366.77 370.20 401.94 430.91 438.53 446.93 465.56 475.56 500.16 514.26 520.61 524.31 532.73 534.44 538.61 541.83 554.64 562.45 572.41 576.70 592.69 607.55 615.86 624.61 631.15 638.76 660.33 681.57 702.09 703.82 704.96 728.47 752.51 756.05 768.76 769.75 771.13 777.40 780.72 792.92 798.78 815.49 833.37 837.30 846.85 856.87 869.36 889.46 897.92 910.78	0.1798 0.0917 0.0612

				911.55 918.32 977.73 978.51 979.17 980.25 987.10 987.56 998.70 1013.64 1033.42 1077.05 1094.05 1098.62 1113.14 1144.54 1152.58 1167.67 1175.18 1178.70 1187.33 1197.97 1207.32 1216.82 1235.33 1252.91 1265.31 1281.87 1287.84 1294.15 1316.91 1329.71 1340.40 1345.68 1357.64 1360.86 1374.94 1397.09 1406.78 1417.57 1421.72 1426.23 1438.69 1442.43 1450.39 1453.61 1470.59 1477.73 1487.67 1507.32 1510.59 1520.70 1528.97 1585.49 1594.47 1604.28 1605.56 1620.20 1628.76 1635.82 1645.55 1660.83 1669.55 2201.30 3134.46 3157.36 3158.05 3159.06 3161.11 3162.41 3163.95 3164.90 3176.57 3177.59 3177.97 3178.43 3181.36 3191.38 3207.94	
Extended-armchair (**4**)	-1343.13983	0.37627	0.79(0.75)	24.91 59.31 86.11 119.71 134.29 167.29 168.22 187.61 211.27 240.00 259.81 264.44 289.08 295.13 316.55 337.70 362.16 362.42 367.17 389.18 426.10 451.43 459.50 467.10 481.59 488.66 497.66 516.69 523.05 530.45 532.59 546.94 555.06 566.79 569.03 587.02 605.16 611.27 617.18 627.86 642.21 665.00 682.24 701.92 704.99 710.37 721.86 725.84 733.88 754.79 756.51 763.70 769.40 770.64 785.29 795.33 798.28 812.95 828.47 832.47 837.33 856.27 871.25 873.36 886.74 906.75 910.35 912.85 945.24 974.39 975.02 978.89 982.53 983.66 984.11 1002.37 1008.29 1040.64 1082.77 1094.78 1106.94 1126.97 1147.46 1160.98 1166.47 1187.30 1189.35 1194.11 1207.28 1211.37 1221.62 1234.65 1253.17 1256.67 1267.93 1280.50 1283.60 1321.60 1330.04 1346.38 1353.27 1368.36 1380.22 1396.42 1404.74 1410.40 1419.72 1427.39 1435.03 1439.35 1448.13 1468.84 1471.65 1484.09	0.2263 0.1001 0.0694

				1498.99 1507.55 1513.95 1545.34 1556.58 1569.36 1583.93 1596.48 1600.79 1613.70 1625.59 1629.03 1632.86 1657.96 1694.72 3154.52 3155.89 3156.29 3158.20 3159.13 3162.06 3162.72 3171.98 3173.13 3173.35 3175.10 3176.09 3186.30 3187.84 3214.17	
Extended-armchair **(TS 1-3)**	-1456.43491	0.38471	0.8(0.75)	36.16 58.38 66.37 86.69 100.19 127.11 164.87 166.59 185.89 192.52 210.91 243.49 260.80 287.08 294.37 312.69 326.91 335.82 353.03 363.54 370.66 381.35 394.87 428.01 447.78 453.72 460.17 464.20 495.60 509.13 517.33 529.09 535.37 536.88 548.14 552.56 559.86 568.36 586.72 599.27 615.13 617.82 625.88 633.64 669.76 674.25 692.44 708.71 711.11 722.16 735.64 757.06 764.44 766.36 770.53 775.47 785.98 798.15 802.96 807.62 823.47 835.20 847.17 856.99 867.54 879.25 885.75 891.87 902.34 906.36 909.94 956.85 975.37 976.72 979.59 984.25 985.47 989.24 1006.43 1022.43 1043.43 1068.07 1091.38 1098.83 1104.70 1118.59 1150.50 1167.78 1170.18 1184.36 1193.25 1194.79 1203.24 1208.64 1224.31 1233.49 1249.04 1257.87 1278.01 1283.97 1293.00 1317.00 1323.33 1338.98 1347.94 1359.03 1383.39 1399.53 1405.71 1412.52 1419.94 1426.92 1434.93 1440.85 1449.29 1458.99 1475.01 1487.33 1502.75 1515.07 1517.13 1549.86 1565.85 1587.05 1588.94 1597.22 1612.56 1616.29 1628.22 1637.98 1641.27 1656.00 1664.96 1895.51 3003.50 3154.98 3156.52 3157.28 3158.18 3159.84 3162.43 3164.08 3171.88 3173.69 3174.41 3175.89 3176.58 3186.13 3188.57	0.1901 0.0972 0.0658

Extended-armchair **(TS 3-4)**	-1456.46174	0.38380	0.77(0.75)	33.11 39.70* 58.58 68.43 87.83 95.63 132.88 150.24 171.29 172.94 189.75 214.88 243.18 256.91 286.97 294.22 309.26 316.20 331.03 346.14 364.54 372.08 376.15 384.30 436.14 455.65 460.92 469.90 489.63 498.01 505.34 517.87 530.49 535.02 535.51 553.63 554.30 567.89 571.91 595.72 600.73 614.19 619.55 630.52 646.59 675.35 695.51 705.49 709.47 713.62 717.53 732.03 758.55 765.29 767.97 771.90 776.23 792.46 794.67 798.57 815.62 832.29 837.14 841.56 857.38 873.24 885.72 892.63 902.60 904.41 905.54 929.60 943.05 977.03 977.46 978.76 986.32 986.54 989.00 1006.09 1027.04 1067.15 1092.20 1101.24 1112.08 1118.06 1150.52 1163.42 1171.00 1175.56 1188.07 1195.02 1207.22 1209.50 1235.45 1237.18 1254.55 1266.33 1280.13 1282.93 1317.92 1322.79 1328.54 1337.67 1357.91 1365.13 1390.52 1400.94 1407.47 1412.56 1422.61 1428.43 1438.91 1444.58 1453.61 1471.30 1472.57 1490.58 1513.09 1517.16 1526.13 1549.80 1582.50 1591.89 1595.77 1607.74 1619.37 1621.88 1630.58 1642.79 1645.48 1663.11 1680.23 1989.24 3150.06 3155.03 3155.82 3156.68 3157.86 3158.52 3161.47 3163.32 3171.54 3174.25 3175.44 3175.61 3178.01 3185.52 3192.67	0.1826 0.0976 0.0649
	*Vibration replaced by unsymmetrical hindered rotor (hrd 5 3 1)			'Vhrd2' 1 0 238.84 -55.23 103.613 -114.60 -7.304	'Ihrd1' 1 0 14.66 0.085 0.277

Extended-armchair **(TS 1-5)**	-1456.42949	0.384153	0.77(0.75)	24.17 37.38 57.54 80.39 103.54 134.82 139.39 159.23 178.34 198.28 212.38 250.05 265.36 272.28 274.87 289.48 306.62 336.09 345.94 363.14 367.81 371.00 400.16 427.31 441.46 442.76 456.19 477.65 498.79 513.18 517.77 519.96 531.92 534.09 538.06 542.83 553.48 562.77 573.11 577.60 588.88 606.44 615.35 623.54 630.79 640.18 669.73 675.48 683.33 701.07 706.56 727.02 740.79 764.06 767.72 768.30 771.78 776.40 780.44 791.04 797.14 814.39 831.34 836.65 855.89 857.53 874.87 889.04 897.98 899.24 909.10 911.97 977.08 978.42 980.03 982.97 986.26 987.85 999.11 1013.93 1030.70 1075.03 1094.41 1098.58 1110.61 1140.67 1153.37 1169.26 1173.49 1179.41 1185.79 1198.09 1205.73 1215.95 1230.93 1252.96 1265.58 1278.91 1285.37 1293.05 1318.38 1325.74 1336.97 1345.22 1357.11 1360.79 1388.06 1396.19 1407.00 1417.04 1422.59 1424.88 1436.08 1442.29 1450.21 1453.31 1471.10 1476.41 1486.48 1507.78 1509.70 1520.58 1529.36 1586.19 1595.21 1604.57 1605.81 1621.00 1629.14 1636.68 1646.07 1661.43 1670.05 2203.30 3140.16 3157.01 3157.78 3159.04 3161.01 3162.46 3163.88 3164.09 3176.95 3177.67 3178.28 3179.05 3180.34 3195.03 3203.30	0.1873 0.0915 0.0623
Extended-armchair **(TS 5-3)**	-1456.42548	0.384004	0.78(0.75)	32.30 43.98 53.68 79.74 84.01 119.66 145.19 162.28 183.74 184.66 207.19 220.95 251.39 277.94 284.76 296.08 309.64 336.18 340.26 362.27 367.58 370.34 374.92 402.45 431.67 446.44 450.21 464.69 497.19 512.64 519.50 525.84 531.84 535.79 538.05 548.50 554.07 572.98 577.21 588.48 608.63 614.75 615.81 629.05 638.15 640.50 688.12 695.20 702.44 706.73	0.1815 0.0944 0.0629

				712.84 730.42 746.89 766.03 770.21 771.03 773.43 779.30 783.55 795.10 801.65 817.28 834.77 839.05 857.01 867.94 870.16 888.55 897.42 909.43 911.41 917.21 977.86 978.92 980.00 983.87 987.42 987.62 994.88 1011.59 1021.81 1072.37 1085.19 1096.36 1104.31 1130.99 1151.01 1169.59 1173.56 1186.04 1189.48 1199.31 1206.20 1216.99 1236.20 1251.81 1269.00 1277.89 1282.18 1293.36 1297.58 1330.31 1333.81 1340.76 1350.90 1360.08 1381.09 1395.17 1414.89 1417.78 1422.04 1425.14 1437.61 1443.24 1451.30 1463.10 1469.57 1484.08 1506.10 1512.88 1517.60 1528.10 1529.83 1593.78 1597.96 1601.46 1613.77 1622.17 1626.92 1629.83 1643.06 1660.46 1663.08 2130.72 3101.19 3155.78 3156.58 3157.81 3159.43 3160.37 3162.28 3164.07 3173.92 3175.83 3176.42 3176.86 3178.77 3188.12 3192.40	

Table A.7. Cartesian coordinates for optimized structures at B3LYP/6-311G(d,p) level of theory.

Species Name (stationary point)	Geometry (Å)			
Phenanthrene I (**1**)	C	1.28311	2.08501	-0.00007
	C	-0.06888	2.30236	0.00019
	C	-0.98533	1.22478	0.00013
	C	-0.49961	-0.12610	-0.00018
	C	0.94429	-0.35762	-0.00011
	C	1.82464	0.76261	-0.00020
	C	-2.39851	1.47303	0.00025
	C	-3.30374	0.46316	0.00015
	C	-2.86186	-0.92640	0.00006
	C	-1.43254	-1.15702	-0.00068
	C	1.51287	-1.64672	0.00040
	C	2.88328	-1.82653	0.00039
	C	3.74816	-0.71976	-0.00000
	C	3.22247	0.55393	-0.00034
	O	-3.66830	-1.87718	-0.00005
	H	1.97028	2.92433	-0.00013
	H	-0.45727	3.31514	0.00038
	H	-2.72850	2.50722	0.00030
	H	-4.37235	0.64149	0.00025
	H	-1.13983	-2.19882	-0.00141
	H	0.87247	-2.51900	0.00073
	H	3.29183	-2.83055	0.00111
	H	4.82161	-0.86901	-0.00029
	H	3.87814	1.41824	-0.00051
Phenanthrene I (**2**)	C	1.21896	2.09847	0.30916
	C	-0.11130	2.37177	0.18350
	C	-1.01818	1.31645	-0.14811
	C	-0.52157	0.00032	-0.32149
	C	0.84884	-0.30432	-0.17600
	C	1.74305	0.77702	0.13520
	C	-2.40818	1.36081	-0.33620
	C	-2.93214	0.01271	-0.64323
	C	-2.71616	-1.04994	0.38492
	C	-1.64495	-0.92610	-0.63685
	C	1.38536	-1.61107	-0.32201
	C	2.73531	-1.83892	-0.18182
	C	3.61349	-0.77531	0.11269
	C	3.12082	0.50403	0.26847
	O	-3.16378	-1.66579	1.29813
	H	1.91589	2.89425	0.55117
	H	-0.48642	3.37925	0.32331
	H	-3.03791	2.23265	-0.22956
	H	-3.75306	-0.13024	-1.34138

	H	-1.52257	-1.74158	-1.34421
	H	0.71684	-2.43646	-0.53826
	H	3.12802	-2.84320	-0.29472
	H	4.67489	-0.96672	0.22017
	H	3.79453	1.32293	0.49909
Phenanthrene I (**3**) Note: Same structure as Phenanthrene II 3	C	0.98129	2.22870	0.35681
	C	-0.37207	2.45751	0.29374
	C	-1.23104	1.38140	-0.01592
	C	-0.72595	0.10672	-0.25311
	C	0.66166	-0.15962	-0.20176
	C	1.53136	0.94062	0.11300
	C	-2.68873	1.35152	-0.16543
	C	-3.08893	0.11146	-0.48641
	C	-1.88669	-0.81142	-0.56690
	C	-2.09991	-2.01922	0.37714
	C	1.23848	-1.43442	-0.44704
	C	2.59864	-1.61551	-0.38679
	C	3.45478	-0.53407	-0.07605
	C	2.93041	0.71142	0.16834
	O	-1.39879	-2.43504	1.22534
	H	1.66032	3.04135	0.59278
	H	-0.77532	3.44796	0.47346
	H	-3.33305	2.21216	-0.03886
	H	-4.10045	-0.23117	-0.65031
	H	-1.80731	-1.25989	-1.56639
	H	0.59466	-2.27513	-0.67324
	H	3.02146	-2.59598	-0.57473
	H	4.52610	-0.69325	-0.03063
	H	3.58411	1.54383	0.40757
Phenanthrene I (**4**) Note: Same structure as Phenanthrene II 4	C	0.27925	2.04120	0.00003
	C	-1.10318	1.95576	-0.00001
	C	-1.70621	0.69288	-0.00002
	C	-0.92866	-0.48412	-0.00002
	C	0.48578	-0.42368	0.00000
	C	1.09529	0.88273	0.00003
	C	-3.10990	0.29182	-0.00015
	C	-3.16639	-1.09726	0.00024
	C	-1.85000	-1.59956	-0.00015
	C	1.32936	-1.56629	-0.00003
	C	2.69592	-1.43496	-0.00001
	C	3.29677	-0.15230	0.00002
	C	2.51347	0.97405	0.00004
	H	0.76181	3.01273	0.00002
	H	-1.70671	2.85725	-0.00006
	H	-3.95258	0.97022	-0.00018
	H	-4.06564	-1.69583	0.00055
	H	-1.57876	-2.64653	-0.00017
	H	0.88155	-2.55346	-0.00006

	H	3.32412	-2.31884	-0.00003
	H	4.37735	-0.06581	0.00003
	H	2.96994	1.95852	0.00005
CO	C	0.00000	0.00000	-0.64398
	O	0.00000	0.00000	0.48298
Phenanthrene I (**5**)	C	-0.79220	-2.36222	0.18979
	C	0.57036	-2.41770	0.11438
	C	1.36651	-1.24877	-0.02879
	C	0.74222	0.00424	-0.11749
	C	-0.69524	0.07801	-0.09968
	C	-1.46184	-1.11770	0.08401
	C	2.82307	-1.45499	-0.05365
	C	3.81108	-0.58641	-0.11226
	C	1.58046	1.19525	-0.24186
	C	-1.40922	1.29312	-0.27632
	C	-2.78259	1.33689	-0.22550
	C	-3.52843	0.16043	-0.00244
	C	-2.87647	-1.03938	0.13931
	O	1.21558	3.54270	0.45854
	H	-1.37565	-3.26659	0.32203
	H	1.07567	-3.37505	0.18507
	H	3.11427	-2.51181	-0.01390
	H	4.88969	-0.62191	-0.13026
	H	2.60677	1.05559	-0.59150
	H	-0.87532	2.21066	-0.48229
	H	-3.29535	2.28100	-0.36975
	H	-4.61065	0.20536	0.04084
	H	-3.43766	-1.95549	0.29069
	C	1.34956	2.43200	0.14396
Phenanthrene I (**6**)	C	-1.12985	2.01783	0.10968
	C	0.21423	1.93142	0.11125
	C	0.92452	0.66781	0.09694
	C	0.11469	-0.57577	0.21822
	C	-1.36799	-0.44874	0.04512
	C	-1.96412	0.83385	0.03714
	C	2.28602	0.69933	-0.02538
	C	3.17294	-0.42907	-0.09115
	C	0.66194	-1.75166	0.51210
	C	-2.19192	-1.57272	-0.09453
	C	-3.57073	-1.44868	-0.20810
	C	-4.16091	-0.18365	-0.18891
	C	-3.36029	0.94225	-0.07242
	O	5.64816	-0.28860	-0.21452
	H	-1.61787	2.98624	0.12231
	H	0.81463	2.83553	0.11515
	H	2.74703	1.67954	-0.09487
	H	2.77230	-1.44154	-0.07575
	H	0.35567	-2.76451	0.71586

	H	-1.74782	-2.56027	-0.12872
	H	-4.18404	-2.33587	-0.31698
	H	-5.23663	-0.08068	-0.27536
	H	-3.80775	1.93083	-0.07317
	C	4.49132	-0.33895	-0.16202
Phenanthrene I (**7**)	C	-1.38657	2.05911	-0.22860
	C	-0.07765	2.36716	-0.10590
	C	0.88062	1.31725	0.14018
	C	0.41389	-0.08497	0.25883
	C	-1.00794	-0.38681	0.11807
	C	-1.89401	0.69578	-0.12386
	C	2.22588	1.35927	0.29508
	C	2.71912	-0.03846	0.54844
	C	3.85837	-0.48484	-0.40895
	C	1.48142	-0.88620	0.49587
	C	-1.52637	-1.68425	0.21206
	C	-2.88749	-1.92217	0.07210
	C	-3.76153	-0.85882	-0.16561
	C	-3.26571	0.43402	-0.26176
	O	4.06626	-1.56058	-0.83574
	H	-2.11353	2.84314	-0.41465
	H	0.26419	3.39271	-0.19031
	H	2.86905	2.22632	0.25278
	H	3.20826	-0.10537	1.53392
	H	1.50029	-1.96003	0.60751
	H	-0.85402	-2.51443	0.39612
	H	-3.26954	-2.93380	0.14747
	H	-4.82434	-1.04185	-0.27508
	H	-3.94262	1.26150	-0.44744
Phenanthrene I (**TS 1-2**)	C	1.31715	2.08754	0.27426
	C	-0.01126	2.38146	0.18045
	C	-0.94883	1.34076	-0.08874
	C	-0.51002	0.00601	-0.22465
	C	0.86947	-0.31889	-0.12437
	C	1.79765	0.74920	0.12086
	C	-2.33332	1.46251	-0.30884
	C	-3.04237	0.22609	-0.47410
	C	-2.79105	-0.97887	0.33913
	C	-1.58596	-0.96321	-0.46723
	C	1.37283	-1.64092	-0.24699
	C	2.72165	-1.89641	-0.15652
	C	3.63317	-0.84439	0.06962
	C	3.17502	0.44794	0.20790
	O	-3.47108	-1.77875	0.92115
	H	2.03997	2.87374	0.46389
	H	-0.36316	3.40115	0.29077
	H	-2.84625	2.41127	-0.40663
	H	-3.95049	0.18041	-1.07181

	H	-1.43184	-1.81886	-1.12109
	H	0.68114	-2.45993	-0.40443
	H	3.08676	-2.91250	-0.25352
	H	4.69386	-1.05620	0.14036
	H	3.87385	1.25805	0.38859
Phenanthrene I (**TS 1-5**)	C	1.13640	2.13744	0.35361
	C	-0.21377	2.33006	0.25338
	C	-1.10066	1.26266	-0.06282
	C	-0.58026	-0.01596	-0.25858
	C	0.82980	-0.24081	-0.16002
	C	1.70049	0.85473	0.14460
	C	-2.53113	1.59129	-0.19597
	C	-3.52606	0.78640	-0.50674
	C	-1.47504	-1.15587	-0.61759
	C	1.41326	-1.52210	-0.35653
	C	2.77183	-1.70602	-0.26623
	C	3.62666	-0.62067	0.03028
	C	3.09787	0.63012	0.23304
	O	-2.80597	-2.38857	1.06654
	H	1.79275	2.96811	0.59093
	H	-0.63175	3.31891	0.40855
	H	-2.76257	2.64915	-0.02550
	H	-4.59181	0.91120	-0.63599
	H	-1.56224	-1.49834	-1.64436
	H	0.76481	-2.36094	-0.57480
	H	3.19331	-2.69310	-0.42028
	H	4.69670	-0.78001	0.09964
	H	3.74458	1.47009	0.46449
	C	-2.18207	-1.81071	0.27706
Phenanthrene I (**TS 1-6**)	C	1.19708	2.03691	0.21705
	C	-0.13409	2.13769	0.05907
	C	-0.97876	0.98186	-0.19956
	C	-0.32696	-0.36211	-0.25623
	C	1.16025	-0.42291	-0.10572
	C	1.89141	0.76338	0.13496
	C	-2.30570	1.17396	-0.40377
	C	-3.29059	0.10865	-0.69778
	C	-1.06915	-1.45006	-0.44163
	C	1.86392	-1.63115	-0.18738
	C	3.24408	-1.67745	-0.03541
	C	3.96224	-0.50552	0.20583
	C	3.28499	0.70184	0.28907
	O	-4.44007	-1.15820	1.09525
	H	1.79246	2.92413	0.40654
	H	-0.62058	3.10536	0.11920
	H	-2.68041	2.19443	-0.38076
	H	-3.62279	-0.09212	-1.71357
	H	-0.88642	-2.51107	-0.51880

	H	1.32636	-2.55258	-0.37461
	H	3.76015	-2.62830	-0.10532
	H	5.03904	-0.53741	0.32583
	H	3.83116	1.62110	0.47400
	C	-3.90180	-0.56478	0.25575
Phenanthrene I (**TS 2-3**)	C	1.26264	2.10844	0.33509
	C	-0.05859	2.44080	0.22418
	C	-1.00353	1.43061	-0.11476
	C	-0.57092	0.11055	-0.31745
	C	0.78665	-0.26400	-0.18558
	C	1.72663	0.77093	0.13728
	C	-2.42061	1.50376	-0.25246
	C	-2.93303	0.22240	-0.48825
	C	-1.73782	-0.76718	-0.68470
	C	-2.46189	-1.19409	0.49209
	C	1.26155	-1.58882	-0.36472
	C	2.60068	-1.87827	-0.23761
	C	3.52732	-0.86000	0.07173
	C	3.09499	0.43494	0.25485
	O	-2.91644	-2.12041	1.07809
	H	1.99433	2.86981	0.58498
	H	-0.38986	3.45971	0.38960
	H	-3.02062	2.39247	-0.11501
	H	-3.93215	-0.00413	-0.83513
	H	-1.65368	-1.41703	-1.56377
	H	0.55581	-2.37927	-0.59406
	H	2.94844	-2.89615	-0.37338
	H	4.57965	-1.10139	0.16755
	H	3.80532	1.21888	0.49639
Phenanthrene I (**TS 2-7**)	C	1.25626	2.07259	0.27692
	C	-0.06548	2.33581	0.12594
	C	-0.96331	1.26388	-0.20683
	C	-0.45316	-0.08203	-0.34152
	C	0.94677	-0.35706	-0.16259
	C	1.80488	0.74239	0.13804
	C	-2.32828	1.27216	-0.39272
	C	-2.80891	-0.10311	-0.74323
	C	-3.05101	-0.77284	0.51788
	C	-1.53093	-0.94462	-0.57615
	C	1.50539	-1.64621	-0.27417
	C	2.86162	-1.85016	-0.10076
	C	3.70761	-0.76840	0.18903
	C	3.18206	0.50593	0.30586
	O	-3.83054	-1.39809	1.15798
	H	1.94557	2.87603	0.51571
	H	-0.45056	3.34253	0.24154
	H	-2.99648	2.11315	-0.27606
	H	-3.48105	-0.24188	-1.59983

	H	-1.49149	-1.98885	-0.84827
	H	0.86031	-2.48828	-0.49738
	H	3.27296	-2.84933	-0.18850
	H	4.77067	-0.93253	0.32254
	H	3.83332	1.34386	0.53220
Phenanthrene I (**TS 5-3**)	C	-1.14409	-2.19457	0.33519
	C	0.19653	-2.46320	0.25067
	C	1.12049	-1.42637	-0.02753
	C	0.67046	-0.12551	-0.22900
	C	-0.72063	0.18019	-0.16674
	C	-1.64029	-0.88156	0.13123
	C	2.56837	-1.64754	-0.10564
	C	3.34706	-0.61732	-0.39003
	C	1.73414	0.88785	-0.54499
	C	-1.25358	1.47812	-0.39877
	C	-2.60417	1.71720	-0.32073
	C	-3.50378	0.67337	-0.00869
	C	-3.02748	-0.59579	0.20835
	O	2.23752	2.79960	0.97902
	H	-1.84929	-2.98827	0.55865
	H	0.56666	-3.47101	0.40560
	H	2.94663	-2.65457	0.08288
	H	4.42052	-0.51806	-0.49024
	H	1.99332	1.07022	-1.58690
	H	-0.57952	2.28821	-0.64633
	H	-2.98485	2.71580	-0.50379
	H	-4.56670	0.87708	0.05205
	H	-3.71038	-1.40628	0.44108
	C	1.90088	1.96347	0.24247
Phenanthrene I (**TS 6-7**)	C	-1.27845	2.04785	-0.12344
	C	0.05599	2.17698	0.01138
	C	0.90358	1.01669	0.18416
	C	0.28614	-0.33409	0.21295
	C	-1.18728	-0.43112	0.07017
	C	-1.94405	0.75451	-0.09742
	C	2.25118	1.08544	0.30599
	C	2.99324	-0.17098	0.56153
	C	1.13996	-1.35438	0.34132
	C	-1.86049	-1.65831	0.09653
	C	-3.24097	-1.72618	-0.04217
	C	-3.98618	-0.55742	-0.21047
	C	-3.33829	0.66885	-0.23643
	O	4.91569	-0.88221	-0.86679
	H	-1.90002	2.92750	-0.25632
	H	0.52183	3.15650	-0.00902
	H	2.78417	2.02560	0.23133
	H	3.00741	-0.59290	1.56846
	H	1.00365	-2.42537	0.41323

	H	-1.29338	-2.57239	0.22765
	H	-3.73781	-2.68953	-0.01841
	H	-5.06361	-0.60697	-0.31884
	H	-3.90907	1.58261	-0.36645
	C	4.08250	-0.47573	-0.16363
Phenanthrene I (**TS 3-4**) Note: Same structure as Phenanthrene II TS 3-4	C	0.98609	2.13549	0.42363
	C	-0.36697	2.34989	0.27944
	C	-1.18477	1.28665	-0.14835
	C	-0.63562	0.02921	-0.42453
	C	0.74950	-0.22285	-0.27856
	C	1.57591	0.87047	0.15315
	C	-2.62154	1.22924	-0.41651
	C	-2.94580	-0.01605	-0.84507
	C	-1.74326	-0.86598	-0.81686
	C	-1.96186	-1.96853	0.70362
	C	1.35588	-1.48145	-0.52796
	C	2.70996	-1.65433	-0.36721
	C	3.52668	-0.57808	0.05012
	C	2.96989	0.65196	0.30369
	O	-2.32195	-1.59198	1.72903
	H	1.63146	2.94395	0.75078
	H	-0.79476	3.32491	0.48555
	H	-3.30293	2.06187	-0.30151
	H	-3.92815	-0.36823	-1.12526
	H	-1.59681	-1.63416	-1.56638
	H	0.73707	-2.31353	-0.84444
	H	3.15829	-2.62239	-0.56088
	H	4.59332	-0.72905	0.17076
	H	3.59364	1.47878	0.62749
Phenanthrene I (**TS 7-4**)	C	1.37368	2.04969	0.26442
	C	0.06392	2.34799	0.09701
	C	-0.86864	1.29975	-0.21107
	C	-0.38765	-0.09256	-0.33575
	C	1.02329	-0.38847	-0.14648
	C	1.89429	0.69530	0.15080
	C	-2.21548	1.32743	-0.44487
	C	-2.65615	-0.05075	-0.67150
	C	-3.53787	-0.62446	0.86761
	C	-1.45160	-0.89272	-0.65005
	C	1.55480	-1.68228	-0.24417
	C	2.91061	-1.91471	-0.05804
	C	3.76864	-0.85046	0.23263
	C	3.26159	0.43738	0.33529
	O	-4.41914	-1.36676	0.80780
	H	2.08481	2.83606	0.49589
	H	-0.28980	3.36885	0.19046
	H	-2.86591	2.18941	-0.42451
	H	-3.47248	-0.26766	-1.35461

	H	-1.45478	-1.95899	-0.82024
	H	0.89485	-2.51275	-0.46775
	H	3.30214	-2.92242	-0.13754
	H	4.82771	-1.02975	0.37867
	H	3.92615	1.26461	0.56234
Phenanthrene II				
Species Name (Stationary point)	Geometry (Å)			
Phenanthrene II (**1**)	C	-0.92123	2.21768	-0.00027
	C	0.43501	2.30687	0.00015
	C	1.24759	1.13115	0.00027
	C	0.64725	-0.15313	0.00011
	C	-0.79063	-0.25546	0.00006
	C	-1.57091	0.94987	-0.00028
	C	2.66114	1.28010	0.00035
	C	3.51757	0.17840	0.00006
	C	2.98485	-1.08872	-0.00022
	C	1.55025	-1.33294	-0.00020
	C	-1.49646	-1.49139	0.00050
	C	-2.87262	-1.52522	0.00047
	C	-3.62877	-0.33679	-0.00005
	C	-2.98308	0.87686	-0.00041
	O	1.15382	-2.51204	-0.00050
	H	-1.53267	3.11384	-0.00052
	H	0.92501	3.27436	0.00036
	H	3.07039	2.28444	0.00068
	H	4.59169	0.32624	0.00003
	H	3.60471	-1.97716	-0.00050
	H	-0.92793	-2.40691	0.00081
	H	-3.38010	-2.48342	0.00088
	H	-4.71204	-0.38103	-0.00010
	H	-3.54939	1.80223	-0.00077
Phenanthrene II (**2**)	C	0.74017	2.16946	0.42219
	C	-0.63117	2.28280	0.29042
	C	-1.40301	1.16519	-0.03143
	C	-0.77374	-0.17814	-0.04361
	C	0.70278	-0.25020	-0.14805
	C	1.43220	0.93509	0.14709
	C	-2.75420	1.05518	-0.46940
	C	-3.04809	-0.21540	-0.86308
	C	-1.89204	-1.14389	-0.68855
	C	-1.48020	-1.29788	0.70998
	C	1.38953	-1.42441	-0.46111
	C	2.78010	-1.45239	-0.48759
	C	3.50629	-0.29585	-0.18998
	C	2.84027	0.87812	0.12158
	O	-1.45754	-1.97521	1.68667
	H	1.33498	3.04350	0.66160

	H	-1.10861	3.25196	0.39119
	H	-3.45180	1.88262	-0.49007
	H	-4.00664	-0.56693	-1.21985
	H	-1.68564	-1.93583	-1.40664
	H	0.83544	-2.32998	-0.68480
	H	3.29663	-2.37233	-0.73545
	H	4.59003	-0.31637	-0.20508
	H	3.40245	1.77889	0.34488
Phenanthrene II (**3**) Note: Same structure as Phenanthrene I 3	C	0.98129	2.22870	0.35681
	C	-0.37207	2.45751	0.29374
	C	-1.23104	1.38140	-0.01592
	C	-0.72595	0.10672	-0.25311
	C	0.66166	-0.15962	-0.20176
	C	1.53136	0.94062	0.11300
	C	-2.68873	1.35152	-0.16543
	C	-3.08893	0.11146	-0.48641
	C	-1.88669	-0.81142	-0.56690
	C	-2.09991	-2.01922	0.37714
	C	1.23848	-1.43442	-0.44704
	C	2.59864	-1.61551	-0.38679
	C	3.45478	-0.53407	-0.07605
	C	2.93041	0.71142	0.16834
	O	-1.39879	-2.43504	1.22534
	H	1.66032	3.04135	0.59278
	H	-0.77532	3.44796	0.47346
	H	-3.33305	2.21216	-0.03886
	H	-4.10045	-0.23117	-0.65031
	H	-1.80731	-1.25989	-1.56639
	H	0.59466	-2.27513	-0.67324
	H	3.02146	-2.59598	-0.57473
	H	4.52610	-0.69325	-0.03063
	H	3.58411	1.54383	0.40757
Phenanthrene II (**4**) Note: Same structure as Phenanthrene I 4	C	0.27925	2.04120	0.00003
	C	-1.10318	1.95576	-0.00001
	C	-1.70621	0.69288	-0.00002
	C	-0.92866	-0.48412	-0.00002
	C	0.48578	-0.42368	0.00000
	C	1.09529	0.88273	0.00003
	C	-3.10990	0.29182	-0.00015
	C	-3.16639	-1.09726	0.00024
	C	-1.85000	-1.59956	-0.00015
	C	1.32936	-1.56629	-0.00003
	C	2.69592	-1.43496	-0.00001
	C	3.29677	-0.15230	0.00002
	C	2.51347	0.97405	0.00004
	H	0.76181	3.01273	0.00002
	H	-1.70671	2.85725	-0.00006
	H	-3.95258	0.97022	-0.00018

	H	-4.06564	-1.69583	0.00055
	H	-1.57876	-2.64653	-0.00017
	H	0.88155	-2.55346	-0.00006
	H	3.32412	-2.31884	-0.00003
	H	4.37735	-0.06581	0.00003
	H	2.96994	1.95852	0.00005
Phenanthrene II (**5**)	C	1.88760	1.92063	-0.00008
	C	0.56688	2.28338	-0.00008
	C	-0.49071	1.30822	-0.00004
	C	-0.05364	0.01155	-0.00010
	C	1.26033	-0.45544	-0.00007
	C	2.28563	0.55626	-0.00005
	C	-1.87773	1.76142	0.00007
	C	-3.00396	1.01618	0.00016
	C	-3.07336	-0.42958	0.00002
	C	-4.20312	-1.11394	0.00035
	C	1.63869	-1.82499	-0.00004
	C	2.96548	-2.17936	0.00005
	C	3.97513	-1.18843	0.00009
	C	3.64112	0.14520	0.00003
	O	-5.18478	-1.73169	-0.00030
	H	2.65679	2.68559	-0.00011
	H	0.29140	3.33364	-0.00013
	H	-2.00557	2.83895	0.00009
	H	-3.95240	1.54339	0.00028
	H	-2.16347	-1.02407	0.00006
	H	0.86306	-2.58181	-0.00008
	H	3.24516	-3.22678	0.00007
	H	5.01724	-1.48693	0.00017
	H	4.41600	0.90506	0.00005
Phenanthrene II (**TS 1-2**)	C	0.76413	2.20076	0.37017
	C	-0.61100	2.28885	0.33607
	C	-1.39849	1.15826	0.08350
	C	-0.76366	-0.16682	0.04914
	C	0.70494	-0.23594	-0.08437
	C	1.44653	0.96384	0.10440
	C	-2.76991	1.12241	-0.30708
	C	-3.12884	-0.09530	-0.78891
	C	-2.08479	-1.13160	-0.69741
	C	-1.47452	-1.36338	0.59695
	C	1.39009	-1.42944	-0.33837
	C	2.77536	-1.45202	-0.42757
	C	3.51098	-0.27507	-0.24719
	C	2.85320	0.91226	0.01850
	O	-1.27157	-2.23167	1.39524
	H	1.36119	3.08977	0.53907
	H	-1.09736	3.25246	0.44616
	H	-3.42457	1.98253	-0.25835

	H	-4.10166	-0.34346	-1.19456
	H	-1.97962	-1.90372	-1.45808
	H	0.83475	-2.35167	-0.46364
	H	3.28550	-2.38618	-0.63197
	H	4.59281	-0.29485	-0.31170
	H	3.41736	1.82757	0.16417
Phenanthrene II (**TS 1-5**)	C	1.53141	2.02322	0.33607
	C	0.19825	2.33305	0.25537
	C	-0.78474	1.33166	-0.03825
	C	-0.30083	0.06688	-0.23080
	C	1.03554	-0.33347	-0.16454
	C	1.99744	0.69650	0.13219
	C	-2.19864	1.70093	-0.12507
	C	-3.22923	0.89196	-0.40920
	C	-3.10690	-0.56116	-0.70316
	C	-3.17275	-1.47855	0.23672
	C	1.48653	-1.66572	-0.36748
	C	2.82304	-1.96805	-0.28294
	C	3.77076	-0.95780	0.00719
	C	3.36734	0.34031	0.20943
	O	-3.22466	-2.28775	1.06832
	H	2.25510	2.79956	0.56028
	H	-0.13331	3.35458	0.41566
	H	-2.41856	2.75152	0.04845
	H	-4.22644	1.32224	-0.45792
	H	-3.01512	-0.92193	-1.72367
	H	0.75479	-2.43407	-0.58713
	H	3.15917	-2.98698	-0.43796
	H	4.82226	-1.21439	0.06995
	H	4.09604	1.11299	0.43252
Phenanthrene II (**TS 2-3**)	C	0.78212	2.20297	0.40390
	C	-0.58450	2.34290	0.28914
	C	-1.37027	1.22984	-0.04163
	C	-0.77069	-0.07698	-0.13608
	C	0.67545	-0.20781	-0.17864
	C	1.43923	0.95623	0.14275
	C	-2.76543	1.11283	-0.34299
	C	-3.07635	-0.16058	-0.69681
	C	-1.86375	-1.05453	-0.69009
	C	-1.55209	-1.40755	0.67283
	C	1.34268	-1.40700	-0.48189
	C	2.72470	-1.47367	-0.46760
	C	3.48188	-0.33698	-0.14112
	C	2.84913	0.85249	0.15750
	O	-1.37176	-2.25873	1.47908
	H	1.39660	3.06183	0.64972
	H	-1.05027	3.31252	0.42863
	H	-3.47826	1.92364	-0.26301

	H	-4.06134	-0.54914	-0.91464
	H	-1.69350	-1.74850	-1.52121
	H	0.76862	-2.29549	-0.72046
	H	3.22257	-2.40648	-0.70572
	H	4.56429	-0.39501	-0.12559
	H	3.43267	1.73339	0.40395
Phenanthrene II (**TS 2-4**)	C	0.61985	2.10212	0.28687
	C	-0.71084	2.15423	-0.02888
	C	-1.41989	0.97283	-0.35530
	C	-0.75856	-0.35815	-0.03603
	C	0.74614	-0.35240	-0.13251
	C	1.39067	0.88156	0.13222
	C	-2.64792	0.71496	-0.98420
	C	-2.83979	-0.66148	-1.12276
	C	-1.75418	-1.37126	-0.57186
	C	-1.35137	-0.72699	1.25309
	C	1.48159	-1.49838	-0.40509
	C	2.87589	-1.45835	-0.40042
	C	3.52804	-0.25828	-0.11579
	C	2.79682	0.89469	0.14093
	O	-1.92201	-0.88369	2.25445
	H	1.15683	3.01059	0.53406
	H	-1.22205	3.11012	-0.08256
	H	-3.34066	1.47843	-1.31123
	H	-3.70892	-1.12799	-1.56560
	H	-1.58428	-2.43674	-0.57284
	H	0.96708	-2.42850	-0.62106
	H	3.44607	-2.35581	-0.60958
	H	4.61167	-0.22111	-0.10365
	H	3.31165	1.82981	0.33534
Phenanthrene II (**TS 5-3**)	C	-1.59199	2.04304	-0.26399
	C	-0.29017	2.47534	-0.21376
	C	0.76105	1.53952	0.00312
	C	0.44162	0.21293	0.15469
	C	-0.86881	-0.28600	0.11723
	C	-1.92460	0.66949	-0.10407
	C	2.18014	1.87492	0.07407
	C	3.04913	0.88100	0.30639
	C	2.49535	-0.48701	0.55575
	C	2.97476	-1.54520	-0.12734
	C	-1.20649	-1.65817	0.27185
	C	-2.51516	-2.06984	0.21661
	C	-3.55252	-1.13185	0.00060
	C	-3.26262	0.20218	-0.15684
	O	3.16108	-2.46872	-0.81161
	H	-2.39526	2.75380	-0.42748
	H	-0.05687	3.52909	-0.33321
	H	2.51450	2.89805	-0.06247

	H	4.11998	1.03807	0.34230
	H	2.19950	-0.74388	1.57314
	H	-0.40834	-2.37505	0.42762
	H	-2.75968	-3.11948	0.33500
	H	-4.58094	-1.47250	-0.04270
	H	-4.05970	0.91952	-0.32527
Phenanthrene II (**TS 3-4**) Note: Same structure as Phenanthrene I TS 3-4	C	0.98609	2.13549	0.42363
	C	-0.36697	2.34989	0.27944
	C	-1.18477	1.28665	-0.14835
	C	-0.63562	0.02921	-0.42453
	C	0.74950	-0.22285	-0.27856
	C	1.57591	0.87047	0.15315
	C	-2.62154	1.22924	-0.41651
	C	-2.94580	-0.01605	-0.84507
	C	-1.74326	-0.86598	-0.81686
	C	-1.96186	-1.96853	0.70362
	C	1.35588	-1.48145	-0.52796
	C	2.70996	-1.65433	-0.36721
	C	3.52668	-0.57808	0.05012
	C	2.96989	0.65196	0.30369
	O	-2.32195	-1.59198	1.72903
	H	1.63146	2.94395	0.75078
	H	-0.79476	3.32491	0.48555
	H	-3.30293	2.06187	-0.30151
	H	-3.92815	-0.36823	-1.12526
	H	-1.59681	-1.63416	-1.56638
	H	0.73707	-2.31353	-0.84444
	H	3.15829	-2.62239	-0.56088
	H	4.59332	-0.72905	0.17076
	H	3.59364	1.47878	0.62749
Phenanthrene III				
Species Name (Stationary point)	Geometry (Å)			
Phenanthrene III (**1**)	C	3.69495	-0.15795	0.00016
	C	3.13275	-1.44455	-0.00047
	C	1.75411	-1.61474	-0.00059
	C	0.87803	-0.52122	-0.00012
	C	1.45149	0.79500	0.00033
	C	2.86609	0.94087	0.00055
	H	4.77145	-0.03416	0.00030
	H	3.77807	-2.31552	-0.00088
	H	1.36198	-2.62304	-0.00110
	H	3.27927	1.94353	0.00097
	C	-0.58408	-0.66624	-0.00002
	C	-1.40612	0.48529	-0.00020
	C	-0.81428	1.84775	-0.00042
	C	0.62189	1.92982	0.00040
	O	-1.51816	2.86847	-0.00040

	H	1.05010	2.92595	0.00080
	C	-1.21824	-1.92390	0.00033
	C	-2.59964	-2.03172	0.00039
	C	-3.40015	-0.88489	0.00012
	C	-2.80045	0.36309	-0.00012
	H	-0.62965	-2.83184	0.00066
	H	-3.05899	-3.01388	0.00067
	H	-4.48043	-0.97359	0.00015
	H	-3.38456	1.27511	-0.00033
Phenanthrene III (**2**)	C	3.57895	0.04172	-0.24980
	C	3.23543	-1.21783	0.25377
	C	1.90389	-1.56955	0.43823
	C	0.89958	-0.64931	0.11167
	C	1.25551	0.62478	-0.38205
	C	2.58922	0.97330	-0.56259
	H	4.62217	0.29764	-0.39453
	H	4.01727	-1.92707	0.50055
	H	1.64701	-2.54813	0.82772
	H	2.85775	1.95245	-0.94312
	C	-0.54103	-0.78539	0.15615
	C	-1.17714	0.50832	-0.15310
	C	-0.71756	1.81242	0.52936
	C	0.06588	1.49500	-0.64482
	O	-1.11829	2.66899	1.25545
	H	0.03747	2.14334	-1.52001
	C	-1.32586	-1.91585	0.28991
	C	-2.69792	-1.86482	0.01760
	C	-3.28784	-0.66932	-0.46243
	C	-2.56498	0.48683	-0.59189
	H	-0.86470	-2.86347	0.54775
	H	-3.30071	-2.75940	0.11239
	H	-4.33563	-0.67307	-0.74228
	H	-3.03115	1.40393	-0.93224
Phenanthrene III (**3**)	C	-3.54376	0.04822	0.05663
	C	-3.23681	-1.28869	-0.20517
	C	-1.91255	-1.72355	-0.23866
	C	-0.89498	-0.80019	-0.00359
	C	-1.21045	0.54289	0.26824
	C	-2.52736	0.97605	0.29636
	H	-4.57914	0.36879	0.07238
	H	-4.03826	-1.99568	-0.38784
	H	-1.68368	-2.76267	-0.44744
	H	-2.76553	2.01583	0.49130
	C	0.56616	-0.95509	0.01233
	C	1.15274	0.29206	0.29949
	C	0.19221	2.59765	-0.36899
	C	0.06432	1.32977	0.50258
	O	1.17782	3.12743	-0.73541

	H	0.08692	1.73756	1.52338
	C	1.37080	-2.07235	-0.20331
	C	2.75605	-1.92722	-0.13832
	C	3.33229	-0.68517	0.13611
	C	2.53130	0.43753	0.35741
	H	0.93203	-3.03998	-0.42028
	H	3.39392	-2.78765	-0.30648
	H	4.41139	-0.59043	0.17559
	H	2.98005	1.40350	0.55599
Phenanthrene III (**4**)	C	3.45372	0.17644	-0.00006
	C	3.03209	-1.15753	0.00002
	C	1.66878	-1.48284	0.00004
	C	0.73374	-0.46061	0.00001
	C	1.15949	0.90602	-0.00007
	C	2.52605	1.21572	-0.00011
	H	4.51417	0.40138	-0.00002
	H	3.77069	-1.95117	0.00003
	H	1.35997	-2.52274	0.00000
	H	2.85771	2.24854	-0.00009
	C	-0.73374	-0.46061	0.00001
	C	-1.15949	0.90602	-0.00007
	C	0.00000	1.74278	0.00031
	H	0.00000	2.82469	0.00031
	C	-1.66878	-1.48284	0.00004
	C	-3.03209	-1.15753	0.00002
	C	-3.45372	0.17644	-0.00006
	C	-2.52605	1.21572	-0.00011
	H	-1.35997	-2.52274	0.00001
	H	-3.77069	-1.95117	0.00003
	H	-4.51417	0.40138	-0.00002
	H	-2.85771	2.24854	-0.00009
Phenanthrene III (**5**)	C	-3.64730	-0.43800	0.08905
	C	-2.98214	-1.66068	0.06308
	C	-1.59156	-1.67501	0.04489
	C	-0.84228	-0.49334	0.05048
	C	-1.51637	0.74993	0.04812
	C	-2.92150	0.74537	0.07833
	H	-4.73071	-0.40301	0.11228
	H	-3.53637	-2.59186	0.06960
	H	-1.06285	-2.62160	0.05537
	H	-3.44732	1.69412	0.07769
	C	0.64229	-0.59436	0.07752
	C	1.42069	-0.03888	1.07528
	C	0.39281	2.36326	-0.32222
	C	-0.85412	2.05631	-0.01522
	O	1.45816	2.73772	-0.58889
	H	-1.46871	2.94022	0.12973
	C	1.35594	-1.32266	-0.89697

	C	2.74102	-1.45125	-0.82477
	C	3.46006	-0.86198	0.21469
	C	2.78395	-0.12940	1.19973
	H	0.80756	-1.77655	-1.71613
	H	3.26471	-2.01250	-1.59019
	H	4.53878	-0.96499	0.26339
	H	3.32070	0.33846	2.01748
Phenanthrene III (**8**)	C	2.74872	-1.94273	0.13853
	C	1.62497	-2.75831	0.25952
	C	0.36218	-2.18277	0.21750
	C	0.18152	-0.80054	0.06218
	C	1.32447	0.02610	-0.06213
	C	2.59467	-0.57467	-0.02501
	H	3.74400	-2.37161	0.16707
	H	1.73142	-3.82840	0.39291
	H	-0.51402	-2.80933	0.33810
	H	3.47773	0.04621	-0.13848
	C	-1.20508	-0.26477	0.03763
	C	-1.61488	0.85664	0.73624
	C	2.18733	2.33507	-0.21935
	C	1.19132	1.47417	-0.25906
	O	3.05306	3.10884	-0.18656
	H	0.21783	1.91640	-0.43714
	C	-2.23049	-0.90482	-0.69156
	C	-3.53774	-0.42501	-0.67444
	C	-3.87498	0.70945	0.06277
	C	-2.88300	1.37791	0.79319
	H	-1.98352	-1.77702	-1.28774
	H	-4.29976	-0.93871	-1.24944
	H	-4.89540	1.07703	0.07247
	H	-3.11682	2.26033	1.37880
Phenanthrene III (**TS 1-2**)	C	3.58212	0.04051	-0.25552
	C	3.23792	-1.21365	0.25994
	C	1.90574	-1.55908	0.45305
	C	0.90297	-0.63843	0.12487
	C	1.25897	0.63185	-0.37701
	C	2.59342	0.97277	-0.56958
	H	4.62516	0.29238	-0.40846
	H	4.01849	-1.92373	0.50810
	H	1.64748	-2.53426	0.85011
	H	2.86314	1.94829	-0.95850
	C	-0.53792	-0.77927	0.16699
	C	-1.19066	0.50723	-0.12624
	C	-0.72958	1.81673	0.52019
	C	0.08067	1.51266	-0.63549
	O	-1.15740	2.68562	1.21842
	H	0.05513	2.16434	-1.50808
	C	-1.30788	-1.92362	0.27411

	C	-2.67798	-1.89024	-0.00732
	C	-3.28413	-0.69466	-0.46418
	C	-2.57734	0.47474	-0.56232
	H	-0.83310	-2.86840	0.51692
	H	-3.26631	-2.79648	0.06539
	H	-4.33132	-0.70645	-0.74586
	H	-3.05736	1.39411	-0.87596
Phenanthrene III (**TS 1-5**)	C	-3.64288	-0.41683	0.07122
	C	-2.99887	-1.64704	0.18077
	C	-1.61200	-1.68437	0.16767
	C	-0.83095	-0.52492	0.04404
	C	-1.48415	0.73059	-0.05213
	C	-2.89280	0.74306	-0.03963
	H	-4.72542	-0.35880	0.07938
	H	-3.56757	-2.56336	0.28581
	H	-1.10972	-2.63712	0.28474
	H	-3.40209	1.69723	-0.12106
	C	0.64157	-0.66299	0.03235
	C	1.49819	0.27939	0.56024
	C	0.40067	2.48140	-0.18560
	C	-0.84683	2.03841	-0.19620
	O	1.39141	3.09275	-0.22495
	H	-1.52251	2.87904	-0.34688
	C	1.29908	-1.79413	-0.50670
	C	2.68297	-1.91752	-0.45467
	C	3.47490	-0.92044	0.11865
	C	2.86617	0.22804	0.63737
	H	0.70922	-2.56833	-0.98479
	H	3.15275	-2.79778	-0.87842
	H	4.55395	-1.02377	0.15116
	H	3.44958	1.03512	1.06543
Phenanthrene III (**TS 5-8**)	C	3.46998	-0.83966	-0.08414
	C	2.69668	-1.97567	0.13772
	C	1.31080	-1.88017	0.13798
	C	0.65681	-0.65720	-0.07756
	C	1.44663	0.49220	-0.30664
	C	2.84096	0.38143	-0.30250
	H	4.55211	-0.90180	-0.08877
	H	3.17023	-2.93747	0.29938
	H	0.71949	-2.77699	0.27790
	H	3.43224	1.27447	-0.46913
	C	-0.82599	-0.60001	-0.08875
	C	-1.52855	0.31670	-0.85203
	C	0.37446	2.60944	0.37245
	C	0.84063	1.83269	-0.58031
	O	-0.05022	3.29001	1.21189
	H	0.82481	2.24032	-1.58532
	C	-1.62347	-1.48386	0.66696

	C	-3.01387	-1.42067	0.61537
	C	-3.65708	-0.47607	-0.18296
	C	-2.89408	0.42686	-0.93634
	H	-1.14761	-2.20850	1.31904
	H	-3.60002	-2.10929	1.21321
	H	-4.74049	-0.43184	-0.21728
	H	-3.37242	1.17492	-1.55966
Phenanthrene III (**TS 2-3**)	C	3.57390	0.06198	-0.20482
	C	3.23910	-1.21981	0.24756
	C	1.91050	-1.59936	0.39243
	C	0.89940	-0.68429	0.07288
	C	1.24666	0.60823	-0.37465
	C	2.57713	0.98791	-0.50888
	H	4.61604	0.33756	-0.31742
	H	4.02749	-1.92419	0.48756
	H	1.66164	-2.59316	0.74696
	H	2.83723	1.98335	-0.85123
	C	-0.54239	-0.82210	0.10724
	C	-1.15147	0.46622	-0.20450
	C	-0.66683	1.84678	0.54458
	C	0.03572	1.45816	-0.65148
	O	-1.10418	2.74061	1.19757
	H	0.00833	2.07701	-1.55210
	C	-1.34564	-1.93466	0.28795
	C	-2.72427	-1.84733	0.06352
	C	-3.29742	-0.64434	-0.40222
	C	-2.54086	0.49080	-0.58302
	H	-0.90184	-2.88757	0.55615
	H	-3.34848	-2.72265	0.19462
	H	-4.35551	-0.61870	-0.63841
	H	-2.99259	1.41414	-0.92624
Phenanthrene III (**TS 8-3**)	C	-3.28715	-1.12044	0.03167
	C	-2.48693	-2.23677	-0.20163
	C	-1.10133	-2.11840	-0.19265
	C	-0.48802	-0.88351	0.04697
	C	-1.30362	0.24015	0.29887
	C	-2.69256	0.11333	0.28565
	H	-4.36731	-1.20884	0.02232
	H	-2.94314	-3.20106	-0.39537
	H	-0.49249	-2.99305	-0.38843
	H	-3.30825	0.98308	0.48587
	C	0.96718	-0.65214	0.02944
	C	1.39443	0.65369	0.22464
	C	-0.95464	2.64143	-0.10845
	C	-0.62942	1.54895	0.59531
	O	-1.06383	3.57977	-0.78758
	H	-0.31970	1.76416	1.61553
	C	1.95511	-1.63047	-0.17657

	C	3.29999	-1.26996	-0.18773
	C	3.68721	0.05726	0.00777
	C	2.71590	1.04300	0.22416
	H	1.68188	-2.66982	-0.32539
	H	4.05517	-2.03086	-0.34998
	H	4.73900	0.32436	-0.00807
	H	3.00855	2.07713	0.37947
Phenanthrene III (**TS 3-4**)	C	3.55189	0.09731	-0.15147
	C	3.27411	-1.21070	0.25260
	C	1.95717	-1.66368	0.35512
	C	0.92046	-0.78835	0.04852
	C	1.20284	0.53654	-0.35806
	C	2.51602	0.98179	-0.45749
	H	4.58145	0.42834	-0.22581
	H	4.09176	-1.88291	0.48730
	H	1.75376	-2.68323	0.66380
	H	2.73609	1.99954	-0.76116
	C	-0.53714	-0.97029	0.03136
	C	-1.12886	0.24690	-0.38863
	C	-0.33426	2.57751	0.77891
	C	-0.06752	1.25219	-0.58899
	O	-1.29522	3.21311	0.75370
	H	-0.14409	1.96817	-1.40288
	C	-1.33425	-2.07525	0.30911
	C	-2.71930	-1.96136	0.16871
	C	-3.30172	-0.76030	-0.24534
	C	-2.51066	0.35456	-0.52391
	H	-0.89373	-3.01509	0.62335
	H	-3.35121	-2.81621	0.38173
	H	-4.37873	-0.69431	-0.34857
	H	-2.96613	1.28961	-0.82997
Benzoperylene				
Species Name (Stationary point)	Geometry (Å)			
Benzoperylene (**1**)	C	2.76367	-0.89524	0.00052
	C	3.12975	-2.25264	0.00027
	C	2.15562	-3.23792	-0.00038
	C	1.38201	-0.54037	0.00013
	C	0.37296	-1.56090	-0.00032
	C	0.80481	-2.90827	-0.00068
	C	1.02491	0.83857	-0.00005
	C	-0.34612	1.21234	-0.00030
	C	-1.36451	0.20341	-0.00007
	C	-1.02091	-1.17812	-0.00024
	C	-2.12365	-2.17865	-0.00026
	C	-3.49303	-1.67257	0.00122
	C	-3.77723	-0.35290	0.00133
	C	-2.73226	0.62654	0.00045

	H	-4.26418	-2.43331	0.00188
	H	-4.80587	-0.00583	0.00217
	C	2.03513	1.84379	0.00014
	C	-3.04581	1.99927	0.00016
	C	-2.06165	2.95991	-0.00046
	C	-0.69450	2.59176	-0.00061
	H	-2.32221	4.01273	-0.00066
	H	-4.09056	2.29118	0.00052
	C	1.65440	3.21012	-0.00047
	C	0.33509	3.57160	-0.00086
	C	3.75283	0.13530	0.00099
	C	3.40365	1.45288	0.00079
	H	4.79794	-0.15538	0.00155
	H	4.16563	2.22473	0.00117
	H	2.43086	3.96737	-0.00077
	H	0.05363	4.61919	-0.00144
	H	0.05792	-3.68470	-0.00109
	H	2.44335	-4.28317	-0.00063
	H	4.18221	-2.51592	0.00038
	O	-1.94747	-3.40554	-0.00137
Benzoperylene (**2**)	C	2.82483	-0.27960	-0.11954
	C	3.48398	-1.50890	-0.33955
	C	2.76261	-2.67104	-0.50964
	C	1.40201	-0.25242	-0.06828
	C	0.67168	-1.47398	-0.22156
	C	1.35938	-2.65456	-0.44557
	C	0.74451	1.01533	0.10201
	C	-0.68206	1.08772	0.04616
	C	-1.41475	-0.08167	-0.08533
	C	-0.80392	-1.41495	-0.02820
	C	-1.47009	-2.42798	0.86571
	C	-2.05102	-2.37613	-0.48879
	C	-3.18326	-1.42195	-0.65856
	C	-2.79162	-0.10401	-0.38526
	H	-1.95316	-3.25610	-1.12199
	H	-4.17930	-1.76153	-0.90696
	C	1.47885	2.20953	0.21809
	C	-3.48613	1.14781	-0.39085
	C	-2.79056	2.31157	-0.17023
	C	-1.37321	2.33068	0.02853
	H	-3.31996	3.25879	-0.17496
	H	-4.55310	1.17713	-0.58035
	C	0.77038	3.44906	0.28701
	C	-0.59818	3.51085	0.18068
	C	3.54744	0.94607	0.04711
	C	2.90670	2.13754	0.21366
	H	4.63148	0.90767	0.02808
	H	3.47662	3.05405	0.32462

	H	1.34386	4.36379	0.39367
	H	-1.09902	4.47323	0.19784
	H	0.81303	-3.58404	-0.56380
	H	3.27616	-3.60916	-0.68609
	H	4.56789	-1.52527	-0.37684
	O	-1.35623	-3.04656	1.87514
Benzoperylene (**3**)	C	1.87454	-2.15467	-0.03873
	C	1.44019	-3.48536	-0.13200
	C	0.08680	-3.78206	-0.25926
	C	0.90948	-1.10677	-0.07539
	C	-0.49110	-1.42180	-0.20790
	C	-0.86879	-2.77165	-0.29891
	C	1.36481	0.24413	0.01766
	C	0.42867	1.29870	-0.02117
	C	-0.93164	0.96389	-0.14602
	C	-1.40396	-0.31765	-0.24329
	C	-3.58879	-0.89284	0.84236
	C	-2.91253	-0.20764	-0.37656
	C	-3.17001	1.28907	-0.37306
	C	-1.99033	1.95330	-0.22112
	H	-3.30401	-0.70169	-1.27424
	H	-4.16163	1.71096	-0.45526
	C	2.74549	0.56563	0.14239
	C	-1.58521	3.34137	-0.14134
	C	-0.26656	3.65398	-0.01120
	C	0.79618	2.65681	0.05167
	H	0.02615	4.69763	0.04882
	H	-2.33021	4.12764	-0.18456
	C	3.10946	1.92545	0.22056
	C	2.16580	2.94665	0.17575
	C	3.26521	-1.80857	0.09202
	C	3.68472	-0.51627	0.17850
	H	3.98871	-2.61672	0.11973
	H	4.74122	-0.28932	0.27547
	H	4.16041	2.17738	0.31684
	H	2.49305	3.97944	0.23599
	H	-1.91763	-3.02827	-0.39005
	H	-0.23042	-4.81648	-0.32849
	H	2.17215	-4.28536	-0.10413
	O	-4.20155	-1.89968	0.83626
Benzoperylene (**4**)	C	-2.70617	0.24119	-0.00002
	C	-3.69052	-0.77203	0.00000
	C	-3.33059	-2.11411	0.00001
	C	-1.33278	-0.12712	-0.00004
	C	-0.96146	-1.52738	-0.00006
	C	-1.99043	-2.49117	-0.00001
	C	-0.35212	0.91099	-0.00003
	C	1.02245	0.56534	-0.00003

	C	1.35615	-0.77998	-0.00006
	C	0.42658	-1.84604	-0.00006
	C	1.22591	-3.06529	0.00021
	C	2.55628	-2.72601	-0.00005
	C	2.67695	-1.26150	-0.00005
	H	0.83936	-4.07475	0.00041
	H	3.38344	-3.42279	-0.00011
	C	-0.70812	2.28015	0.00001
	C	3.70857	-0.31785	-0.00001
	C	3.39837	1.05158	0.00002
	C	2.06421	1.52985	0.00001
	H	4.20945	1.77244	0.00004
	H	4.74995	-0.62263	-0.00001
	C	0.34001	3.25636	0.00004
	C	1.66632	2.90437	0.00003
	C	-3.04828	1.63059	0.00001
	C	-2.09198	2.61126	0.00002
	H	-4.09943	1.89964	0.00002
	H	-2.38511	3.65599	0.00004
	H	0.06312	4.30544	0.00006
	H	2.42906	3.67629	0.00006
	H	-1.72698	-3.54257	-0.00000
	H	-4.10112	-2.87670	0.00003
	H	-4.73784	-0.48950	0.00003
Benzoperylene (**5**)	C	2.76962	-1.66925	-0.00000
	C	2.74862	-3.07253	-0.00001
	C	1.54333	-3.76940	-0.00001
	C	1.53451	-0.95826	0.00000
	C	0.30004	-1.68898	0.00001
	C	0.32857	-3.09476	0.00000
	C	1.51408	0.46729	0.00000
	C	0.28191	1.18213	0.00001
	C	-0.98220	0.45166	0.00001
	C	-0.86224	-0.90029	0.00002
	C	-5.02892	-1.25943	-0.00001
	C	-3.80174	-0.76152	0.00010
	C	-3.49595	0.64084	0.00004
	C	-2.24695	1.20626	0.00001
	H	-3.00057	-1.49875	0.00025
	H	-4.34135	1.32126	0.00003
	C	2.75009	1.18369	-0.00001
	C	-2.14835	2.65091	-0.00001
	C	-0.96742	3.30562	-0.00001
	C	0.29111	2.59567	-0.00000
	H	-0.94327	4.38997	-0.00002
	H	-3.07684	3.21247	-0.00001
	C	2.72227	2.58799	-0.00001
	C	1.52256	3.27444	-0.00001

	C	3.99027	-0.91474	-0.00001
	C	3.97724	0.44492	-0.00001
	H	4.93082	-1.45541	-0.00001
	H	4.90950	1.00015	-0.00001
	H	3.66004	3.13346	-0.00002
	H	1.51977	4.35944	-0.00002
	H	-0.60541	-3.64382	0.00000
	H	1.55193	-4.85359	-0.00001
	H	3.68850	-3.61386	-0.00001
	O	-6.09198	-1.72060	-0.00011
Benzoperylene (**TS 1-2**)	C	2.82316	-0.31353	-0.13598
	C	3.46052	-1.55660	-0.33776
	C	2.71903	-2.71205	-0.46583
	C	1.40140	-0.26306	-0.06866
	C	0.65049	-1.47451	-0.18479
	C	1.31854	-2.67248	-0.38146
	C	0.76345	1.01313	0.10001
	C	-0.66316	1.10243	0.06802
	C	-1.42209	-0.05872	-0.04921
	C	-0.82034	-1.39382	0.01359
	C	-1.50865	-2.44604	0.80017
	C	-2.20281	-2.34994	-0.49028
	C	-3.24236	-1.32333	-0.66058
	C	-2.80092	-0.03303	-0.34508
	H	-2.17767	-3.23585	-1.12246
	H	-4.23731	-1.58810	-0.99361
	C	1.51931	2.19626	0.19755
	C	-3.46836	1.23140	-0.34002
	C	-2.74908	2.37841	-0.12032
	C	-1.32990	2.35991	0.05955
	H	-3.25479	3.33826	-0.11764
	H	-4.53562	1.28060	-0.52430
	C	0.83415	3.44671	0.27620
	C	-0.53420	3.52810	0.19590
	C	3.56677	0.90266	0.00358
	C	2.94563	2.10421	0.16854
	H	4.64970	0.84779	-0.03099
	H	3.52935	3.01392	0.26203
	H	1.42399	4.35243	0.36982
	H	-1.02169	4.49707	0.21993
	H	0.75683	-3.59625	-0.46134
	H	3.21574	-3.66249	-0.62340
	H	4.54341	-1.59038	-0.38973
	O	-1.30693	-3.20671	1.69910
Benzoperylene (**TS 1-5**)	C	2.64278	-1.55758	-0.01786
	C	2.65366	-2.95745	-0.10488
	C	1.46866	-3.67610	-0.24588
	C	1.39474	-0.87249	-0.07669

	C	0.18143	-1.62135	-0.22456
	C	0.24348	-3.02356	-0.30651
	C	1.34437	0.54864	0.01296
	C	0.09955	1.23483	-0.04439
	C	-1.13282	0.47874	-0.19454
	C	-1.00985	-0.87008	-0.27683
	C	-3.97235	-1.67304	0.44307
	C	-3.80510	-0.88199	-0.59672
	C	-3.61634	0.57956	-0.44561
	C	-2.42010	1.19793	-0.26334
	H	-3.89953	-1.34681	-1.57549
	H	-4.50496	1.20191	-0.51864
	C	2.55699	1.28869	0.16168
	C	-2.36806	2.64823	-0.15515
	C	-1.20836	3.32082	-0.00999
	C	0.07085	2.64397	0.04950
	H	-1.21361	4.40344	0.06496
	H	-3.30908	3.18597	-0.19784
	C	2.49253	2.68859	0.25125
	C	1.27659	3.34817	0.19686
	C	3.84209	-0.78221	0.12989
	C	3.79857	0.57399	0.21537
	H	4.79192	-1.30466	0.17358
	H	4.71462	1.14441	0.32787
	H	3.41185	3.25302	0.36463
	H	1.24571	4.43054	0.26748
	H	-0.67658	-3.58501	-0.41441
	H	1.50296	-4.75787	-0.30857
	H	3.60264	-3.48110	-0.05958
	O	-4.10823	-2.37022	1.36127
Benzoperylene (**TS 2-3**)	C	2.77690	-0.62460	-0.07000
	C	3.26653	-1.93575	-0.23081
	C	2.39588	-2.99515	-0.41573
	C	1.37036	-0.40065	-0.09261
	C	0.47595	-1.51442	-0.26708
	C	1.01221	-2.79046	-0.43424
	C	0.88916	0.94452	0.03360
	C	-0.50618	1.20538	-0.03792
	C	-1.36978	0.12703	-0.20628
	C	-0.94739	-1.21871	-0.22568
	C	-1.95750	-2.37858	0.81150
	C	-2.21047	-2.06285	-0.55932
	C	-3.31257	-1.01371	-0.53404
	C	-2.77749	0.25558	-0.36050
	H	-2.21675	-2.83823	-1.33823
	H	-4.35454	-1.29503	-0.58142
	C	1.77203	2.03694	0.19133
	C	-3.31974	1.58396	-0.27614

	C	-2.47736	2.65092	-0.09314
	C	-1.04835	2.51192	0.02394
	H	-2.89517	3.65115	-0.03857
	H	-4.38800	1.74399	-0.36677
	C	1.22232	3.34600	0.27779
	C	-0.13606	3.58004	0.19340
	C	3.65213	0.49825	0.10929
	C	3.17638	1.76913	0.23802
	H	4.72074	0.31241	0.13577
	H	3.86354	2.59884	0.36735
	H	1.90164	4.18259	0.40382
	H	-0.51101	4.59664	0.25261
	H	0.35123	-3.63962	-0.56936
	H	2.78633	-3.99817	-0.54541
	H	4.33767	-2.10523	-0.21206
	O	-1.90969	-3.08226	1.75500
Benzoperylene (**TS 5-3**)	C	2.33831	-1.87771	-0.01142
	C	2.13235	-3.26356	-0.07989
	C	0.84714	-3.78937	-0.18559
	C	1.21013	-1.00824	-0.05730
	C	-0.11491	-1.55712	-0.16931
	C	-0.26326	-2.95413	-0.22728
	C	1.40440	0.40262	0.01563
	C	0.28891	1.27487	-0.02691
	C	-1.02252	0.71200	-0.15112
	C	-1.19559	-0.63606	-0.20408
	C	-4.16296	-1.31266	0.27228
	C	-3.35172	-0.54188	-0.48965
	C	-3.39123	0.94087	-0.32552
	C	-2.19882	1.57751	-0.20355
	H	-3.20805	-0.95035	-1.49223
	H	-4.33991	1.46249	-0.32112
	C	2.71553	0.95082	0.13338
	C	-1.98223	3.00729	-0.11317
	C	-0.73093	3.51339	0.00445
	C	0.45419	2.67446	0.04830
	H	-0.58947	4.58773	0.06883
	H	-2.84095	3.66910	-0.14529
	C	2.85860	2.34856	0.20558
	C	1.75615	3.18955	0.16513
	C	3.64822	-1.29795	0.10603
	C	3.82874	0.04879	0.17518
	H	4.50276	-1.96576	0.14114
	H	4.82771	0.46275	0.26472
	H	3.85415	2.77000	0.29616
	H	1.89724	4.26384	0.22614
	H	-1.26011	-3.37331	-0.29973
	H	0.71070	-4.86402	-0.23193

	H	2.98946	-3.92774	-0.04598
	O	-4.61932	-2.06838	1.03154
Benzoperylene (**TS 2-4**)	C	2.79599	0.11340	-0.17017
	C	3.62289	-0.99468	-0.46584
	C	3.07748	-2.24081	-0.68351
	C	1.38859	-0.07525	-0.08621
	C	0.84569	-1.38470	-0.28353
	C	1.68804	-2.43763	-0.58391
	C	0.55309	1.07780	0.13480
	C	-0.86764	0.94377	0.07815
	C	-1.42147	-0.32200	-0.06824
	C	-0.61261	-1.56415	0.01997
	C	-0.99792	-2.32886	1.22561
	C	-1.71458	-2.62421	-0.39147
	C	-2.89724	-1.94562	-0.72219
	C	-2.74126	-0.54618	-0.46068
	H	-1.49531	-3.66012	-0.61175
	H	-3.81116	-2.43721	-1.02554
	C	1.10374	2.36513	0.25676
	C	-3.61048	0.57991	-0.52594
	C	-3.11151	1.83779	-0.26181
	C	-1.72992	2.06730	0.01379
	H	-3.77687	2.69406	-0.30267
	H	-4.65552	0.45291	-0.78484
	C	0.21872	3.48907	0.32281
	C	-1.13793	3.35331	0.18199
	C	3.33308	1.42608	0.02960
	C	2.52621	2.50541	0.23820
	H	4.41024	1.55011	-0.00733
	H	2.95636	3.49354	0.36315
	H	0.65190	4.47686	0.44010
	H	-1.77391	4.23237	0.18026
	H	1.27796	-3.43055	-0.73209
	H	3.71925	-3.08127	-0.92163
	H	4.69588	-0.84765	-0.52707
	O	-0.50806	-2.90153	2.14255
Benzoperylene (**TS 3-4**)	C	2.75417	-0.88955	-0.02289
	C	3.12149	-2.23967	-0.13192
	C	2.15762	-3.22304	-0.33526
	C	1.37751	-0.53521	-0.12352
	C	0.38386	-1.55942	-0.33848
	C	0.80995	-2.89477	-0.43860
	C	1.01669	0.84166	-0.00539
	C	-0.34115	1.21607	-0.10090
	C	-1.28650	0.20201	-0.30973
	C	-0.97776	-1.13230	-0.43746
	C	-2.48201	-2.61690	1.00850
	C	-2.29656	-1.83039	-0.61055

	C	-3.31171	-0.77283	-0.68694
	C	-2.70406	0.44755	-0.45027
	H	-2.36951	-2.69496	-1.26069
	H	-4.36426	-0.96165	-0.84107
	C	1.98909	1.85982	0.20150
	C	-3.12902	1.81613	-0.35266
	C	-2.20386	2.80443	-0.14232
	C	-0.77974	2.55335	-0.01027
	H	-2.54014	3.83411	-0.07032
	H	-4.17883	2.07057	-0.44678
	C	1.54709	3.19701	0.29892
	C	0.20413	3.53943	0.19530
	C	3.72128	0.15403	0.18912
	C	3.36202	1.46378	0.29590
	H	4.76605	-0.12940	0.26323
	H	4.11740	2.22633	0.45455
	H	2.28413	3.97734	0.45728
	H	-0.08897	4.58141	0.27265
	H	0.07582	-3.67753	-0.59284
	H	2.46104	-4.26098	-0.41467
	H	4.16848	-2.51254	-0.05496
	O	-2.74080	-2.10747	2.01016
Extended-armchair				
Species Name (Stationary point)	Geometry (Å)			
Extended-armchair (**1**)	C	4.987451	-0.393435	0.000017
	C	5.739360	-1.572434	0.000178
	C	5.103361	-2.807907	0.000346
	C	3.560589	-0.467210	-0.000001
	C	2.905198	-1.740079	0.000090
	C	3.719835	-2.897814	0.000308
	C	2.800715	0.735905	-0.000088
	C	1.383994	0.684391	-0.000062
	C	0.706388	-0.588847	-0.000029
	C	1.459857	-1.787929	0.000012
	C	0.718336	-3.070978	0.000004
	C	-0.721455	-3.012635	0.000117
	C	-1.449687	-1.850649	-0.000029
	C	-0.734909	-0.600928	-0.000039
	H	-1.188414	-3.987615	0.000226
	C	3.470526	2.004033	-0.000173
	C	-1.466279	0.621918	0.000015
	C	-0.779219	1.866101	-0.000001
	C	0.644440	1.894062	-0.000068
	C	2.719130	3.177243	-0.000196
	C	1.324386	3.151986	-0.000128
	C	5.626537	0.891221	-0.000113
	C	4.903357	2.037533	-0.000207

	H	6.710884	0.923247	-0.000129
	H	5.396140	3.003737	-0.000299
	H	3.231509	4.133968	-0.000252
	H	3.241138	-3.862237	0.000409
	H	5.691682	-3.718579	0.000510
	H	6.822434	-1.509523	0.000192
	O	1.256086	-4.194512	-0.000131
	C	-1.513599	3.090353	0.000065
	C	-2.907229	3.051644	0.000184
	C	-3.612586	1.842529	0.000209
	C	-2.895757	0.612724	0.000100
	H	-3.461875	3.984694	0.000253
	C	-3.616245	-0.621481	0.000037
	C	-2.918759	-1.859025	-0.000115
	C	-3.662431	-3.042463	-0.000359
	C	-5.056595	-3.024809	-0.000350
	C	-5.744119	-1.823090	-0.000114
	C	-5.043897	-0.607365	0.000061
	H	-3.160363	-4.000218	-0.000587
	H	-5.600956	-3.962167	-0.000539
	H	-6.828583	-1.809255	-0.000089
	C	-5.731052	0.651191	0.000236
	C	-5.047039	1.822056	0.000309
	H	-6.815699	0.645559	0.000299
	H	-5.574545	2.769807	0.000435
	C	0.555982	4.362874	-0.000099
	C	-0.799912	4.334663	0.000006
	H	1.087706	5.308268	-0.000152
	H	-1.371796	5.256319	0.000040
Extended-armchair (**3**)	C	4.840907	-0.537922	-0.141634
	C	5.491164	-1.774500	-0.224925
	C	4.759078	-2.960766	-0.270945
	C	3.416697	-0.502986	-0.103106
	C	2.657147	-1.741886	-0.152566
	C	3.370813	-2.952243	-0.237297
	C	2.787317	0.778134	-0.022453
	C	1.391985	0.837408	0.010528
	C	0.693425	-0.376379	-0.030576
	C	1.226832	-1.632531	-0.117565
	C	0.093612	-3.580663	1.030644
	C	0.018852	-2.609949	-0.171083
	C	-1.208463	-1.671439	-0.119053
	C	-0.718770	-0.398369	-0.035461
	C	3.511248	2.014168	0.015083
	C	-1.455591	0.792299	0.011525
	C	-0.769678	2.024426	0.066432
	C	0.666359	2.047033	0.065300
	C	2.795837	3.218688	0.078491

	C 1.379310 3.268629 0.100823 C 5.564961 0.711840 -0.095525 C 4.946267 1.920855 -0.021804 H 6.648687 0.663364 -0.123823 H 5.533421 2.832721 0.008121 H 3.350719 4.151761 0.105983 H 2.826098 -3.888461 -0.263924 H 5.282314 -3.908302 -0.333467 H 6.575066 -1.804670 -0.253668 O 0.564964 -4.661384 1.034720 C -1.521673 3.222341 0.104597 C -2.936048 3.126688 0.086557 C -3.611854 1.899483 0.024342 C -2.847998 0.687905 -0.017645 H -3.520764 4.041274 0.116946 C -3.435045 -0.613207 -0.095070 C -2.633934 -1.825199 -0.147972 C -3.308244 -3.058232 -0.224369 C -4.695250 -3.115209 -0.250337 C -5.466368 -1.953603 -0.202355 C -4.857455 -0.695741 -0.125242 H -2.733255 -3.976922 -0.259642 H -5.187102 -4.079713 -0.308167 H -6.548759 -2.020571 -0.224308 C -5.622192 0.529596 -0.076078 C -5.043192 1.758426 -0.005863 H -6.703881 0.445637 -0.098487 H -5.660106 2.650343 0.026926 C 0.593681 4.475199 0.149436 C -0.775007 4.453439 0.151508 H 1.110910 5.428614 0.182307 H -1.322272 5.389889 0.185924 H 0.036834 -3.228275 -1.076526
Extended-armchair (**5**)	C -5.063482 0.720812 -0.033822 C -5.693815 1.969561 -0.038945 C -4.948606 3.150630 -0.054686 C -3.638446 0.664286 -0.049770 C -2.882488 1.881563 -0.069703 C -3.563135 3.115955 -0.067950 C -2.960181 -0.586792 -0.036977 C -1.541822 -0.645951 -0.051522 C -0.768928 0.580235 -0.098273 C -1.485236 1.738634 -0.089290 C 0.984156 4.019412 0.401814 C 0.808593 2.980470 -0.388650 C 1.476319 1.668756 -0.223621 C 0.696457 0.518970 -0.134151 H 0.111053 3.137515 -1.206581

	C	-3.723002	-1.801226	-0.002407
	C	1.326098	-0.774784	-0.050429
	C	0.545717	-1.961658	0.006488
	C	-0.886930	-1.898882	-0.009888
	C	-3.057613	-3.021064	0.029595
	C	-1.656058	-3.097100	0.034826
	C	-5.797075	-0.516643	-0.009285
	C	-5.158554	-1.713245	0.006093
	H	-6.881045	-0.471943	0.000130
	H	-5.726686	-2.637257	0.028352
	H	-3.633986	-3.940352	0.060456
	H	-2.988328	4.034282	-0.074391
	H	-5.461159	4.105961	-0.054200
	H	-6.777592	2.014019	-0.026941
	O	1.124310	4.944559	1.089073
	C	1.186828	-3.230346	0.085821
	C	2.587074	-3.296892	0.12912
	C	3.372600	-2.152678	0.088621
	C	2.740371	-0.868404	-0.011667
	H	3.066426	-4.268379	0.197307
	C	3.535955	0.308018	-0.075540
	C	2.914539	1.588088	-0.202952
	C	3.746459	2.721672	-0.322636
	C	5.126878	2.610149	-0.276124
	C	5.735353	1.366619	-0.124242
	C	4.961443	0.207027	-0.034010
	H	3.302883	3.696744	-0.468797
	H	5.737363	3.501376	-0.367803
	H	6.816510	1.287116	-0.089972
	C	5.562656	-1.093589	0.085921
	C	4.806872	-2.216631	0.141088
	H	6.645053	-1.155802	0.123465
	H	5.273988	-3.192220	0.224417
	C	-0.972716	-4.355404	0.095651
	C	0.383498	-4.417520	0.124341
	H	-1.565559	-5.263412	0.126166
	H	0.887912	-5.376400	0.178721
Extended-armchair (**4**)	C	-4.816710	-0.916697	0.000023
	C	-5.431851	-2.179630	0.000053
	C	-4.667825	-3.346191	0.000054
	C	-3.396837	-0.835385	-0.000007
	C	-2.594666	-2.057756	0.000004
	C	-3.279963	-3.290203	0.000027
	C	-2.817517	0.472067	-0.000030
	C	-1.422965	0.570620	-0.000062
	C	-0.693612	-0.609529	-0.000082
	C	-1.165780	-1.927736	-0.000027
	C	0.048007	-2.783563	-0.000005

	C	1.178015	-1.956495	-0.000049
	C	0.683703	-0.606525	-0.000077
	C	-3.572401	1.683686	-0.000006
	C	1.398640	0.570873	-0.000054
	C	0.691185	1.801739	-0.00003
	C	-0.731616	1.800693	-0.000050
	C	-2.888944	2.922978	-0.000005
	C	-1.482023	3.010249	-0.000016
	C	-5.579910	0.306741	0.000033
	C	-4.999790	1.542053	0.000021
	H	-6.661968	0.223141	0.000054
	H	-5.620039	2.432383	0.000033
	H	-3.473996	3.837485	0.000018
	H	-2.704273	-4.208921	0.000031
	H	-5.164050	-4.310074	0.000077
	H	-6.514987	-2.241835	0.000074
	C	1.430706	3.015178	0.000003
	C	2.834211	2.933452	0.000033
	C	3.539101	1.693793	0.000024
	C	2.804344	0.484260	-0.000016
	H	3.414535	3.851507	0.000064
	C	3.409975	-0.821902	-0.000014
	C	2.638786	-2.055052	-0.000040
	C	3.339490	-3.259240	-0.000019
	C	4.740781	-3.293760	0.000013
	C	5.478294	-2.125164	0.000032
	C	4.830129	-0.870562	0.000023
	H	2.785215	-4.191288	-0.000023
	H	5.248277	-4.251901	0.000027
	H	6.562428	-2.160856	0.000058
	C	5.571639	0.362716	0.000054
	C	4.968087	1.586530	0.000056
	H	6.654864	0.298191	0.000079
	H	5.568451	2.490267	0.000083
	C	-0.712340	4.232083	0.000011
	C	0.656500	4.234945	0.000021
	H	-1.244176	5.178156	0.000029
	H	1.185402	5.182688	0.000047
	H	0.043259	-3.864519	0.000034
Extended-armchair (**TS 1-3**)	C	4.827493	-0.534584	-0.259340
	C	5.494102	-1.759162	-0.430858
	C	4.783394	-2.949302	-0.479363
	C	3.408907	-0.525116	-0.131216
	C	2.677414	-1.774673	-0.172565
	C	3.393501	-2.959909	-0.348260
	C	2.762659	0.749392	0.002932
	C	1.359308	0.790588	0.074831
	C	0.666793	-0.414927	0.040761

	C	1.228943	-1.705136	0.020748
	C	0.507151	-2.958270	1.113022
	C	-0.026607	-2.696936	-0.201925
	C	-1.219714	-1.729674	-0.146213
	C	-0.723903	-0.448724	-0.027313
	C	3.468690	1.985972	0.010695
	C	-1.477292	0.734292	0.025176
	C	-0.803407	1.970329	0.098456
	C	0.626332	2.001587	0.110113
	C	2.742390	3.193720	0.089231
	C	1.332672	3.230977	0.129333
	C	5.535271	0.720585	-0.217939
	C	4.900402	1.917485	-0.088431
	H	6.616682	0.690366	-0.302183
	H	5.473026	2.838875	-0.070957
	H	3.292816	4.129515	0.098535
	H	2.864902	-3.906151	-0.368431
	H	5.311010	-3.886474	-0.615073
	H	6.574518	-1.765149	-0.526873
	O	0.850209	-3.791489	1.882184
	C	-1.569167	3.165874	0.120324
	C	-2.975783	3.059402	0.077972
	C	-3.642357	1.822680	-0.000155
	C	-2.869380	0.619676	-0.034032
	H	-3.570026	3.968176	0.097183
	C	-3.449398	-0.685228	-0.133592
	C	-2.641478	-1.892980	-0.184901
	C	-3.304595	-3.129940	-0.286112
	C	-4.692049	-3.195188	-0.336085
	C	-5.469851	-2.040297	-0.291789
	C	-4.868915	-0.776409	-0.192441
	H	-2.721303	-4.043411	-0.318251
	H	-5.176521	-4.162333	-0.410609
	H	-6.551243	-2.112462	-0.333800
	C	-5.641583	0.441653	-0.148580
	C	-5.069761	1.674026	-0.058641
	H	-6.722108	0.352161	-0.192965
	H	-5.692327	2.562254	-0.032172
	C	0.536377	4.433123	0.169989
	C	-0.830861	4.402802	0.168069
	H	1.047884	5.389839	0.197091
	H	-1.384973	5.335535	0.194066
	H	-0.018197	-3.485077	-0.96443
Extended-armchair (**TS 3-4**)	C	4.825630	-0.500994	-0.221542
	C	5.488858	-1.729091	-0.338216
	C	4.768314	-2.919771	-0.400991
	C	3.401644	-0.481868	-0.165359
	C	2.652573	-1.727391	-0.236239

	C 3.378600 -2.924641 -0.354416
	C 2.763918 0.793235 -0.044801
	C 1.366608 0.839370 0.011385
	C 0.681584 -0.373886 -0.047046
	C 1.216145 -1.637996 -0.182783
	C 0.138215 -3.570105 1.418724
	C 0.039517 -2.567763 -0.217146
	C -1.193267 -1.695116 -0.177364
	C -0.727968 -0.410000 -0.047767
	C 3.475335 2.034523 0.006365
	C -1.476879 0.766080 0.022402
	C -0.805034 2.005624 0.098543
	C 0.629226 2.042561 0.092024
	C 2.748461 3.232085 0.099805
	C 1.330746 3.269698 0.137852
	C 5.538449 0.754202 -0.157947
	C 4.910348 1.956171 -0.051675
	H 6.622139 0.716271 -0.201173
	H 5.489857 2.872552 -0.011344
	H 3.295605 4.169471 0.135874
	H 2.844733 -3.866211 -0.396788
	H 5.299506 -3.860959 -0.488989
	H 6.572602 -1.746850 -0.379785
	O 0.998750 -4.317348 1.579154
	C -1.570614 3.193804 0.151983
	C -2.985198 3.081292 0.127690
	C -3.646189 1.847120 0.039374
	C -2.868464 0.645069 -0.020985
	H -3.580994 3.988188 0.170631
	C -3.435908 -0.662020 -0.135983
	C -2.618300 -1.863686 -0.215584
	C -3.278735 -3.101096 -0.325367
	C -4.665004 -3.174156 -0.360155
	C -5.450860 -2.023515 -0.289160
	C -4.857242 -0.761012 -0.177919
	H -2.691956 -4.011119 -0.381078
	H -5.145031 -4.142828 -0.444125
	H -6.532222 -2.102853 -0.319907
	C -5.637457 0.453734 -0.105455
	C -5.075465 1.688400 -0.004085
	H -6.717858 0.356530 -0.137395
	H -5.704604 2.571119 0.043322
	C 0.533217 4.466815 0.208253
	C -0.836337 4.431006 0.215199
	H 1.040151 5.425362 0.252005
	H -1.392164 5.361808 0.264163
	H 0.059432 -3.451780 -0.848331
Extended-armchair	C 5.038902 -0.514976 -0.156469

(**TS 1-5**)	C	5.726514	-1.731152	-0.219044
	C	5.037520	-2.945910	-0.250745
	C	3.612835	-0.526559	-0.129560
	C	2.915327	-1.776793	-0.167520
	C	3.652462	-2.977223	-0.224397
	C	2.875407	0.687917	-0.058413
	C	1.455145	0.678003	-0.032598
	C	0.741189	-0.583927	-0.077734
	C	1.513569	-1.702370	-0.138707
	C	-0.166740	-3.719026	0.690721
	C	-0.820463	-3.106316	-0.275627
	C	-1.467995	-1.773388	-0.146424
	C	-0.730158	-0.596682	-0.061392
	H	-0.971445	-3.698674	-1.174188
	C	3.581214	1.936145	-0.008634
	C	-1.417371	0.673261	0.003173
	C	-0.690049	1.894165	0.065585
	C	0.744227	1.897940	0.047476
	C	2.860682	3.121178	0.071602
	C	1.457371	3.129957	0.101853
	C	5.713533	0.754908	-0.113181
	C	5.019198	1.917746	-0.041604
	H	6.798222	0.762687	-0.136043
	H	5.542781	2.867330	-0.006094
	H	3.393286	4.066112	0.111554
	H	3.120799	-3.920659	-0.241466
	H	5.594311	-3.875115	-0.294627
	H	6.811097	-1.723787	-0.239499
	O	0.415092	-4.280749	1.521012
	C	-1.386558	3.134553	0.133632
	C	-2.788591	3.144216	0.128763
	C	-3.524161	1.970315	0.047664
	C	-2.835645	0.712859	-0.017650
	H	-3.308924	4.095402	0.181470
	C	-3.583861	-0.491688	-0.111174
	C	-2.907219	-1.745443	-0.172875
	C	-3.683388	-2.921217	-0.246068
	C	-5.067912	-2.866611	-0.277293
	C	-5.732714	-1.643462	-0.226220
	C	-5.012400	-0.449348	-0.137385
	H	-3.187207	-3.882228	-0.262498
	H	-5.638080	-3.787101	-0.334581
	H	-6.816587	-1.608696	-0.247325
	C	-5.669528	0.827409	-0.067732
	C	-4.960692	1.978489	0.022033
	H	-6.753982	0.848033	-0.087596
	H	-5.468244	2.935869	0.074622
	C	0.718870	4.355143	0.182366

	C -0.638578 4.355972 0.197641 H 1.270513 5.288089 0.228457 H -1.186930 5.290226 0.255334
Extended-armchair (**TS 5-3**)	C 4.970519 -0.644452 -0.098999 C 5.609749 -1.887057 -0.163883 C 4.870415 -3.069578 -0.233812 C 3.545255 -0.596389 -0.107132 C 2.785429 -1.819951 -0.183823 C 3.484084 -3.042620 -0.243978 C 2.887728 0.665681 -0.037007 C 1.479530 0.722180 -0.039662 C 0.743005 -0.499775 -0.117233 C 1.372281 -1.704364 -0.190687 C -0.558525 -3.870410 0.630562 C -0.453063 -2.872293 -0.285226 C -1.364484 -1.673969 -0.180546 C -0.699085 -0.469701 -0.118037 H -0.237645 -3.252883 -1.284161 C 3.633880 1.888152 0.038549 C -1.379035 0.779337 -0.046773 C -0.638591 1.985234 0.027404 C 0.795979 1.957495 0.029301 C 2.948252 3.100907 0.106637 C 1.540236 3.164921 0.104084 C 5.700034 0.596411 -0.023107 C 5.069414 1.797308 0.041801 H 6.784165 0.549777 -0.018465 H 5.645339 2.715071 0.098643 H 3.515170 4.024968 0.165018 H 2.919418 -3.966474 -0.292418 H 5.388189 -4.021107 -0.279560 H 6.693875 -1.925999 -0.157395 O -0.340161 -4.625503 1.489447 C -1.328545 3.223968 0.103532 C -2.737323 3.221926 0.106574 C -3.477823 2.042749 0.038664 C -2.787807 0.787834 -0.039583 H -3.262562 4.170385 0.165469 C -3.498708 -0.444459 -0.110407 C -2.799149 -1.699198 -0.187908 C -3.561779 -2.881031 -0.278819 C -4.948169 -2.840632 -0.276496 C -5.629871 -1.628001 -0.188441 C -4.926104 -0.422255 -0.108260 H -3.054530 -3.834735 -0.353831 H -5.508169 -3.766428 -0.346942 H -6.714353 -1.611365 -0.186699 C -5.598250 0.849593 -0.026784

	C -4.914916 2.020144 0.043204 H -6.683219 0.850623 -0.023814 H -5.447678 2.963363 0.103335 C 0.812428 4.400888 0.176861 C -0.549886 4.428681 0.177046 H 1.373701 5.327709 0.234450 H -1.073046 5.377460 0.235119

Appendix B

Details of Singlet OH Oxidation of Soot

Table B.1. High-pressure rate coefficients (in s^{-1}) of the elementary reactions in the OH + phenanthrene radical reaction system.

Reaction	1500 K	2000 K	2500 K
$k_{2\to1}$	9.6E+00	7.0E+04	1.3E+07
$k_{2\to18}$	7.0E-03	1.2E+02	4.2E+04
$k_{2\to22}$	5.4E-02	3.6E+02	7.5E+04
$k_{2\to23}$	9.2E+00	1.2E+04	9.3E+05
$k_{2\to3}$	2.9E-01	8.3E+02	9.9E+04
$k_{2\to5}$	8.5E+06	2.1E+08	1.5E+09
$k_{2\to7}$	2.2E+04	3.4E+06	7.2E+07
$k_{2\to4}$	1.2E+03	1.4E+06	9.5E+07
$k_{5\to2}$	1.4E+12	2.2E+12	2.9E+12
$k_{5\to24}$	7.6E+02	1.9E+06	2.1E+08
$k_{5\to25}$	8.9E+01	1.6E+05	1.5E+07
$k_{5\to6}$	1.3E+09	1.7E+10	8.1E+10
$k_{6\to5}$	1.3E+11	4.6E+11	9.9E+11
$k_{6\to27}$	1.3E+04	1.2E+07	7.1E+08
$k_{6\to28}$	6.1E+07	1.8E+09	1.3E+10
$k_{7\to2}$	9.7E+04	7.6E+06	1.1E+08
$k_{7\to13}$	3.1E+05	1.9E+07	2.3E+08
$k_{7\to19}$	5.1E+01	1.3E+05	1.5E+07
$k_{7\to8}$	8.0E+05	4.2E+07	4.5E+08

$k_{7\rightarrow4}$	8.6E+03	5.1E+06	2.2E+08
$k_{8\rightarrow7}$	1.7E+12	2.7E+12	3.5E+12
$k_{8\rightarrow12}$	1.8E+06	3.0E+08	6.5E+09
$k_{8\rightarrow9}$	3.3E+10	1.2E+11	2.6E+11
$k_{9\rightarrow12}$	1.4E+07	1.2E+09	1.8E+10
$k_{9\rightarrow8}$	1.5E+12	2.2E+12	2.8E+12
$k_{9\rightarrow10}$	1.2E+11	5.1E+11	1.2E+12
$k_{10\rightarrow11}$	8.6E+11	3.6E+12	8.6E+12
$k_{10\rightarrow9}$	1.2E+09	2.5E+10	1.6E+11
$k_{12\rightarrow9}$	1.7E+11	3.2E+11	4.8E+11
$k_{12\rightarrow8}$	9.1E+11	1.4E+12	1.9E+12
$k_{13\rightarrow14}$	9.6E+10	3.9E+11	9.2E+11
$k_{13\rightarrow7}$	5.8E+08	7.2E+09	3.3E+10
$k_{14\rightarrow13}$	3.0E+09	8.2E+09	1.5E+10
$k_{14\rightarrow15}$	1.0E+12	1.4E+12	1.7E+12
$k_{15\rightarrow14}$	5.5E+11	9.7E+11	1.4E+12
$k_{15\rightarrow16}$	2.6E+03	3.7E+05	7.3E+06
$k_{16\rightarrow15}$	4.2E+10	2.9E+11	9.1E+11
$k_{16\rightarrow17}$	5.1E+08	9.8E+09	5.8E+10
$k_{24\rightarrow5}$	1.2E+06	9.8E+07	1.4E+09
$k_{25\rightarrow26}$	2.1E+10	1.4E+11	4.5E+11
$k_{25\rightarrow5}$	3.6E+07	1.3E+09	1.2E+10
$k_{27\rightarrow29}$	5.6E+10	1.9E+11	4.0E+11
$k_{6\rightarrow27}$	3.3E+11	8.5E+11	1.5E+12
$k_{28\rightarrow29}$	3.2E+11	1.0E+12	2.1E+12
$k_{6\rightarrow28}$	3.4E+12	4.2E+12	4.7E+12
$k_{20\rightarrow19}$	7.2E+03	1.7E+06	4.4E+07
$k_{20\rightarrow21}$	1.9E+06	1.1E+09	4.4E+10
$k_{19\rightarrow20}$	4.1E+12	5.5E+12	6.5E+12

$k_{4\rightarrow30}$	4.0E+05	4.5E+07	7.7E+08
$k_{4\rightarrow32}$	6.8E+05	2.3E+08	7.7E+09
$k_{30\rightarrow4}$	4.4E+12	4.8E+12	5.1E+12
$k_{30\rightarrow31}$	3.5E+12	4.4E+12	5.1E+12
$k_{30\rightarrow33}$	6.0E+10	2.9E+11	7.5E+11
$k_{31\rightarrow30}$	4.8E+08	4.3E+09	1.7E+10
$k_{31\rightarrow33}$	1.3E+13	1.8E+13	2.2E+13
$k_{31\rightarrow32}$	1.3E+08	3.7E+09	2.8E+10
$k_{32\rightarrow4}$	6.6E+11	1.2E+12	1.8E+12
$k_{32\rightarrow31}$	8.6E+10	1.9E+11	3.0E+11

Table B.2. The total energies, zero-point energies, expectation values of S^2, vibrational frequencies, rotational constants, unsymmetrical hindered rotor MultiWell parameters, and Cartesian coordinate geometries for the geometries discussed in Chapter 4. These parameters for Figure 4.8 are reported in Appendix A.

(reaction) Species	Information	Frequencies (unscaled) (cm^{-1})	Cartesian coordinates, (angstroms)			
			Atom	X	Y	Z
(OH + benzene) 2	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0696622 ZPE (hartree): 0.1106050 $<S^2>$: 0.755 Rotational constants (GHz): 3.9483 2.2440 1.8373	26.733 65.528 134.63 151.38 409.08 414.72 470.24 620.14 620.39 690.78 716.4 859.24 869.14 976.03 984.47 1005.9 1008.1 1023.1 1054 1059.2 1176 1195.2 1197.2 1331.7 1381.1 1505.7 1509.8 1620.2 1628.6 3162.4 3172.5 3180 3190.7 3191.4 3209.7 3738.5	C	0.089528	1.211186	0.546266
			C	0.694974	0.000029	0.902492
			C	0.089545	-1.211152	0.546314
			C	-1.110978	-1.209919	-0.157810
			C	-1.712761	-0.000015	-0.508102
			C	-1.110995	1.209909	-0.157854
			H	-1.579186	-2.147910	-0.434298
			H	-2.648690	-0.000033	-1.055667
			H	-1.579216	2.147881	-0.434382
			H	0.564477	-2.146721	0.816398
			O	2.459067	0.000036	-0.837824
			H	1.760593	-0.000543	-1.514251
			H	0.564457	2.146768	0.816303
			H	1.609152	0.000045	1.480660
(OH + benzene) 2-3_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0674256 ZPE (hartree): 0.1112250 $<S^2>$: 0.781 Rotational constants (GHz): 4.2325 2.5527 1.9572	-347.06 124.31 133.17 231.78 390.57 407.21 610.57 612.66 663.92 724.7 809.08 835.73 899.87 965.95 978.16 992.91 1012.6 1029.1 1040 1053.2 1172.5 1181 1194.7 1322.2 1377.2 1487.1 1498.4 1582.8 1605.7 3164.9 3174.1 3184.4 3194.8 3195.5 3211.9 3759.6	C	-0.176667	1.220519	-0.472455
			C	-0.859882	-0.000075	-0.715843
			C	-0.176547	-1.220591	-0.472406
			C	1.087856	-1.214351	0.092340
			C	1.724727	0.000077	0.376901
			C	1.087737	1.214428	0.092293
			H	1.592106	-2.150394	0.304081
			H	2.716848	0.000133	0.814045
			H	1.591889	2.150530	0.304005
			H	-0.676101	-2.154386	-0.698665
			O	-2.175677	0.000012	0.799791
			H	-1.537204	-0.000134	1.529706
			H	-0.676316	2.154254	-0.698747
			H	-1.729144	-0.000134	-1.357727

(OH + benzene)	Theory: B3LYP/6-311G(d,p)	-1265.2 77.929 110.62 174.8 358.41	C	-0.025107	1.216508	-0.053391
2-5_TS		409.79 446.23 613.31 642.39 688.2	C	-0.681412	-0.001385	-0.096504
	Energy (hartree): -308.0598408	726.03 793.03 832.72 917.32 975.46	C	-0.022447	-1.217969	-0.053158
		1001.1 1009.7 1018.5 1032.2 1070.4	C	1.373230	-1.209208	0.020609
	ZPE (hartree): 0.1052300	1107 1180 1184.5 1322.5 1324.6 1325.5	C	2.063444	0.001522	0.057209
		1468.9 1500.7 1603.6 1623.4 3161.2	C	1.370594	1.210710	0.020440
	$\langle S^2 \rangle$: 0.757	3169.2 3180.6 3186.4 3191.7 3762.9	H	1.916123	-2.147654	0.049063
			H	3.145996	0.002734	0.116399
	Rotational constants (GHz):		H	1.911444	2.150335	0.048770
	5.5830		H	-0.573625	-2.150534	-0.082904
	1.7212		O	-3.149834	-0.000028	-0.019431
	1.3239		H	-3.164407	0.001107	0.950521
			H	-0.578279	2.147882	-0.083442
			H	-1.928400	-0.004716	-0.214188
(OH + benzene)	Theory: B3LYP/6-311G(d,p)	105.06 286.69 391.56 398.7 442.14	C	0.203406	1.251276	0.241056
3		533.17 584.26 617.19 704.33 759.19	C	1.013549	0.000266	0.417876
	Energy (hartree): -308.0912973	809.4 865.94 946.67 972.21 977.59	C	0.203609	-1.251391	0.241478
		989.88 1023.3 1030.5 1120.1 1168.4	C	-1.128548	-1.225779	-0.049827
	ZPE (hartree): 0.1135330	1190.8 1235 1306.8 1356.6 1399.2	C	-1.825544	-0.000276	-0.190529
		1409.4 1449.7 1541.9 1594.8 2967.1	C	-1.128950	1.225885	-0.049673
	$\langle S^2 \rangle$: 0.786	3154.7 3157.5 3178 3178.4 3194.4	H	-1.667825	-2.157883	-0.185170
		3794.5	H	-2.882654	-0.001020	-0.425752
	Rotational constants (GHz):		H	-1.668192	2.158059	-0.184303
	4.8484		H	0.741769	-2.188431	0.333341
	2.6350		O	2.175134	-0.000073	-0.449752
	1.8517		H	1.838689	0.001049	-1.353825
			H	0.740731	2.188796	0.333263
			H	1.471278	0.000130	1.418174
(OH + benzene)	Theory: B3LYP/6-311G(d,p)	-299.73 96.361 295.87 399.47 441.97	C	-0.180631	-1.260438	0.225558
3-4_TS		530.48 583.62 615.68 700.79 752.19	C	-1.009718	-0.024504	0.415571
	Energy (hartree): -308.0855436	806.8 874.98 947.45 968.35 976.85	C	-0.219645	1.238779	0.242771
		991.76 1010.2 1024.6 1118.6 1169.8	C	1.112651	1.236993	-0.048357
	ZPE (hartree): 0.1123910	1193.5 1221.6 1308.6 1330.6 1376.1	C	1.827657	0.024541	-0.197838
		1437.2 1453 1545.1 1599.3 2896.2	C	1.150323	-1.212220	-0.059366
	$\langle S^2 \rangle$: 0.787		H	1.638523	2.179061	-0.165053

	Rotational constants (GHz): 4.8416 2.6485 1.8509	3141.5 3158.7 3166.1 3182.5 3194.6 3823.7	H 2.885082 0.043150 -0.431009 H 1.703777 -2.135417 -0.196505 H -0.754839 2.175074 0.376355 O -2.137086 -0.103461 -0.497895 H -2.321347 0.788702 -0.808287 H -0.704360 -2.206550 0.301487 H -1.433977 -0.035238 1.436141
(OH + benzene) 4	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0866183 ZPE (hartree): 0.1128650 $\langle S^2 \rangle$: 0.787 Rotational constants (GHz): 4.9037 2.6275 1.8358	99.747 223.72 301.4 403.23 436.51 530.22 584.6 613.17 703.46 747.66 803.54 873.16 953.17 968.05 975.39 991.73 1016.2 1028.8 1117.5 1166.8 1193.3 1211.1 1310.4 1346 1376.9 1423.9 1456.5 1544.6 1599.1 2874 3147.8 3159.7 3167.5 3183.9 3194.6 3814.3	C -0.186882 -1.253087 0.207612 C -1.003918 -0.011826 0.392423 C -0.205770 1.247747 0.205212 C 1.131692 1.234392 -0.056483 C 1.842206 0.014770 -0.172390 C 1.151482 -1.215246 -0.044702 H 1.663980 2.170826 -0.188765 H 2.904686 0.022564 -0.382103 H 1.699642 -2.143746 -0.166063 H -0.744375 2.187064 0.287264 O -2.123741 -0.087239 -0.523261 H -2.767743 0.573796 -0.247914 H -0.723325 -2.192546 0.273430 H -1.415806 -0.020542 1.420203
(OH + benzene) 4-7_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0279118 ZPE (hartree): 0.1108650 $\langle S^2 \rangle$: 0.779 Rotational constants (GHz): 4.3601 2.8612 2.4803	-657.33 188.07 221.32 274.74 461.89 509.18 593.42 642.53 683.89 739.09 756.06 796.43 865.17 900.08 911.27 950.99 1030.6 1049.1 1110.5 1122.3 1158 1186.4 1294.4 1318.5 1378.3 1397.5 1409.4 1437.2 1549.5 3041.7 3153.8 3164.3 3172.3 3178.7 3203.7 3814.1	C -0.191812 -0.877458 0.853777 C -1.216420 0.009684 0.302240 C -0.193973 1.089758 0.602709 C 1.025814 1.153048 -0.087106 C 1.589496 -0.086234 -0.531235 C 0.991167 -1.168414 0.038460 H 1.576414 2.085376 -0.151302 H 2.439690 -0.145142 -1.198228 H 1.336243 -2.188059 -0.086820 H -0.478893 1.861178 1.310413 O -1.590490 -0.222910 -1.038776 H -1.769236 0.635379 -1.437735 H -0.321974 -1.306694 1.841587 H -2.083953 0.118943 0.959209

(OH + benzene) 4-9_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0443806 ZPE (hartree): 0.1062210 $\langle S^2 \rangle$: 0.774 Rotational constants (GHz): 5.3822 2.5557 1.7795	-965.88 208.72 302.72 368.38 420.48 483.96 502.18 529.49 624.59 643.79 682.08 769.11 809.15 827.74 898.67 963.75 983.42 1002.7 1035.1 1094.1 1174 1185 1191.8 1264.5 1337.8 1370.1 1492.8 1510.6 1596.1 1623 3158.5 3170 3178 3193.1 3201.2 3829.1	C C C C C C H H H H O H H H	-0.199051 -0.931307 -0.230267 1.154630 1.872717 1.184174 1.681935 2.955832 1.736973 -0.790922 -2.281217 -2.694111 -0.751117 -0.994239	-1.228564 -0.018576 1.212011 1.219299 0.020762 -1.196589 2.166165 0.034904 -2.128836 2.140922 -0.106445 0.736280 -2.159740 0.011811	-0.021189 0.071558 -0.034681 -0.030785 -0.012847 -0.026426 -0.061173 -0.016495 -0.055147 -0.060174 -0.163697 0.051503 -0.040194 1.817472
(OH + benzene) 5	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0740579 ZPE (hartree): 0.1103620 $\langle S^2 \rangle$: 0.757 Rotational constants (GHz): 5.6535 1.4165 1.1385	42.544 52.264 63.727 118 215.61 307.57 409.08 429.84 600.47 622.83 675.1 730.09 825.66 910.78 977.52 987.63 999.63 1016.4 1050 1073.9 1175.8 1176.2 1302.2 1322.3 1462 1469.3 1573.2 1626.8 1648.4 3157.5 3164.7 3175.7 3184.6 3190.2 3810.2 3895.7	C C C C C C H H H H O H H H	0.403011 0.391730 -0.724055 -1.963630 -2.018810 -0.848909 -2.878490 -2.981651 -0.900374 -0.665566 3.550717 3.128733 1.330282 3.125299	-0.755591 0.619451 1.421611 0.765916 -0.627796 -1.386976 1.349160 -1.125845 -2.470698 2.504267 -0.000964 0.422130 -1.315936 0.424952	-0.000235 -0.000232 -0.000049 0.000148 0.000151 -0.000043 0.000299 0.000302 -0.000050 -0.000060 -0.000205 0.754890 -0.000394 -0.751789
(OH + benzene) 7	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0512091 ZPE (hartree): 0.1122500 $\langle S^2 \rangle$: 0.775	102.26 209.09 245.47 457.56 524.21 575.13 692.99 706.22 736.24 742.04 793.27 820.58 921.49 925.98 947.79 998.17 1019.6 1056.2 1062.6 1091.7 1102.8 1212.8 1285.6 1295.2 1320.9 1333.2 1401.1 1402.3 1473.9 3087.5 3144 3153.4 3188.4 3207.2 3220 3815.4	C C C C C C H H	0.130309 1.300889 0.130038 -0.980925 -1.580372 -0.979231 -1.253536 -2.378734	0.824952 0.031543 -0.708545 -1.145584 -0.038763 1.136331 -2.179754 -0.088124	0.806180 0.251187 0.909295 0.033741 -0.560786 -0.125085 -0.128189 -1.290782

	Rotational constants (GHz): 4.4953 2.7937 2.6966		H -1.230034 2.136747 -0.449140 H 0.342453 -1.229773 1.836506 O 1.525279 0.015277 -1.121851 H 1.658067 -0.898408 -1.394189 H 0.329181 1.466873 1.657402 H 2.206120 0.070623 0.856010
(OH + benzene) 7-8_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0328169 ZPE (hartree): 0.1107800 $\langle S^2 \rangle$: 0.785 Rotational constants (GHz): 4.6242 2.6291 2.3729	-453.33 140.51 219.96 362.73 410.47 520.19 540.07 626.55 696.69 735.05 799.01 811.36 823.12 912.2 938.03 940.59 1020 1041 1097.1 1110.9 1159.7 1219.8 1246.4 1293.3 1306.7 1369 1410.8 1452.4 1546.8 3037.9 3167.2 3188.1 3206.7 3223.7 3231 3822.1	C -0.187293 0.130388 1.016267 C -1.404311 0.335498 0.169168 C 0.399499 1.230557 0.165736 C 1.372641 0.679505 -0.656150 C 1.506798 -0.716855 -0.342684 C 0.632601 -1.067414 0.639415 H 1.919594 1.204446 -1.427204 H 2.188033 -1.394134 -0.842861 H 0.481757 -2.053270 1.054678 H 0.153137 2.275321 0.280255 O -1.739383 -0.601316 -0.758392 H -2.287449 -0.191453 -1.435532 H -0.338040 0.305777 2.084802 H -2.121577 1.113774 0.402486
(OH + benzene) 8	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0478501 ZPE (hartree): 0.1118450 $\langle S^2 \rangle$: 0.753 Rotational constants (GHz): 5.2686 2.1763 1.9587	86.215 117.63 267.08 353.93 366.57 534.43 611.82 643.8 703.65 719.05 808.21 842.3 873.99 949.2 953.74 988.2 1008.2 1021.3 1107.5 1117 1178.6 1194.9 1233.7 1301.2 1316.7 1391.6 1439.7 1557.4 1643 2983 3115.9 3183.6 3196 3215.7 3223.3 3846.1	C -0.227010 0.104253 0.778985 C -1.678594 0.084211 0.418711 C 0.607872 1.211076 0.146545 C 1.686320 0.673324 -0.446012 C 1.656819 -0.787614 -0.280997 C 0.557344 -1.137512 0.406063 H 2.466405 1.214817 -0.966643 H 2.413546 -1.461796 -0.661655 H 0.244471 -2.135899 0.678255 H 0.339960 2.257644 0.196982 O -1.953773 -0.204050 -0.893977 H -2.898413 -0.102638 -1.042737 H -0.179346 0.229987 1.872545 H -2.372940 0.743855 0.935291

(OH + benzene) 1 benzene	Theory: B3LYP/6-311G(d,p) Energy (hartree): -232.3085405 ZPE (hartree): 0.1001780 <S^2>: 0 Rotational constants (GHz): 5.7106 5.7099 2.8551	412.46 412.97 622.97 623.07 688.81 723.27 862.26 862.67 981.32 981.6 1013.4 1016.6 1023.4 1059.9 1060.4 1174.7 1197.5 1197.6 1335.3 1381.7 1512.5 1513.1 1637.2 1637.8 3155.8 3165.3 3165.5 3181.1 3181.3 3191.8	C 0.869098 -1.089673 -0.000036 C 1.378263 0.207767 0.000032 C 0.509165 1.297390 0.000004 C -0.869066 1.089697 -0.000034 C -1.378257 -0.207826 0.000029 C -0.509204 -1.297364 0.000005 H -1.545210 1.937462 0.000053 H -2.450525 -0.369473 -0.000061 H -0.905301 -2.306853 0.000016 H 0.905333 2.306842 0.000005 H 1.545199 -1.937472 0.000041 H 2.450510 0.369553 -0.000054
(OH + benzene) H	Theory: B3LYP/6-311G(d,p) Energy (hartree): -0.5021559 ZPE (hartree): 0.0000000 <S^2>: 0.75 Rotational constants (GHz): 0.0000 0.0000 0.0000 CBS-QB3 Energy (hartree): -0.499818	N/A	H 0.000000 0.000000 0.000000
(OH + benzene) H$_2$O	Theory: B3LYP/6-311G(d,p) Energy (hartree): -76.4474480 ZPE (hartree): 0.0213160 <S^2>: 0	1638.2 3810.7 3907.9	O 0.000000 0.118670 0.000000 H 0.757120 -0.474679 0.000000 H -0.757120 -0.474679 0.000000

	Rotational constants (GHz): 801.9134 437.3937 283.0226		
(OH + benzene) OH	Theory: B3LYP/6-311G(d,p) Energy (hartree): -75.7545274 ZPE (hartree): 0.0084400 $\langle S^2 \rangle$: 0.752 Rotational constants (GHz): 0.0000 560.4914 560.4914 CBS-QB3 Energy (hartree): -75.64972	3704.7	O 0.000000 0.000000 0.108357 H 0.000000 0.000000 -0.866857
(OH + benzene) 9 phenoxy	Theory: B3LYP/6-311G(d,p) Energy (hartree): -306.9068598 ZPE (hartree): 0.0911780 $\langle S^2 \rangle$: 0.788 Rotational constants (GHz): 5.5253 2.7889 1.8534	190.65 379.51 445.74 483.98 531.37 597.54 656.34 802.12 803.94 805.05 928.12 983.91 987.72 999.85 1008.8 1088.6 1163.2 1164.6 1271.6 1336.6 1418.7 1442.8 1480.2 1546.2 1587.1 3165.5 3171.8 3187.3 3195.1 3198.3	C -0.288981 1.237850 0.000129 C 1.085679 1.223510 0.000039 C 1.782219 0.000000 -0.000121 C 1.085679 -1.223510 0.000059 C -0.288981 -1.237850 0.000139 C -1.048571 0.000000 -0.000461 O -2.300041 0.000000 0.000049 H -0.856681 2.160890 0.000489 H 1.642609 2.153980 0.000109 H 2.866209 0.000000 -0.000181 H 1.642609 -2.153980 0.000139 H -0.856681 -2.160890 0.000369
(OH + benzene) 6	Theory: B3LYP/6-311G(d,p)	400.83 426.76 601.79 620.31 673.26 721.29 812.8 892.18 964.35 988.68	C -1.223869 -0.770644 -0.000011 C -0.000003 -1.395903 0.000003

phenyl radical	Energy (hartree): -231.6194243 ZPE (hartree): 0.0870270 $<S^2>$: 0.757 Rotational constants (GHz): 6.2967 5.6215 2.9700	992.85 1016.4 1049.4 1072.8 1175 1175.8 1301.7 1323.6 1462.5 1470.4 1574.7 1629.3 3155.3 3161 3173.5 3175.9 3187.7	C	1.223873	-0.770637	0.000009
			C	1.211875	0.631400	-0.000010
			C	-0.000003	1.321976	0.000002
			C	-1.211871	0.631409	0.000006
			H	2.150419	1.176021	-0.000013
			H	0.000008	2.405944	0.000006
			H	-2.150425	1.176013	0.000013
			H	2.157649	-1.321801	0.000008
			H	-2.157659	-1.321785	-0.000004
OH + Bi-layer						
(OH + Bi-layer) 2	Theory: M062X/6-311G(d,p) Energy (hartree): -539.6196977 ZPE (hartree): 0.2078280 $<S^2>$: 0 Rotational constants (GHz): 1.4347 0.5491 0.5302	25.323 49.562 58.38 69.726 100.61 135.99 238.39 346.11 408.32 412.36 415.72 421.75 515.82 538.27 620.87 622.19 632.85 697.29 700.01 720.71 767.5 836.84 840.06 874.27 882.36 898.84 978.65 998.81 1002.8 1005.6 1015 1016.5 1031.1 1032.5 1062.2 1077.1 1079.9 1109.8 1177.6 1180 1199.7 1207.6 1209.7 1217.3 1311.8 1339.3 1353.9 1375.9 1385.7 1520.7 1527.7 1530.3 1552.8 1673.4 1676.8 1677.5 1693.6 3181.9 3186.6 3193.5 3199.4 3200.9 3206.3 3209.8 3214.7 3217.2 3224.2 3226.7 3912.9	C	0.456136	1.119122	1.345574
			C	0.786114	-0.196786	1.654742
			C	1.746198	-0.879157	0.921152
			C	2.383301	-0.240856	-0.139786
			C	2.066090	1.078947	-0.452962
			C	1.105323	1.752374	0.293166
			H	-0.308149	1.638553	1.909264
			H	0.279717	-0.703519	2.468004
			H	2.011376	-1.905382	1.144104
			H	2.568036	1.574949	-1.278583
			H	0.856886	2.776473	0.039118
			H	-1.454703	-2.588431	0.166746
			C	-1.727433	-1.572335	-0.094621
			C	-1.071410	-0.925002	-1.137304
			H	-0.283930	-1.433929	-1.681184
			C	-1.414562	0.380467	-1.467572
			H	-0.896953	0.887945	-2.273405
			C	-2.409751	1.042008	-0.754080
			H	-2.674545	2.061360	-1.010857
			C	-3.060716	0.397091	0.291756
			H	-3.835341	0.911991	0.848300
			C	-2.719204	-0.911574	0.621471
			H	-3.227309	-1.415428	1.435752
			O	3.305338	-0.958439	-0.841035
			H	3.681695	-0.402874	-1.528195

(OH + Bi-layer) 2-3_TS	Theory: M062X/6-311G(d,p) Energy (hartree): -539.4595781 ZPE (hartree): 0.2024110 <S^2>: 0 Rotational constants (GHz): 1.5503 0.4935 0.4812	-557.24 9.4077 36.774 48.622 51.801 74.325 108.32 185.8 336.53 398.91 407.26 411.61 461.66 511.3 561.12 615.98 617.94 660.33 688.49 719.64 723.71 728.09 811.51 846.76 867.22 876.46 938.36 944.04 986.56 992.07 995.94 999.46 1016.1 1024.8 1034.2 1060 1069.7 1071.8 1118.3 1128 1153 1162.7 1191.8 1199.3 1201.1 1277.7 1334.3 1336.2 1370.9 1409.3 1497.2 1518.9 1521.7 1580 1626.3 1670.2 1676.6 3084.2 3171.9 3177.9 3186.7 3192.9 3195 3202.7 3205.3 3211 3229.1 3235.4 3889.8	C C C C C C H H H H H H C C H C H C H C H C H O H	0.415000 1.238677 2.522805 2.283289 2.006334 0.961460 -0.570774 1.011063 3.507138 2.706050 0.622063 -2.497274 -2.380973 -1.329744 -0.606811 -1.177692 -0.333786 -2.079069 -1.956861 -3.128212 -3.829267 -3.278503 -4.095882 3.335978 3.036285	1.526829 0.913251 0.423623 -0.669270 0.614607 1.496243 1.903083 0.677047 0.736918 0.605412 2.098961 -1.094960 -0.806330 -1.320102 -1.988625 -0.944356 -1.318195 -0.057617 0.238350 0.460735 1.154317 0.086855 0.489978 -1.465786 -2.122810	0.540726 1.414258 0.813966 0.009620 -0.876806 -0.784958 0.784350 2.445601 1.175293 -1.703662 -1.615354 2.263343 1.225145 0.472808 0.924462 -0.856975 -1.424634 -1.437399 -2.473014 -0.684852 -1.134725 0.647602 1.234260 -0.304596 -0.937966
(OH + Bi-layer) 3	Theory: M062X/6-311G(d,p) Energy (hartree): -539.4869670 ZPE (hartree): 0.2049050 <S^2>: 0 Rotational constants (GHz): 1.4779 0.4837 0.4502	37.208 49.002 54.388 64.022 71.454 79.852 110.95 140.34 337.06 409.27 414.9 446.76 499.3 569.99 619.9 622.31 692.27 721.47 741.55 747.2 807.77 826.97 837.67 870.63 881.03 951.94 970.31 976.68 994.78 1004.8 1011.9 1015.4 1027.6 1032.6 1033.1 1035.4 1079.3 1081.9 1114.3 1118.5 1175.2 1177 1206.6 1212.7 1257.2 1310.9 1341.4 1343.8 1352.1 1386.8 1413.1 1529.7 1531.4 1569.4 1662 1675 1678.8 3072.9 3179.2 3189 3193.9 3205.4	C C C C C C H H H H H H C	0.364834 1.280393 2.429977 2.342165 2.052113 0.847293 -0.599638 1.198920 3.422010 2.664169 0.306007 -2.002963 -2.120236	1.241828 0.368722 0.301228 -0.986641 1.330410 1.841426 1.448003 -0.262431 0.461529 1.559362 2.583237 -2.150476 -1.391974	1.041171 1.491157 0.528570 -0.264345 -0.511552 -0.202474 1.487210 2.364655 0.966288 -1.372008 -0.775038 1.499336 0.733733

		3206.5 3209.6 3217.1 3218.2 3236 3247.4 3843	C H C H C H C H C H O H	-1.229107 -0.390214 -1.377551 -0.665105 -2.411355 -2.526292 -3.297251 -4.101350 -3.152773 -3.843846 3.577839 3.544576	-1.338680 -2.021085 -0.361363 -0.309816 0.565210 1.327339 0.517735 1.240923 -0.463524 -0.502932 -1.369098 -2.167136	-0.332622 -0.387247 -1.311097 -2.126070 -1.220422 -1.983174 -0.147370 -0.074787 0.829046 1.663145 -0.502787 -1.042780
(OH + Bi-layer) 4	Theory: M062X/6-311G(d,p) Energy (hartree): -539.4833951 ZPE (hartree): 0.2047230 $<S^2>$: 0 Rotational constants (GHz): 1.7312 0.3588 0.3247	16.042 26.592 42.549 51.646 75.193 88.072 96.216 182.05 292.23 413.63 417.15 434.77 541.91 620.24 620.41 666.2 702.03 715.11 726.21 740.75 786.83 821.17 861.38 879.21 888.01 918.97 970.48 984.94 994.73 1004.8 1010.4 1015.7 1017.4 1034.3 1041.2 1043.3 1074.4 1080.4 1108.3 1113.4 1168.2 1172.2 1202.4 1207.1 1230.5 1305.4 1340.1 1358.3 1369.4 1379.7 1406.2 1523.9 1528.1 1585.8 1667.8 1674.4 1679.1 3052.1 3175.9 3183.1 3189.2 3197.8 3203.4 3209.7 3209.9 3221 3240.8 3248.5 3814.8	C C C C C C H H H H H H C C H C H C H C H C H O H	2.047596 1.709860 2.754532 2.392834 3.746767 3.313652 1.483788 0.821673 3.265453 4.636439 3.815336 -3.353833 -3.133782 -1.839123 -1.043729 -1.555929 -0.542241 -2.571632 -2.352600 -3.866806 -4.657323 -4.148031 -5.156688 1.134765 0.905978	1.554788 0.302838 -0.650921 -1.721572 0.264173 1.528727 2.451047 0.002630 -1.173981 -0.095327 2.403390 -1.884025 -1.023790 -0.809401 -1.500209 0.295657 0.454384 1.185351 2.046665 0.971224 1.664785 -0.133176 -0.298804 -1.555573 -2.209365	0.641656 0.986189 0.480318 -0.528851 -0.209770 -0.105869 0.865017 1.524806 1.302076 -0.704666 -0.497758 1.379087 0.757532 0.295673 0.550475 -0.502079 -0.851042 -0.837659 -1.458056 -0.376964 -0.638598 0.421046 0.780939 -0.856385 -1.528524

(OH + Bi-layer) 1 benzene	Theory: M062X/6-311G(d,p) Energy (hartree): -232.1961506 ZPE (hartree): 0.1009610 $<S^2>$: 0 Rotational constants (GHz): 5.7316 5.7311 2.8657	407.8 413.39 618.21 618.97 693.43 723.95 870.68 883.02 998.51 1007 1016.1 1032.9 1033.7 1072.2 1074.1 1167.5 1200.2 1200.9 1333.8 1376.8 1523.1 1525.2 1674.2 1676.8 3175.5 3180.1 3194.4 3200.4 3209 3214.7	C C C C C C H H H H H H	0.939731 1.358145 0.418450 -0.939732 -1.358145 -0.418451 1.671620 2.416093 0.744526 -1.671609 -2.416096 -0.744518	1.025713 -0.300902 -1.326573 -1.025711 0.300904 1.326572 1.824870 -0.535647 -2.359951 -1.824880 0.535640 2.359955	-0.000009 -0.000027 -0.000005 -0.000011 -0.000027 -0.000002 0.000104 0.000003 0.000138 0.000105 0.000007 0.000123
(OH + Bi-layer) 1 phenol	Theory: M062X/6-311G(d,p) Energy (hartree): -307.4173554 ZPE (hartree): 0.1056000 $<S^2>$: 0 Rotational constants (GHz): 5.6955 2.6365 1.8022	233.67 376.67 414.55 422.79 520.02 537.23 630.84 704.39 773.66 840.96 841.77 905.2 983.97 1006.4 1017.5 1059.8 1107.1 1175.2 1193.2 1214.1 1315.1 1355.1 1371.5 1520.1 1550.5 1683.5 1693.1 3174.7 3190.2 3196.2 3211.8 3218.7 3913.4	C C C C C C H H H H H O H	1.849521 1.166292 -0.220153 -0.937423 -0.263482 1.127236 2.931761 1.718869 -0.769202 -0.825166 1.644723 -2.295367 -2.669996	0.027634 -1.186018 -1.218569 -0.023860 1.194458 1.213993 0.046247 -2.118109 -2.151752 2.123542 2.165921 -0.110671 0.773687	0.000014 0.000019 -0.000032 -0.000044 -0.000019 0.000006 0.000045 0.000012 -0.000085 -0.000040 -0.000001 0.000057 -0.000052

OH + phenanthrene radical

(OH + phen. rad.) 1 phenanthrene rad.	Theory: B3LYP/6-311G(d,p) Energy (hartree): -538.9768311 ZPE (hartree): 0.1806060 $<S^2>$: 0.758 Rotational constants (GHz):	99.663 116.17 222.14 225.65 247.91 406.89 410.22 447.55 451.16 494.86 500.23 555.45 555.91 588.13 629.11 706.77 720.95 725.21 743.07 770.15 802.63 828.08 835.76 884.47 889.2 889.27 963.08 968.29 981.43 996.58 1012.8 1050.4 1065.2 1099.6 1162.5 1172.1 1179.7 1190 1230.6 1243 1281.7 1314.3 1355.2 1367.4 1424 1431.8	C C C C C C H H H	3.539185 2.858944 1.479556 0.728306 1.414009 2.826567 3.421399 0.952837 4.623153	-0.319849 -1.551187 -1.583017 -0.389252 0.855603 0.860690 -2.478030 -2.530807 -0.301201	0.000077 0.000037 -0.000070 -0.000039 0.000048 0.000075 0.000067 -0.000095 0.000124

	1.6504 0.5540 0.4148 CBS-QB3 Energy (hartree): -537.839563	1450.2 1476.4 1515.6 1533.5 1585.6 1637.5 1650.6 1655.7 3155.4 3159.1 3159.7 3167.1 3169.8 3174.8 3178.1 3182.5 3189.2	H 3.345972 1.813398 0.000140 C -0.719430 -0.394105 -0.000111 C -1.441036 0.841191 -0.000104 C -0.700264 2.069652 -0.000108 C 0.658181 2.075425 -0.000029 H -1.253453 3.003200 -0.000260 H 1.200481 3.015235 0.000028 C -1.507020 -1.541281 -0.000120 C -2.865732 -1.603599 -0.000027 C -3.558579 -0.368318 0.000165 C -2.854954 0.818459 0.000092 H -3.405285 -2.544158 0.000076 H -4.643265 -0.363195 0.000411 H -3.388233 1.763080 0.000203
(OH + phen. rad.) 2	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.9029022 ZPE (hartree): 0.1979190 $<S^2>$: 0 Rotational constants (GHz): 1.1839 0.5325 0.3673 CBS-QB3 Energy (hartree): -613.662247	60.272 93.889 194.27 226.58 254.34 288.34 346.56 358.4* 404.33 412.44 489.06 502.37 513.01 525.85 549.99 569.55 581.5 631.29 683.36 714.58 727.96 750.51 771.01 792.85 812.38 823.58 859.27 863.8 884.03 958.83 962.82 983.03 998.57 1011.1 1024.6 1073.4 1115.7 1155.9 1175.9 1189.8 1195.8 1206.6 1235 1250.4 1283 1311.2 1336.6 1362.4 1372.6 1441.6 1450.9 1473.7 1493.4 1536.7 1569.9 1607.8 1643.7 1654.2 1666.3 3141.4 3156.2 3158.9 3168.2 3170.4 3177.8 3185.1 3189.3 3276.2 3825.9	C 3.646447 -0.326611 0.000147 C 2.892586 -1.508853 0.000413 C 1.511311 -1.471125 0.000291 C 0.800847 -0.244131 -0.000076 C 1.580994 0.954170 -0.000198 C 2.990862 0.884449 -0.000155 H 3.395361 -2.469756 0.000758 H 0.966673 -2.398812 0.000526 H 4.729894 -0.366157 0.000280 H 3.552505 1.812926 -0.000379 C -0.657463 -0.131305 -0.000115 C -1.249368 1.171392 0.000036 C -0.411903 2.334512 -0.000063 C 0.937438 2.232489 -0.000253 H -0.892543 3.306805 0.000011 H 1.558863 3.121930 -0.000325 C -1.567917 -1.229389 -0.000208 C -2.940880 -1.033889 0.000069 C -3.489025 0.252138 0.000360 C -2.650487 1.342223 0.000267 H -3.594075 -1.902395 0.000091 H -4.565401 0.378589 0.000494 H -3.051940 2.349064 0.000414 O -1.079566 -2.508583 -0.000613

			H	-1.823450	-3.119963	-0.000060
	*Vibration replaced by unsymmetrical hindered rotor (hrd 2 4 1). The same representation of the hindered rotor potential was also used in VariFlex	Multiwell hindered rotor parameters: Vhrd2 1 0.0 948.0 -948.0 Ihrd1 1 0.0 1.655 -0.4777 -0.4924 0.595662				
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-498.39 99.553 107.48 190.71 211.02	C	3.483530	-0.292522	-0.212940
2-3_TS		221.62 267.31 313.46 398.78 428.69	C	2.707639	-1.452761	-0.401593
	Energy (hartree): -614.7500511	450.08 465.1 490.35 516.21 538.69	C	1.333139	-1.397565	-0.312661
		542.72 567.94 590.56 670.84 674.47	C	0.661079	-0.181001	-0.044379
	ZPE (hartree): 0.1937850	700.19 734.32 761.24 788.06 797.45	C	1.449577	1.006268	0.120899
		818.62 829.95 882.26 920.22 938.68	C	2.861802	0.906156	0.043315
	$\langle S^2 \rangle$: 0	953.33 970.6 971.43 980.97 993.9 1021.8	H	3.192946	-2.397671	-0.619011
		1059.8 1112.8 1125.8 1140.2 1166.7	H	0.758208	-2.301868	-0.452190
	Rotational constants (GHz):	1183.6 1186.6 1231.1 1246.2 1282	H	4.564579	-0.345737	-0.275864
	1.0823	1305.9 1337.6 1363.5 1371.6 1397.8	H	3.448430	1.809072	0.178098
	0.5910	1454.8 1482.6 1513.4 1551.1 1558.5	C	-0.781465	-0.052301	0.081788
	0.4065	1600.9 1622.7 1650.5 3047.7 3157.8	C	-1.349734	1.253208	0.076566
		3161.4 3169.5 3180.7 3184.9 3187.2	C	-0.542172	2.391564	0.250421
		3207.6 3214.9 3795.8	C	0.823322	2.271449	0.307667
			H	-1.013342	3.367344	0.306324
			H	1.449554	3.148052	0.428903
			C	-1.624543	-1.338972	0.610421
			C	-2.046675	-1.037221	-0.679240
			C	-3.146164	-0.015265	-0.601820
			C	-2.759156	1.210731	-0.196524
			H	-1.897830	-1.665178	-1.563432
			H	-4.166024	-0.329676	-0.786056
			H	-3.426956	2.049871	-0.047935
			O	-1.077614	-2.552598	0.854227
			H	-0.709738	-2.544033	1.745824
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-1224.8 89.942 140.91 214.59 228.21	C	-3.527189	-0.282437	-0.281427
2-5_TS		270.03 329.27 382.16 410.34 441.42	C	-2.855549	-1.435068	0.033290
	Energy (hartree): -614.8375810	481.48 496.23 511.77 545.86 563.97	C	-1.443340	-1.420607	0.327643
		567.39 575.18 626.77 681.99 707 727.65	C	-0.734362	-0.142630	0.206211
	ZPE (hartree): 0.1924100	748.41 773.82 787.91 811.76 841 856.35	C	-1.487812	1.059232	0.004336
		881.2 901.69 946.38 980.93 988.65	C	-2.855969	0.958386	-0.236147
	$\langle S^2 \rangle$: 0	996.13 997.84 1030.6 1059.7 1086.3	H	-3.390913	-2.374903	0.114851
		1116.5 1164.1 1184 1187.1 1203 1243.7	H	-1.214015	-1.972058	1.251465

	Rotational constants (GHz):	1263.4 1293.7 1345.5 1370.4 1384.7	H	-4.587039	-0.305211	-0.506391
	1.1655	1396 1436.4 1450 1468.8 1475.7 1509	H	-3.421812	1.869468	-0.405235
	0.5590	1547.6 1588.2 1594.7 1626.2 1658.3	C	0.670912	-0.107585	0.176844
	0.3821	1878.1 3000.3 3158 3159.2 3161 3171.3	C	1.353319	1.154868	0.128708
		3177.6 3180.3 3189.4 3195.6	C	0.562428	2.357878	0.126442
			C	-0.789687	2.317412	0.026646
			H	1.081401	3.310640	0.134034
			H	-1.367126	3.231887	-0.057280
			C	1.410334	-1.348025	-0.023100
			C	2.814339	-1.237456	-0.229052
			C	3.451379	-0.014533	-0.155407
			C	2.739905	1.183180	0.012751
			H	3.364880	-2.154942	-0.396701
			H	4.531249	0.024820	-0.257135
			H	3.261492	2.133334	0.007428
			O	0.814346	-2.481903	-0.047840
			H	-0.625122	-2.163502	-0.208750
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-2165.7 82.512 100.78 195.96 212.02	C	-3.656533	-0.396678	0.064512
2-7_TS		217.01 288.48 368.47 401.67 406.99	C	-2.873935	-1.566897	0.081792
	Energy (hartree): -614.8028751	469.76 481.81 496.77 539.55 551.56	C	-1.496604	-1.498082	0.060974
		561.16 597.78 627.18 679.37 702.04	C	-0.837283	-0.245837	0.023804
	ZPE (hartree): 0.1915140	716.45 752.31 770.46 805.61 817.03	C	-1.632357	0.938283	-0.005224
		841.15 852.27 866.8 893.86 962 971.81	C	-3.042019	0.834305	0.018051
	$<S^2>$: 0	990.68 998.08 1010.1 1034.1 1061.3	H	-3.359443	-2.536135	0.105581
		1083.4 1136.6 1154.5 1178.4 1184.4	H	-0.902313	-2.401306	0.058226
	Rotational constants (GHz):	1184.6 1220.7 1239.2 1258.1 1304.9	H	-4.738085	-0.467750	0.080492
	1.2046	1364.8 1381.6 1389.6 1414.1 1452.5	H	-3.632659	1.744288	-0.001149
	0.5236	1463.1 1485.3 1517.5 1532.6 1572.5	C	0.598655	-0.112931	0.039126
	0.3675	1617.3 1640.7 1657.6 1807.8 3077	C	1.212893	1.166477	-0.020872
		3158.4 3161.2 3165.5 3171.6 3179.1	C	0.373863	2.318727	-0.088222
		3184.2 3187.3 3214.5	C	-0.984819	2.208171	-0.066767
			H	0.841244	3.295342	-0.147949
			H	-1.602623	3.099818	-0.103078
			C	1.511402	-1.213716	0.003212
			C	2.930173	-1.049206	0.221428
			C	3.487655	0.269738	0.108073
			C	2.644229	1.329267	-0.037468
			H	3.317001	-1.672834	1.032366

			H	4.558214	0.420708	0.193399
			H	3.034181	2.337209	-0.122120
			O	1.301874	-2.429812	-0.381153
			H	2.657573	-2.270577	-0.461048
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-252.74 45.326 98.014 160.2 169.08	C	-3.472334	0.516933	-0.059828
2-18_TS		196.36 214.02 254.44 334.94 412.34	C	-2.570320	1.617684	-0.110710
	Energy (hartree): -614.7158495	420.29 445.19 475.99 488.24 493.96	C	-1.216482	1.380958	-0.082157
		500.5 548.33 557.04 574.45 578.47	C	-0.780256	0.043833	-0.008998
	ZPE (hartree): 0.1915290	684.99 703.22 719 736.66 760.34 803.41	C	-1.646755	-1.067553	0.032771
		806.93 822.86 837.23 866.98 896.05	C	-3.033387	-0.792838	0.008835
	$<S^2>$: 0	905.04 959.76 969.29 981.15 1001.9	H	-2.978986	2.621843	-0.174333
		1029.4 1058.5 1093.3 1159.5 1165.6	H	0.189552	2.823599	-0.100927
	Rotational constants (GHz):	1179.8 1208.1 1229.3 1250.6 1308.7	H	-4.539043	0.719119	-0.081609
	0.9431	1337.7 1353.6 1392.4 1426.9 1438	H	-3.749376	-1.607373	0.039608
	0.5772	1479.4 1499.2 1514.7 1531.4 1614	C	0.609239	-0.128250	0.002151
	0.3593	1633.2 1649.1 1660.4 3141.9 3154.5	C	1.228737	-1.402987	0.028831
		3156.1 3164.7 3172.1 3173.8 3181.6	C	0.330873	-2.527644	0.078598
		3229.9 3250.6 3811.5	C	-1.028018	-2.367256	0.084721
			H	0.757044	-3.525274	0.106467
			H	-1.666798	-3.244300	0.121947
			C	1.426642	0.993731	-0.059243
			C	2.778187	1.008098	-0.117328
			C	3.385838	-0.284190	-0.094212
			C	2.642052	-1.445728	-0.016524
			H	3.368626	1.909917	-0.175115
			H	4.468647	-0.332339	-0.133035
			H	3.147891	-2.404965	0.002197
			O	1.014055	3.307297	0.145350
			H	0.965915	3.312644	1.110571
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-1247.3 88.026 133.45 166.88 217.84	C	3.498460	-0.248634	-0.201207
2-22_TS		251.3 297.07 343.33 400.4 425.51 453.72	C	2.774292	-1.446262	0.019415
	Energy (hartree): -614.7300698	486.84 489.63 513.98 521.22 547.67	C	1.427611	-1.284141	0.127297
		564.56 573.42 600.17 640.71 671.17	C	0.706944	-0.102678	0.107575
	ZPE (hartree): 0.1859690	701.38 711.86 740.02 757.68 787.25	C	1.476514	1.093952	-0.008027
		800.06 812.55 832.32 851.68 875 886.62	C	2.873219	0.985212	-0.170964
	$<S^2>$: 0	944.46 955.09 973.46 981.62 999.31	H	3.268080	-2.405157	0.085124
		1050.8 1064.3 1079.4 1147.6 1167.3	H	0.545339	-2.547791	0.962202
	Rotational constants (GHz):	1187.4 1198.3 1233.3 1251.6 1313.4	H	4.567301	-0.320129	-0.365812

	1.1827	1324.5 1341.3 1375.2 1406.8 1443.6	H	3.463114	1.888385	-0.279590
	0.5691	1450 1453.4 1500.5 1521.2 1557.5	C	-0.706533	-0.067656	0.110775
	0.3876	1599.4 1636.1 1646.3 3159.8 3160.5	C	-1.404339	1.156933	0.106375
		3172.1 3177.9 3181.6 3188.2 3195.5	C	-0.615469	2.360641	0.111071
		3219 3229.9	C	0.745900	2.331315	0.031961
			H	-1.131348	3.314969	0.133091
			H	1.308193	3.257771	-0.017421
			C	-1.347176	-1.337958	-0.058867
			C	-2.746608	-1.325952	-0.178620
			C	-3.446304	-0.115277	-0.101633
			C	-2.809361	1.114120	0.028525
			H	-3.269167	-2.265432	-0.309457
			H	-4.529248	-0.140891	-0.165922
			H	-3.382475	2.033962	0.034679
			O	-0.574814	-2.381295	-0.132217
			H	1.195826	-2.447024	1.438773
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-358.89 76.335 97.968 183.39 217.94	C	-3.630146	0.369332	-0.007952
2-23_TS		228.66 266.66 297.84 406.86 410.62	C	-2.855161	1.535310	-0.119713
	Energy (hartree): -614.7637731	427.72 473.94 479.96 503.34 530.02	C	-1.476556	1.460651	-0.131873
		552.25 567.88 594.54 636.95 710.45	C	-0.803424	0.219969	-0.028711
	ZPE (hartree): 0.1929780	718.28 730.91 760.82 793.9 812.6 823.7	C	-1.596651	-0.964047	0.046860
		857.98 876.85 887.27 892.13 964.62	C	-3.005130	-0.856202	0.065976
	<S^{2}>: 0	971.23 977.06 986.81 996.32 1001.1	H	-3.340461	2.500736	-0.208967
		1064.3 1085.5 1143.2 1168.7 1174.1	H	-0.910646	2.371641	-0.264843
	Rotational constants (GHz):	1187.1 1229.8 1244.3 1270.1 1310.3	H	-4.712151	0.433995	0.005321
	1.1420	1356.6 1358.4 1401.8 1439.2 1452	H	-3.592201	-1.766345	0.131476
	0.5319	1471.7 1494.4 1507.6 1542.8 1586.9	C	0.641595	0.085443	-0.018360
	0.3640	1631.9 1652.8 1664.6 2511 3133.6	C	1.239370	-1.217933	-0.021009
		3154.6 3159.4 3161.7 3170.6 3179.2	C	0.387405	-2.367371	0.027680
		3186.8 3218.6 3679	C	-0.963721	-2.248456	0.078800
			H	0.852628	-3.347261	0.033320
			H	-1.592927	-3.130566	0.129460
			C	1.633122	1.071716	0.001565
			C	2.973046	1.053365	-0.028188
			C	3.497359	-0.264748	-0.081865
			C	2.650174	-1.356964	-0.057618
			H	2.318210	2.743771	0.083721
			H	4.570699	-0.429674	-0.123602

			H	3.056723	-2.364424	-0.064804
			O	1.278483	2.629784	0.113536
			H	0.974569	2.829478	1.017088
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	32.259 71.003 109.18 164.1 211.22	C	3.426700	-0.879103	-0.034280
3		242.56 281.04 353.36 403.89 430.18	C	2.442733	-1.864563	-0.280163
	Energy (hartree): -614.7840160	445.61 488.56 491.74 524.41 552.62	C	1.112679	-1.525266	-0.333261
		563.46 627.75 680.07 689.52 739.69	C	0.696841	-0.180048	-0.141671
	ZPE (hartree): 0.1956300	756.58 764.48 802.93 822.81 836.41	C	1.695357	0.822546	0.103828
		852.13 878.98 895.05 952.41 962.41	C	3.058141	0.430983	0.151897
	<S^2>: 0	972.63 977.29 990.24 995.8 998.9 1045.6	H	2.743996	-2.895522	-0.429322
		1057.2 1117.1 1157.4 1168.4 1180.7	H	0.365510	-2.287525	-0.518931
	Rotational constants (GHz):	1186.1 1229.7 1239.8 1250.1 1280.9	H	4.472521	-1.162081	0.004348
	0.9726	1288.8 1346.5 1363.9 1378.2 1399	H	3.810753	1.190172	0.338576
	0.5761	1410.4 1467 1487.2 1551.1 1579.7 1618	C	-0.651810	0.245086	-0.193575
	0.3749	1633.9 1663.4 2996.8 3157.3 3160.4	C	-0.999827	1.581718	-0.020500
		3167.7 3179.2 3182 3191.7 3194 3224	C	-0.012802	2.562251	0.226782
		3757.3	C	1.304124	2.177866	0.288118
			H	-0.292815	3.600872	0.363995
			H	2.078007	2.914996	0.475616
			C	-2.139913	-1.426372	0.809415
			C	-1.913580	-0.564485	-0.424205
			C	-2.986645	0.506034	-0.421243
			C	-2.447330	1.711319	-0.166153
			H	-1.893286	-1.150540	-1.353626
			H	-4.035153	0.283777	-0.561224
			H	-2.988777	2.645736	-0.087045
			O	-2.181429	-2.685720	0.399844
			H	-2.317336	-3.241918	1.178937
(OH + phen. rad.)	CBS-QB3 Energy (hartree):					
4	-613.030277					
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	60.326 112.51 180.66 215.17 234.03	C	3.614606	-0.270675	-0.000090
5		241.86 327.57 363.93 402.22 459.22	C	2.946118	-1.444024	0.000326
	Energy (hartree): -614.8482363	486.91 487.64 513.17 518.4 536.69	C	1.465564	-1.508473	0.000224
		557.35 582.75 649.63 694.47 716.82	C	0.725606	-0.197499	0.000066
	ZPE (hartree): 0.1958870	717.04 769.05 791.16 799.84 832.74	C	1.509748	1.021732	-0.000103
		853.32 884.8 907.15 939.06 965.54	C	2.889877	0.958904	-0.000288
	<S^2>: 0	984.49 987.91 1001.1 1003.9 1033.2	H	3.481386	-2.387556	0.000646

	Rotational constants (GHz): 1.1716 0.5394 0.3701	1075.9 1096.4 1155.8 1175.1 1179.6 1189.2 1195.8 1231.8 1262.9 1270.6 1314.8 1369.4 1381.2 1416.2 1436.1 1452.7 1468.1 1497.9 1508.5 1586.6 1610.9 1627.8 1657.4 1680 2963 2987.4 3155.6 3158.6 3161 3169.3 3176.2 3179.5 3187.9 3193.5	H H H C C C C H H C C C C H H H O H	1.107048 4.698247 3.446425 -0.662736 -1.324060 -0.517272 0.832008 -1.023779 1.433678 -1.499129 -2.936815 -3.498551 -2.701994 -3.535992 -4.579313 -3.179618 -1.001560 1.106574	-2.126843 -0.244868 1.890909 -0.128945 1.165790 2.356761 2.292013 3.316144 3.194557 -1.362106 -1.171348 0.071545 1.244880 -2.073862 0.173941 2.218097 -2.500621 -2.126885	-0.837735 -0.000231 -0.000502 0.000051 0.000099 0.000098 -0.000061 0.000207 -0.000175 -0.000058 -0.000178 0.000004 0.000168 -0.000350 -0.000005 0.000336 -0.000205 0.837899
(OH + phen. rad.) 5-6_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7983302 ZPE (hartree): 0.1920010 $<S^2>$: 0 Rotational constants (GHz): 1.1872 0.5360 0.3700	-1036.8 76.582 99.09 179.39 213.81 249.51 275.24 364.92 401.82 404.09 461.44 492 510.12 526.89 550.43 559.01 564.39 634.26 672.5 714.01 719.13 751.2 757.41 794.62 813.3 833.46 849.47 857.74 875.36 971.9 983.44 985.88 993.02 994.58 1051.6 1081.2 1089.2 1113.9 1157.7 1170.9 1182.7 1209.1 1228.8 1242.3 1258.9 1267.3 1354.6 1382 1398.7 1417.8 1441 1471.2 1497.2 1509.7 1528.1 1564.3 1596.7 1615 1644.9 2166.5 3104.7 3149.6 3157.3 3166.8 3176.7 3178.8 3181 3185.6 3207.1	C C C C C C H H H H C C C C H H C C C C	3.622182 2.879881 1.432262 0.723586 1.519875 2.934125 3.368615 0.833915 4.703636 3.486953 -0.693890 -1.331815 -0.509000 0.854033 -1.004682 1.445934 -1.517874 -2.938499 -3.505601 -2.721848	-0.257464 -1.469389 -1.435972 -0.193731 1.006596 0.934167 -2.426182 -2.344391 -0.287042 1.867950 -0.144186 1.151196 2.318937 2.262848 3.284836 3.171471 -1.368533 -1.150737 0.105864 1.266126	-0.021170 -0.023590 -0.061670 -0.008801 -0.004847 -0.010307 -0.169399 -0.103396 -0.021412 -0.003464 -0.007189 -0.001595 0.005648 0.006896 0.011862 0.014700 -0.003873 -0.000639 0.001138 0.001095

			H	-3.553289	-2.043485	0.000404
			H	-4.587646	0.198439	0.002652
			H	-3.180659	2.247742	0.002303
			O	-1.031383	-2.528116	-0.001340
			H	2.253784	-1.598747	1.049894
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-179.63 31.763 48.621 79.138 137.69	C	3.771158	-0.926229	0.195297
5-24_TS		175.68 182.95 205.42 282.08 300.62	C	3.007503	-1.848604	-0.433856
	Energy (hartree): -614.6987468	398.74 410.71 428.19 474 480.57 511.3	C	1.544897	-1.656243	-0.647096
		540.84 547.98 581.45 642.15 674.4	C	1.000071	-0.301904	-0.232155
	ZPE (hartree): 0.1896640	703.29 704.43 723.53 765.67 787.97	C	1.893391	0.658698	0.402132
		811.18 886 898.49 909.62 928.72 961.01	C	3.233587	0.347363	0.564864
	<S^2>: 0	970.05 993.6 996.33 1002.7 1064.7	H	3.456281	-2.762734	-0.808815
		1128.9 1136.6 1164.4 1181.4 1183.9	H	1.246161	-1.904147	-1.678467
	Rotational constants (GHz):	1198.3 1239 1250.1 1320.1 1357.3 1375	H	4.832118	-1.102483	0.335607
	1.0144	1406 1422.7 1429.9 1435.2 1448.1	H	3.928781	1.142936	0.816932
	0.3959	1504.3 1537.7 1618.1 1641.8 1674.4	C	-0.262760	0.101119	-0.500607
	0.3051	2207.7 2965.6 2989 3118 3136.7 3137.7	C	-0.756540	1.366185	-0.284493
		3142.7 3149.5 3160.3 3171.1 3179.9	C	0.206593	2.394855	0.034291
			C	1.443015	2.023292	0.476694
			H	-0.102599	3.435549	0.084152
			H	2.126502	2.766783	0.873419
			C	-3.242520	-1.483161	0.357523
			C	-3.118384	-0.589174	-0.594313
			C	-3.221678	0.871325	-0.346410
			C	-2.175426	1.702045	-0.198221
			H	-2.924310	-0.969461	-1.594162
			H	-4.221235	1.299287	-0.323131
			H	-2.399054	2.754831	-0.039295
			O	-3.362397	-2.276897	1.200843
			H	1.019089	-2.402781	-0.034880
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-476.06 77.11 91.534 119.92 153.7	C	3.512909	-0.196626	-0.253216
5-25_TS		165.12 222.49 258.15 346.1 400.04	C	2.874879	-1.390792	-0.414229
	Energy (hartree): -614.7040920	436.94 467.06 494.39 498.13 510.16	C	1.394062	-1.455193	-0.297274
		540.6 561.58 588.72 629.76 655.89	C	0.672420	-0.158541	-0.099607
	ZPE (hartree): 0.1891570	677.97 700.48 709.39 753.34 767.81	C	1.387276	1.042403	0.129981
		805.71 828.55 854.42 890.72 899.84	C	2.807176	0.993368	0.002178
	<S^2>: 0	909.34 946.21 968.99 973.02 974.79	H	3.413415	-2.312779	-0.590738
		1018.3 1036.2 1097.9 1105 1133.2	H	0.947415	-2.004746	-1.141619

	Rotational constants (GHz): 1.1148 0.5616 0.4161	1178.7 1187.6 1201.8 1230.8 1239.5 1259.3 1284.5 1314.8 1379 1386.9 1389.8 1397.1 1430.8 1464.5 1508.7 1556.9 1587.9 1604.3 1904.7 2942.1 2963.2 3059.1 3156.1 3159.5 3177 3181.7 3194.9 3198.3 3222.5	H 4.593875 -0.149018 -0.334909 H 3.354258 1.927337 0.063535 C -0.762746 -0.120206 -0.039111 C -1.480893 1.159354 0.059639 C -0.724780 2.296267 0.322297 C 0.657486 2.245698 0.396863 H -1.230002 3.249763 0.442690 H 1.220880 3.151300 0.587683 C -1.429133 -1.389385 0.590523 C -1.984779 -1.175082 -0.703671 C -3.127542 -0.232793 -0.807861 C -2.840102 1.010281 -0.334025 H -1.757928 -1.917460 -1.473005 H -4.067190 -0.566999 -1.223198 H -3.554952 1.823151 -0.306934 O -1.224655 -2.111992 1.510170 H 1.140072 -2.077138 0.580210
(OH + phen. rad.) 6	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8235691 ZPE (hartree): 0.1948880 $\langle S^2 \rangle$: 0 Rotational constants (GHz): 1.1957 0.5259 0.3660	76.904 82.707 177.3 185.34 238.89 256.37 301.19 363.25 398.82 408.06 474.27 486.92 512.63 520.07 549.65 555.22 618.16 661.64 668.45 712.9 720.65 754.38 801.66 807.12 814.73 841.73 866.9 891.7 917.69 949.05 979.15 983.74 989.04 1007.1 1024.7 1085.1 1099.3 1161.6 1167.1 1174.5 1184.6 1232.9 1240.8 1267.6 1283.7 1352.6 1361.6 1378.1 1388.3 1393.3 1440.1 1455.3 1510.3 1519.9 1525.3 1569.9 1593.2 1606.4 1671.8 2955.4 2958.3 3155.6 3159 3160.8 3168.2 3178.2 3179.9 3181.2 3188.1	C -3.633697 -0.183837 0.000116 C -2.918638 -1.482559 0.000125 C -1.441132 -1.416179 0.000145 C -0.735478 -0.221563 0.000014 C -1.504477 1.007618 -0.000116 C -2.949836 0.973610 -0.000022 H -3.250299 -2.090538 0.860026 H -0.862235 -2.332464 0.000295 H -4.718377 -0.189612 0.000272 H -3.472542 1.924549 0.000006 C 0.709672 -0.160929 -0.000045 C 1.339615 1.121407 -0.000065 C 0.541486 2.283412 -0.000026 C -0.842292 2.237154 -0.000099 H 1.039892 3.248057 0.000027 H -1.419471 3.155042 -0.000078 C 1.530036 -1.369049 -0.000095 C 2.953744 -1.137095 0.000223 C 3.537009 0.123321 0.000232 C 2.749601 1.263724 -0.000069 H 3.568832 -2.030423 0.000344

			H	4.618772	0.211649	0.000419
			H	3.186275	2.255091	0.000007
			O	1.068206	-2.536901	-0.000406
			H	-3.250188	-2.090352	-0.859976
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-92.637 37.492 44.939 102.18 130.3	C	3.651731	-0.822537	0.367751
6-27_TS		161.63 191.67 261.9 286.83 350.91	C	2.898531	-1.777248	-0.505738
	Energy (hartree): -614.6933559	396.44 425.2 437.69 446.72 475.9 495.8	C	1.566727	-1.290991	-0.954425
		536.65 545.72 595.81 654.26 676.79	C	1.044286	-0.083879	-0.573097
	ZPE (hartree): 0.1895880	688.73 728.08 750.1 776.81 796.16	C	1.858361	0.823944	0.231602
		809.69 847.55 891.66 896.54 932.34	C	3.158234	0.384938	0.692580
	$\langle S^2 \rangle$: 0	951.07 962.75 982.45 995.3 996.54	H	3.495705	-2.023576	-1.400562
		1037.4 1124 1127.6 1164.8 1178.2	H	0.952125	-1.936796	-1.572925
	Rotational constants (GHz):	1191.1 1223.5 1243.8 1267.2 1300	H	4.617995	-1.142945	0.742002
	0.9979	1346.7 1368.1 1384.4 1407.3 1408.1	H	3.729600	1.054732	1.328732
	0.4139	1425.4 1433.9 1519.7 1559.4 1586	C	-0.330621	0.196437	-0.891082
	0.3282	1667.3 1677.6 2202.6 2955 2963.7	C	-0.917467	1.299141	-0.249843
		3110.1 3125.6 3133 3148.5 3158 3168.5	C	-0.058383	2.295403	0.254471
		3175.2 3176.9	C	1.295922	2.043729	0.543128
			H	-0.447459	3.297128	0.426489
			H	1.879377	2.800964	1.056457
			C	-2.896436	-1.606031	0.533888
			C	-3.100400	-0.836783	-0.509328
			C	-3.331954	0.626847	-0.383345
			C	-2.365366	1.546217	-0.263652
			H	-3.084794	-1.321945	-1.479789
			H	-4.367181	0.960772	-0.396987
			H	-2.674812	2.582378	-0.134921
			O	-2.715728	-2.289120	1.459801
			H	2.786286	-2.752882	-0.004348
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-288.53 70.028 103.26 161.19 164.62	C	3.532775	-0.130940	-0.218854
6-28_TS		250.31 262.47 278.44 349.12 416.89	C	2.845732	-1.448123	-0.398977
	Energy (hartree): -614.7593422	435.91 470.21 485.39 495.27 538.75	C	1.355023	-1.368809	-0.312043
		571.47 612.58 662.09 673.48 699.76	C	0.675773	-0.224817	-0.081030
	ZPE (hartree): 0.1930520	718.94 751.94 778.88 794.7 831.23	C	1.404075	1.038223	0.109477
		849.92 863.52 879.02 910.79 921.66	C	2.852987	1.001029	0.010187
	$\langle S^2 \rangle$: 0	938.48 964.32 988.51 998.75 999.56	H	3.132681	-1.893619	-1.365246
		1029.7 1073 1091.4 1121.2 1134.5 1171	H	0.814634	-2.300624	-0.440525
	Rotational constants (GHz):	1196.1 1203.1 1255.6 1265.6 1279.9	H	4.616227	-0.116773	-0.277177

	1.1236 0.5502 0.4039	1319.5 1374.3 1383.3 1391.8 1425.2 1434.6 1444 1556.7 1607.3 1632.1 1651.3 1705.2 1845.9 2958.2 2961.4 3113.8 3150.1 3160.9 3168.3 3172 3176.1 3185 3210.3	H	3.382729	1.940148	0.138078
			C	-0.806113	-0.175514	0.065698
			C	-1.457558	1.155375	0.100161
			C	-0.701560	2.264554	0.321409
			C	0.728289	2.199158	0.359960
			H	-1.186833	3.232202	0.396111
			H	1.288456	3.115241	0.512685
			C	-1.491266	-1.374491	0.580085
			C	-2.154978	-1.142065	-0.688222
			C	-3.196559	-0.103876	-0.761756
			C	-2.850031	1.101522	-0.267613
			H	-2.067038	-1.909429	-1.456073
			H	-4.164048	-0.344147	-1.185789
			H	-3.508424	1.957776	-0.204113
			O	-1.243445	-2.282074	1.328388
			H	3.219649	-2.171539	0.344052
(OH + phen. rad.) 7	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8880195 ZPE (hartree): 0.1969980 $<S^2>$: 0 Rotational constants (GHz): 1.2041 0.5198 0.3639	9.5396 78.386 107 203.38 241.16 245.72 363.92 379.22 396.92 420.61 480.94 497.83 522.79 534.41 545.26 563.65 626.37 655.79 665.76 711.9 742.21 773.67 794.39 815.32 841.67 853.67 894.6 940.24 960.05 973.74 986.25 999.34 1004.9 1022.9 1025.8 1061.5 1138.4 1174.7 1181.2 1199.7 1206.6 1217.3 1229 1244.4 1301.3 1345 1362.3 1384 1399.8 1416.9 1438.1 1459.7 1496.4 1545.2 1584.8 1632.9 1654.9 1704.1 1725.6 3016.1 3034.4 3153 3158.4 3161 3170.2 3173.6 3179.5 3186.6 3256.3	C	3.671178	-0.345794	0.000118
			C	2.905217	-1.529160	0.000035
			C	1.529097	-1.490757	-0.000038
			C	0.827964	-0.252299	-0.000023
			C	1.617141	0.946303	0.000030
			C	3.032080	0.868711	0.000110
			H	3.407181	-2.490506	0.000015
			H	0.960019	-2.405431	-0.000124
			H	4.754011	-0.397740	0.000184
			H	3.600548	1.792887	0.000155
			C	-0.610983	-0.136234	-0.000040
			C	-1.203822	1.137852	-0.000088
			C	-0.391562	2.300880	-0.000096
			C	0.971301	2.207989	-0.000014
			H	-0.873661	3.272167	-0.000153
			H	1.581476	3.105443	0.000011
			C	-1.507830	-1.326261	-0.000071
			C	-3.021674	-1.102482	0.000449
			C	-3.510588	0.303813	0.000082
			C	-2.652662	1.326466	-0.000157
			H	-3.415158	-1.649356	-0.866004
			H	-4.582273	0.475270	0.000047

			H	-3.013873	2.349604	-0.000390
			O	-1.116626	-2.482239	-0.000411
			H	-3.414405	-1.648584	0.867772
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-917.86 57.807 95.598 159.76 219.78	C	3.650372	-0.327297	0.025168
7-8_TS		253.45 271.54 359.25 398.62 411.4	C	2.897903	-1.511558	0.013602
	Energy (hartree): -614.8114709	452.26 491.55 511.7 529.09 542.29	C	1.517354	-1.478384	-0.006129
		557.36 564.02 638.38 677.13 703.28	C	0.812842	-0.244035	-0.008565
	ZPE (hartree): 0.1927790	720.98 725.01 767.68 802.01 807.6	C	1.592912	0.957867	0.000182
		818.78 837.63 848.84 895.73 924.13	C	2.999797	0.888867	0.016680
	$\langle S^2 \rangle$: 0	974.59 985.78 990.02 1023.3 1031.8	H	3.404340	-2.470441	0.016158
		1049.5 1068.7 1140.9 1159.2 1180.3	H	0.942876	-2.390496	-0.023194
	Rotational constants (GHz):	1186.5 1220.2 1233.4 1238.5 1256.8	H	4.733860	-0.367896	0.037380
	1.1841	1303.5 1340.7 1359.6 1368.4 1401.9	H	3.565306	1.814915	0.022110
	0.5308	1445.1 1454 1488.6 1507.1 1556.9	C	-0.632588	-0.156078	-0.017905
	0.3673	1577.9 1622.6 1644.8 1659.6 2460.6	C	-1.240170	1.142687	-0.021143
		3148 3156.8 3159.3 3169.8 3177.6	C	-0.410776	2.319302	-0.019255
		3185.2 3200.8 3206.8 3242.1	C	0.938603	2.229773	-0.009504
			H	-0.900804	3.286750	-0.026748
			H	1.550429	3.126018	-0.007641
			C	-1.479434	-1.374980	-0.018151
			C	-2.902675	-1.139761	-0.038900
			C	-3.485128	0.197411	0.020322
			C	-2.630779	1.323387	-0.032004
			H	-3.551190	-2.006485	-0.013174
			H	-4.544062	0.309937	-0.196067
			H	-3.049980	2.320789	-0.042458
			O	-1.062753	-2.546200	-0.039234
			H	-3.418151	-0.216712	1.121115
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-1573.4 81.77 97.972 164.99 219.74	C	-3.623578	-0.337230	0.148728
7-13_TS		222.5 280.2 349.74 401.23 416.29 477.77	C	-2.868947	-1.519647	0.175695
	Energy (hartree): -614.8075593	488 500.99 530.58 554.85 562.43 604.82	C	-1.488229	-1.476162	0.112249
		652.67 681.26 703.03 727.1 752.64 782.4	C	-0.807381	-0.243707	0.027416
	ZPE (hartree): 0.1914270	806.85 812.41 840.85 854.53 892.58	C	-1.574888	0.952894	-0.014559
		918.95 971.65 980.52 990.22 1002	C	-2.982013	0.880165	0.050760
	$\langle S^2 \rangle$: 0	1004.9 1035 1064.4 1078.6 1109 1140.9	H	-3.370519	-2.478575	0.240114
		1165.1 1179.9 1183.7 1191.7 1239.7	H	-0.917876	-2.393212	0.106014
	Rotational constants (GHz):	1250.5 1303.9 1320.8 1359.9 1377.4	H	-4.705703	-0.381314	0.197740
	1.1801	1406.1 1449.4 1460.9 1477.7 1514.6	H	-3.554157	1.801583	0.022200

	0.5343 0.3765	1533.4 1569.7 1595.7 1647 1656.2 1773.9 3159.5 3161.7 3161.9 3172.9 3174.2 3179.5 3187.5 3188.5 3227.5	C	0.654165	-0.151828	0.017458
			C	1.272138	1.148692	-0.109172
			C	0.438240	2.312744	-0.196906
			C	-0.912699	2.220718	-0.141533
			H	0.922436	3.278543	-0.291767
			H	-1.524209	3.115420	-0.193515
			C	1.527064	-1.362247	-0.254329
			C	2.813909	-1.093670	0.428864
			C	3.425375	0.168950	0.313920
			C	2.669627	1.270739	-0.034795
			H	1.481775	-0.639793	1.178485
			H	4.475269	0.276476	0.562942
			H	3.122603	2.251408	-0.120373
			O	1.176516	-2.436125	-0.693581
			H	3.401551	-1.963991	0.704034
(OH + phen. rad.) 7-19_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7361361 ZPE (hartree): 0.1844440 $\langle S^2 \rangle$: 0 Rotational constants (GHz): 1.1856 0.5242 0.3663	-216.74 70.659 93.228 125.55 175.39 198.98 229.39 259.42 274.74 336.59 361.15 411.85 425.29 436.27 456.57 492.01 519.73 527.33 540.75 542.74 589.45 654.29 678.11 695.93 732.88 742.93 767.74 811.73 821.6 839.69 844.83 886.94 896.19 940.32 973.49 986.25 1012.4 1028.1 1057.4 1063 1159.3 1164.8 1179.8 1188.1 1229.6 1240.1 1290.4 1320.9 1339.8 1376.8 1389.2 1410.6 1455.4 1481.9 1516.7 1545 1580.1 1626.5 1643.7 1652.7 3155.4 3160.8 3163.8 3169.6 3172.7 3181.8 3187.9 3242.9 4234.3	C	3.646034	-0.454685	-0.032896
			C	2.840835	-1.610058	-0.110622
			C	1.468114	-1.519738	-0.111488
			C	0.821397	-0.255760	-0.038813
			C	1.645085	0.916096	0.042919
			C	3.054691	0.783030	0.041342
			H	3.309751	-2.586046	-0.166516
			H	0.860299	-2.409983	-0.146144
			H	4.726235	-0.546127	-0.029215
			H	3.660303	1.681013	0.103489
			C	-0.602321	-0.083994	-0.110498
			C	-1.168239	1.203825	-0.016657
			C	-0.317344	2.343331	0.079649
			C	1.038415	2.200642	0.106536
			H	-0.767259	3.328032	0.139888
			H	1.678734	3.073758	0.174255
			C	-1.559805	-1.251446	-0.023433
			C	-2.867999	-0.818218	-0.413353
			C	-3.490127	0.336066	-0.029743
			C	-2.590838	1.396451	0.024867
			H	-4.113199	-2.665336	0.371080
			H	-4.555950	0.512814	-0.127557
			H	-2.975052	2.404111	-0.100974

			O	-1.241196	-2.375236	0.361038
			H	-3.401683	-2.903605	0.446519
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	43.316 90.675 147.88 178.33 217.26 257	C	-3.641421	-0.325503	0.000311
8		289.24 355.31 398.02 404.82 483.38	C	-2.894587	-1.510355	0.000210
	Energy (hartree): -614.8204367	493.82 508.14 529.32 531.48 560.61	C	-1.512950	-1.476989	-0.000007
		609.13 659.51 673.74 708.05 710.85	C	-0.807857	-0.240331	-0.000098
	ZPE (hartree): 0.1941540	752.07 781.53 794.84 807.9 827.54	C	-1.588451	0.966062	-0.000029
		842.04 878.81 899.52 974.45 980.08	C	-2.990048	0.895273	0.000176
	<S^2>: 0	992.57 1008.4 1018.5 1026.4 1063	H	-3.402599	-2.468089	0.000278
		1088.2 1095.6 1150.4 1179 1184.1	H	-0.927451	-2.383411	-0.000147
	Rotational constants (GHz):	1224.7 1240.1 1261 1300.2 1315.9	H	-4.725239	-0.362829	0.000491
	1.1709	1335.1 1339.9 1360.7 1409.7 1417.1	H	-3.559000	1.818974	0.000218
	0.5329	1443.3 1469.1 1498.2 1563.7 1580.7	C	0.631490	-0.164907	-0.000170
	0.3670	1611.4 1641.3 1665 2948.1 2948.6	C	1.240268	1.151410	-0.000167
		3159.1 3161.4 3172.6 3178.8 3183.7	C	0.407694	2.334822	-0.000296
		3186.5 3187.7 3224.7	C	-0.936876	2.245679	-0.000204
			H	0.902104	3.300033	-0.000415
			H	-1.553071	3.138558	-0.000246
			C	1.477495	-1.400503	-0.000191
			C	2.875545	-1.163735	0.000525
			C	3.496758	0.157720	0.000431
			C	2.606442	1.314622	0.000126
			H	3.512094	-2.041094	0.000825
			H	4.190137	0.244586	0.858277
			H	3.037475	2.308978	0.000094
			O	1.019358	-2.562410	-0.000644
			H	4.189673	0.243983	-0.857930
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-245.79 92.589 94.05 164.82 204.1	C	3.548562	-0.293628	-0.304628
8-9_TS		228.07 251.48 309.35 389.25 411.9	C	2.811037	-1.471609	-0.433841
	Energy (hartree): -614.7960823	432.67 481.32 502.68 532.5 554 571.05	C	1.427987	-1.446331	-0.302931
		635.65 654.45 674.9 722.34 729.13	C	0.752460	-0.243704	-0.064649
	ZPE (hartree): 0.1941580	757.48 784.87 793.27 813.87 825.65	C	1.499511	0.953184	0.078185
		869.07 886.9 905.38 947.63 956.45	C	2.895566	0.903121	-0.042511
	<S^2>: 0	983.43 992.83 1013.9 1031.5 1067.9	H	3.315419	-2.411408	-0.626535
		1086.9 1123.7 1154.4 1167.1 1187.1	H	0.865011	-2.368591	-0.376353
	Rotational constants (GHz):	1194.2 1219.8 1236.5 1288.3 1302.3	H	4.628243	-0.313315	-0.399099
	1.1108	1309.2 1334.7 1362.4 1373.7 1429.1	H	3.465081	1.819694	0.071015
	0.5527	1446 1483.9 1506.9 1593 1629.5 1647.3	C	-0.707128	-0.177847	0.109836

	0.4060	1669.1 1814.7 2983.1 3019.2 3144.6 3159.9 3162.6 3173.2 3181 3186 3192.8 3196.7	C	-1.359490	1.153539	0.107579
			C	-0.524336	2.302863	0.406569
			C	0.818534	2.205418	0.375629
			H	-1.011161	3.257292	0.574246
			H	1.433107	3.083698	0.542768
			C	-1.449671	-1.334456	0.611847
			C	-2.224069	-1.179448	-0.592433
			C	-3.198998	-0.063223	-0.823111
			C	-2.651684	1.212120	-0.273558
			H	-2.185180	-2.008303	-1.294879
			H	-3.428801	0.043652	-1.890492
			H	-3.245584	2.117001	-0.239606
			O	-1.189230	-2.251253	1.358280
			H	-4.151968	-0.329689	-0.339202
(OH + phen. rad.) 8-12_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7228990 ZPE (hartree): 0.1911840 $<S^2>$: 0 Rotational constants (GHz): 1.0331 0.3869 0.2857	-72.439 32.84 63.9 80.981 148.61 182.29 205.81 217.24 258.76 366.07 391.6 421.55 463.35 485.48 504.27 520.11 541.52 591.08 629.74 640.66 657.97 715.54 737.27 765.01 787.09 808.69 848.56 863.52 897.29 900.18 956.95 979.84 987.28 1010.9 1020.7 1047.2 1065 1120.7 1150.8 1163.8 1176.7 1206.1 1217.8 1238.7 1266.7 1305.9 1341.7 1352.1 1394.1 1428.3 1430.1 1450.6 1454.1 1481.6 1557.5 1574.2 1632.5 1645.3 2219.4 2999.3 3025 3104.1 3137.2 3152.7 3167.4 3169.1 3180.3 3188 3193.7	C	3.788478	1.147762	-0.050941
			C	2.779327	2.122330	-0.123474
			C	1.454695	1.735521	-0.064534
			C	1.085617	0.368576	0.019037
			C	2.130027	-0.615294	0.056871
			C	3.470769	-0.198369	0.049057
			H	3.044735	3.170385	-0.200782
			H	0.649967	2.461372	-0.079373
			H	4.829679	1.452156	-0.066820
			H	4.261845	-0.939747	0.105402
			C	-0.296583	0.032028	0.159476
			C	-0.581705	-1.374987	0.036603
			C	0.474208	-2.388020	0.065322
			C	1.770879	-2.013378	0.094436
			H	0.202471	-3.439122	0.014449
			H	2.565864	-2.752050	0.104280
			C	-3.471342	1.390873	0.173664
			C	-3.331158	0.148410	0.561964
			C	-3.138154	-1.009999	-0.386236
			C	-1.860543	-1.790455	-0.259214
			H	-3.245548	-0.010089	1.629676
			H	-3.958852	-1.726411	-0.250485
			H	-1.980279	-2.848908	-0.494961
			O	-3.597122	2.496407	-0.166202

			H	-3.239992	-0.668824	-1.423945
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	70.332 86.34 139.89 177.97 213.12	C	3.550444	-0.318846	-0.219791
9		238.65 269.63 380.13 393.87 427.98	C	2.828466	-1.474996	-0.506237
	Energy (hartree): -614.8035619	455.52 508.31 513.69 550.73 569.53	C	1.435228	-1.456422	-0.462428
		618.36 664.8 685.46 695.44 732.74	C	0.748526	-0.286672	-0.142794
	ZPE (hartree): 0.1952330	756.75 763.73 785.99 813.13 832.48	C	1.475778	0.894386	0.142741
		857.57 879.3 895.45 914.95 950.56	C	2.875206	0.853866	0.102287
	$\langle S^2 \rangle$: 0	950.87 983.33 991.78 1007 1029 1044.5	H	3.346556	-2.392960	-0.759191
		1062.8 1080.8 1143.3 1157.2 1170.3	H	0.882408	-2.364601	-0.678051
	Rotational constants (GHz):	1185.8 1191.5 1232 1254.1 1288.3	H	4.633866	-0.330910	-0.247908
	1.1229	1303.1 1327.2 1333.1 1354.1 1427.3	H	3.433967	1.758563	0.318979
	0.5380	1482.5 1486.9 1508.1 1596.5 1632.9	C	-0.727146	-0.219849	-0.008546
	0.4296	1645.5 1679 1913.5 3002.3 3032.6	C	-1.373157	1.136506	-0.080535
		3136.6 3157.4 3159.8 3163.9 3176.7	C	-0.569054	2.269591	0.328044
		3178.6 3190.8 3193.5	C	0.768604	2.138620	0.443757
			H	-1.048771	3.230210	0.480617
			H	1.373981	2.997247	0.715758
			C	-1.495035	-1.180352	0.840572
			C	-1.870822	-1.192886	-0.572128
			C	-3.024035	-0.291642	-1.034074
			C	-2.615329	1.093517	-0.593008
			H	-1.624064	-2.081832	-1.146260
			H	-3.166101	-0.342494	-2.121046
			H	-3.262093	1.954354	-0.709810
			O	-1.581086	-1.699755	1.912523
			H	-3.967095	-0.618461	-0.580430
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-564.3 62.535 72.67 142.16 163.74	C	3.565189	-0.306205	-0.062583
9-10_TS		226.32 248.43 262.52 343.9 405.02	C	2.864640	-1.474420	-0.386761
	Energy (hartree): -614.7754758	423.83 455.62 469.91 513.59 532.18	C	1.483385	-1.462578	-0.501493
		545.12 592.04 651.86 680.55 687.1	C	0.749770	-0.277306	-0.289825
	ZPE (hartree): 0.1931210	722.97 750.58 766.94 775.09 823.91	C	1.463888	0.914857	0.048686
		845.52 859.53 872.54 932.22 939.11	C	2.862625	0.871126	0.148955
	$\langle S^2 \rangle$: 0	973.15 975.52 984.08 989.95 1016.1	H	3.406739	-2.398534	-0.556276
		1054.5 1075.2 1125.8 1154.1 1162	H	0.963388	-2.377959	-0.765552
	Rotational constants (GHz):	1180.6 1182 1201.9 1229.8 1250.7	H	4.645362	-0.322229	0.020631
	1.1647	1289.4 1304.3 1345.3 1350.9 1417.4	H	3.395400	1.782690	0.401676
	0.5303	1429.9 1478.4 1490.5 1495.9 1568.2	C	-0.669543	-0.165321	-0.379334
	0.4350	1582.1 1635.5 1649 2067.2 2930.4	C	-1.394318	1.077299	-0.182117

		3089.8 3113.5 3150.2 3151.3 3156.9 3170.7 3177.7 3188.7 3214.6	C	-0.620783	2.235762	0.192706
			C	0.728652	2.139920	0.289718
			H	-1.123790	3.178454	0.377317
			H	1.307853	3.018346	0.558532
			C	-1.672072	-1.199036	0.939016
			C	-1.763621	-1.206981	-0.510683
			C	-3.010453	-0.456505	-0.995008
			C	-2.743515	0.917750	-0.398726
			H	-1.543544	-2.189457	-0.927371
			H	-3.031475	-0.441973	-2.098660
			H	-3.472514	1.715430	-0.399218
			O	-1.461359	-1.333171	2.070262
			H	-3.919628	-0.949571	-0.648473
(OH + phen. rad.) 10	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8343711 ZPE (hartree): 0.1970580 $<S^2>$: 0 Rotational constants (GHz): 1.3287 0.4644 0.3915	69.713 106.17 146.3 206.88 237.76 257.09 405.75 413.82 436.78 463.22 482.71 513.54 538.52 569.17 579.37 626.64 678.69 706.67 730.12 755.78 796.21 809.24 819.63 837.33 843.55 866.96 880.2 910.27 958.61 967.19 968.75 995.03 1003.2 1031.9 1041 1051.2 1066.9 1117 1158.6 1165.5 1169.5 1175.1 1181.2 1226 1236.6 1245.7 1269.5 1290.4 1379.5 1388.1 1415.6 1471 1482.9 1491.4 1559.5 1606.5 1624.9 1665.6 1891.1 3050.7 3120.8 3148.7 3153.8 3158.9 3163.5 3167.8 3179.3 3182.2 3189.8	C	3.713122	-0.464025	0.157711
			C	2.968137	-1.654497	-0.018976
			C	1.602923	-1.607198	-0.155107
			C	0.913074	-0.366157	-0.117586
			C	1.664985	0.845844	0.071546
			C	3.076403	0.751506	0.200097
			H	3.483187	-2.608094	-0.049089
			H	1.037492	-2.521539	-0.294807
			H	4.791061	-0.517322	0.260036
			H	3.647568	1.663838	0.337705
			C	-0.481864	-0.226973	-0.266397
			C	-1.105857	1.016039	-0.198860
			C	-0.377344	2.193801	0.022171
			C	0.994177	2.096758	0.136752
			H	-0.873231	3.155417	0.091235
			H	1.589586	2.991469	0.284770
			C	-2.578981	-0.545161	0.682782
			C	-1.635229	-1.202296	-0.400064
			C	-2.558891	-0.423979	-1.401479
			C	-2.582092	0.690531	-0.298479
			H	-1.459757	-2.272340	-0.459765
			H	-2.093302	-0.140118	-2.346620
			H	-3.324982	1.482556	-0.258651
			O	-3.117997	-0.869593	1.688428
			H	-3.529025	-0.902295	-1.556902

(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-437.49 40.01 69.672 130.77 136 241.73	C	3.663595	-0.325057	0.224510
10-11_TS		252.42 279.75 410.3 425.01 462.55	C	2.999877	-1.544644	0.000917
	Energy (hartree): -614.8067428	474.31 504.41 519.34 529.14 556.29	C	1.638146	-1.563372	-0.224316
		599.22 617.83 688.88 706.6 755.46	C	0.887911	-0.369076	-0.226176
	ZPE (hartree): 0.1939430	761.25 801.22 822.65 823.42 843.99	C	1.557894	0.869699	0.005773
		882.82 885.56 897.42 958.97 977.34	C	2.953703	0.857641	0.223454
	<S^2>: 0	980.41 987.27 990.33 993.47 1016.3	H	3.561455	-2.472028	0.000905
		1054 1099.3 1138 1168.5 1181.8 1196.6	H	1.135007	-2.505923	-0.407726
	Rotational constants (GHz):	1210.4 1232.2 1265.5 1281 1325.9	H	4.733977	-0.316562	0.396279
	1.2095	1344.4 1363.5 1407 1445 1472.1 1480.2	H	3.463694	1.799731	0.396341
	0.4739	1492.4 1558.6 1581.4 1635.3 1654.5	C	-0.527476	-0.321494	-0.469445
	0.4160	1995.5 3011.2 3108.9 3158.4 3161.1	C	-1.224822	0.920511	-0.446649
		3167.4 3178.6 3178.7 3180.5 3189.1	C	-0.535202	2.134625	-0.170125
		3192.1	C	0.813476	2.099929	0.027460
			H	-1.077671	3.072892	-0.133549
			H	1.360232	3.018684	0.212734
			C	-2.493305	-0.577047	1.086416
			C	-1.509913	-1.348507	-0.568524
			C	-2.713536	-0.713040	-1.234765
			C	-2.619588	0.621917	-0.523667
			H	-1.281287	-2.405672	-0.631922
			H	-2.535676	-0.587895	-2.312320
			H	-3.388742	1.385403	-0.567500
			O	-2.458045	-0.524429	2.236638
			H	-3.651184	-1.245702	-1.075517
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	104.5 117.57 235.81 251.61 263.57	C	-3.341189	-0.150714	0.000042
11		362.61 420.07 427.43 453.46 518.97	C	-2.762853	-1.422092	-0.000026
	Energy (hartree): -501.5008044	534.55 553.45 608.07 683.59 691.98	C	-1.380282	-1.556043	-0.000061
		699.96 739.25 755.67 768.57 807.32	C	-0.544943	-0.432273	-0.000005
	ZPE (hartree): 0.1856260	827.77 836.83 874.71 885.81 906.34	C	-1.130825	0.861528	0.000027
		946.86 952.52 981.76 982.91 991.86	C	-2.529765	0.975237	0.000058
	<S^2>: 0	1006.7 1062.7 1111.3 1119.1 1163	H	-3.391073	-2.305678	-0.000061
		1183.8 1201.9 1225.7 1233.6 1270.2	H	-0.939097	-2.546387	-0.000136
	Rotational constants (GHz):	1276.8 1321.1 1334 1382.2 1405.2	H	-4.419847	-0.042364	0.000068
	1.8159	1427.7 1484.7 1503.6 1575 1592 1625.8	H	-2.975949	1.964485	0.000086
	0.6615	1647.2 1678.2 2999.2 3016.4 3154.5	C	0.914078	-0.520575	-0.000006
	0.4863	3158.7 3166.4 3176.2 3178.1 3189.3	C	1.721877	0.720216	-0.000064
		3210.8 3213.9	C	1.057733	2.001377	-0.000075

			C -0.291409 2.054342 -0.000014 H 1.650757 2.909588 -0.000109 H -0.798684 3.013928 0.000027 C 1.752415 -1.586068 0.000021 C 3.172000 -1.096663 0.000026 C 3.039493 0.397547 0.000061 H 1.482785 -2.632974 0.000051 H 3.729186 -1.459990 0.875770 H 3.874750 1.084470 0.000100 H 3.729206 -1.460005 -0.875702
(OH + phen. rad.) 12	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7309444 ZPE (hartree): 0.1911350 $\langle S^2\rangle$: 0 Rotational constants (GHz): 1.1607 0.3222 0.2526	21.552 57.374 64.211 108.6 166.28 189.21 195.24 245.6 260.56 392.58 406.82 428.45 465.61 491.55 520.21 559.73 603.96 634.81 638.44 668.58 679.34 730.03 758.5 773.67 783.19 809.74 828.21 898.27 898.75 931.65 978.09 985.98 993.31 994.26 1012.2 1048.4 1075.5 1129.3 1146.3 1168.9 1180 1206.1 1213.4 1238.4 1272.3 1308.5 1315.3 1353.4 1396.2 1413.8 1433.6 1443 1459.3 1492.2 1561.2 1584.6 1635.6 1651.9 2195.7 2781.9 2950 2951.2 3108.2 3137.6 3155.1 3168.7 3170.6 3181.7 3195.7	C -3.936058 -1.243458 -0.000047 C -2.920826 -2.214075 -0.000066 C -1.599135 -1.814134 -0.000011 C -1.238190 -0.441956 0.000029 C -2.290002 0.534166 0.000010 C -3.627925 0.108312 -0.000007 H -3.179031 -3.266652 -0.000113 H -0.791081 -2.536189 0.000009 H -4.975226 -1.555146 -0.000059 H -4.423824 0.846384 0.000016 C 0.150997 -0.102788 0.000179 C 0.417852 1.323546 0.000052 C -0.651983 2.320546 0.000030 C -1.945462 1.934907 0.000023 H -0.392434 3.375870 0.000045 H -2.747201 2.666089 0.000023 C 4.098314 -1.157093 0.000079 C 3.039596 -0.396563 0.000143 C 3.026080 1.104257 0.000018 C 1.712294 1.794347 -0.000291 H 2.032293 -0.861981 0.000317 H 3.570931 1.521059 0.864492 H 1.826354 2.879341 -0.000630 O 5.011765 -1.886236 -0.000136 H 3.571804 1.521029 -0.863855
(OH + phen. rad.) 12-9_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7185980	-166.66 43.939 60.467 94.503 155.39 192.49 217.5 244.42 291.5 376.18 406.63 440.88 466.44 506.82 518.21 527.11	C 3.506058 1.079546 -0.172696 C 2.487060 2.022044 0.048186 C 1.192301 1.606662 0.285008

	ZPE (hartree): 0.1908100 <S^2>: 0 Rotational constants (GHz): 0.9355 0.5020 0.3360	573.57 619.57 628.87 636.07 675.06 708.67 737.87 746.48 762.71 774.46 814.17 870.19 874.8 883.61 951.06 968.64 971.71 988.07 1004.1 1045.4 1053.2 1118.4 1125.2 1157.1 1177.9 1192.1 1212.5 1231.1 1261.7 1299.8 1313.1 1327.5 1388.2 1392.5 1417.2 1456.5 1462.4 1483 1532.7 1560.6 1628.2 1632.9 2171.3 2981.1 3020 3150.8 3153.8 3165.4 3171.9 3175.2 3179.9 3189.7 3195.5	C 0.847775 0.232356 0.241927 C 1.885068 -0.723353 -0.039040 C 3.205950 -0.272094 -0.198707 H 2.725206 3.079846 0.058577 H 0.412615 2.331657 0.488136 H 4.527317 1.411770 -0.320078 H 3.991766 -0.999916 -0.376173 C -0.416861 -0.276454 0.625797 C -0.822754 -1.565577 0.187503 C 0.248082 -2.534058 -0.045193 C 1.531142 -2.119863 -0.141965 H -0.023938 -3.564567 -0.250635 H 2.318675 -2.831516 -0.367872 C -2.637961 1.706614 -0.052035 C -2.636596 0.497451 0.493582 C -3.106104 -0.733661 -0.269882 C -2.129556 -1.856694 -0.112586 H -2.611100 0.482684 1.575167 H -4.101783 -1.025931 0.087246 H -2.433477 -2.856051 -0.403067 O -2.561950 2.758831 -0.532558 H -3.231300 -0.476129 -1.330226
(OH + phen. rad.) 13	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8574617 ZPE (hartree): 0.1966200 <S^2>: 0 Rotational constants (GHz): 1.1839 0.5271 0.3684	40.531 86.533 151.56 213.53 242.63 267.7 336.23 385.41 407.4 453.02 483.34 488.96 517.99 523.66 552.68 564.39 614.43 670.11 712.5 730.59 753.06 775.7 795.59 818.53 827.81 868.9 890.36 905.77 957.45 968.13 976.87 994.06 1005.2 1014.2 1061.3 1073.5 1131.2 1139.6 1161.6 1177.3 1183.2 1193.1 1211.9 1231.7 1241.1 1265.4 1316.9 1336.3 1376.1 1426.6 1446.1 1486.5 1503.2 1561.7 1599.5 1635.5 1646.5 1666.7 1732.5 2884.4 3155 3156.4 3160.1 3171.7 3173.3 3176.5 3187.5 3193.3 3248	C -3.641264 -0.326491 -0.139370 C -2.915700 -1.502343 0.037214 C -1.530434 -1.466905 0.187286 C -0.832943 -0.255721 0.144240 C -1.573073 0.940245 -0.020931 C -2.968994 0.885602 -0.162764 H -3.426437 -2.458421 0.060896 H -0.982253 -2.386569 0.314876 H -4.719048 -0.356334 -0.251882 H -3.517823 1.813066 -0.289417 C 0.670757 -0.169504 0.378709 C 1.298132 1.183539 0.086447 C 0.444932 2.337022 0.011339 C -0.899624 2.223128 -0.040005 H 0.917657 3.311358 -0.055008 H -1.515501 3.112311 -0.127841

			C	1.549708	-1.380167	-0.042358
			C	2.988583	-1.126508	-0.073223
			C	3.490806	0.133893	-0.086649
			C	2.650513	1.291750	-0.045295
			H	0.799814	-0.254048	1.479070
			H	4.562471	0.279675	-0.182962
			H	3.097765	2.272165	-0.166049
			O	1.097110	-2.492505	-0.248124
			H	3.618081	-1.998414	-0.204546
(OH + phen. rad.) 13-14_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8303822 ZPE (hartree): 0.1940800 $\langle S^2 \rangle$: 0 Rotational constants (GHz): 1.1312 0.5190 0.3710	-501.72 80.245 84.414 144.85 186.55 212.84 286.93 319.33 368.93 415.67 441.62 471.64 503.02 504.83 523.32 561.58 577.76 613.41 674.45 703.2 718 743.5 760.81 785.48 800.16 811.13 832.09 858.61 883.48 942.07 960.39 978.74 986.3 991.71 997.37 1026.5 1054.3 1120 1148.8 1175.5 1182.7 1201.7 1215.6 1245.2 1260.6 1293 1347.2 1369 1403.7 1427.2 1460.6 1475.6 1520.8 1537.1 1556.6 1595.8 1635.1 1653.3 1949.2 3082 3139.5 3156.7 3157.6 3160.9 3171.6 3176 3179 3187 3201.7	C	-3.613609	-0.360957	-0.153333
			C	-2.895793	-1.466159	0.334561
			C	-1.536105	-1.375913	0.568591
			C	-0.841265	-0.176491	0.314497
			C	-1.573126	0.949646	-0.158557
			C	-2.959608	0.830512	-0.391849
			H	-3.412632	-2.399637	0.527032
			H	-0.991269	-2.236706	0.934272
			H	-4.678786	-0.444923	-0.335573
			H	-3.507073	1.694336	-0.754627
			C	0.583121	-0.048232	0.523315
			C	1.233686	1.196177	0.303886
			C	0.449345	2.322384	-0.091991
			C	-0.887322	2.195037	-0.330474
			H	0.945235	3.275591	-0.239517
			H	-1.462051	3.054659	-0.660959
			C	1.701765	-1.565898	-0.368399
			C	3.005114	-1.109532	-0.311097
			C	3.433493	0.179092	0.069713
			C	2.649296	1.271193	0.367782
			H	1.003962	-0.653100	1.327710
			H	4.505525	0.341693	0.011025
			H	3.122456	2.242265	0.458777
			O	1.033745	-2.519263	-0.564160
			H	3.710706	-1.765221	-0.814734
(OH + phen. rad.) 14	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8500507	31.996 44.73 80.924 119.53 149.91 187.85 239.06 291.18 381.91 403.31 425.28 467.48 488.92 501.03 524.42 540.82 585.83 604.95 641.65 667.61	C	3.797090	-0.569201	0.124023
			C	3.060710	-1.586112	-0.527193
			C	1.722826	-1.415916	-0.788330
			C	1.053894	-0.221929	-0.410158

	ZPE (hartree): 0.1942780	691.15 744.41 764.69 781.34 785.67	C	1.800716	0.806702	0.244766
		812.88 840.6 876.53 914.46 928.99	C	3.179663	0.599808	0.499993
	$<S^2>$: 0	934.83 963.6 974.74 979 980.27 994.92	H	3.558316	-2.504331	-0.818403
		1042.2 1132.8 1155.1 1173 1179.5	H	1.156276	-2.197500	-1.283549
	Rotational constants (GHz):	1191.9 1228.8 1265 1273.4 1289.8	H	4.852162	-0.716643	0.325289
	1.1285	1383.5 1394.9 1405.5 1435.3 1447.4	H	3.742422	1.382393	0.998484
	0.4213	1467.5 1503 1539.1 1606 1641.6 1658.2	C	-0.324955	-0.017371	-0.666458
	0.3354	1675.6 2201.5 3133.9 3154.3 3156.1	C	-0.972850	1.146196	-0.291318
		3158 3162.7 3166.9 3169.7 3175.4	C	-0.206077	2.171265	0.339201
		3175.9 3188.1	C	1.127514	2.004595	0.603252
			H	-0.702474	3.094023	0.620376
			H	1.689507	2.794432	1.091200
			C	-2.641176	-1.554550	0.641314
			C	-3.538581	-0.821403	0.005826
			C	-3.443693	0.554627	-0.468228
			C	-2.395607	1.395385	-0.565503
			H	-0.866089	-0.788009	-1.204392
			H	-4.410415	0.955162	-0.756131
			H	-2.632329	2.414054	-0.861408
			O	-1.900951	-2.257660	1.190428
			H	-4.496612	-1.324882	-0.082006
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-78.784 22.532 65.789 120.9 161.76	C	3.922547	-0.963083	0.105546
14-15_TS		185.91 205.73 264.92 365.73 394.2	C	3.014661	-1.966084	-0.310227
	Energy (hartree): -614.8435038	426.01 438.81 479.06 484.17 526.03	C	1.682881	-1.672993	-0.468919
		543.16 561.15 626.31 634.5 669.78	C	1.189909	-0.363405	-0.219574
	ZPE (hartree): 0.1937470	684.78 733.62 767.99 780.08 787.22	C	2.110113	0.648573	0.199694
		798.57 835.19 876.53 915 925.18 960.62	C	3.479406	0.313382	0.354078
	$<S^2>$: 0	964.91 975.13 994.51 996.8 1007.1	H	3.377371	-2.969573	-0.502212
		1041.4 1127.2 1145.6 1172.7 1174.2	H	0.985547	-2.441303	-0.786067
	Rotational constants (GHz):	1187.7 1229.7 1273.4 1277.5 1291.1	H	4.971682	-1.208006	0.227113
	1.1116	1381.9 1389.3 1397.3 1407.2 1438.9	H	4.173918	1.083734	0.672904
	0.3542	1468.5 1501.9 1540.4 1605.5 1641.4	C	-0.179004	-0.039123	-0.373574
	0.2842	1660.5 1684.8 2218 3109.8 3133.4	C	-0.656568	1.238786	-0.130143
		3140.8 3157 3158.7 3163.7 3175.1	C	0.278744	2.236287	0.278628
		3176.4 3188.6 3205.6	C	1.609124	1.953318	0.441545
			H	-0.083213	3.242041	0.465261
			H	2.297949	2.730444	0.756029
			C	-3.614295	-1.307012	0.328974

			C -3.339312 -0.506063 -0.674580 C -3.186140 0.966439 -0.499298 C -2.057224 1.658386 -0.279233 H -0.858880 -0.818291 -0.690105 H -4.104540 1.544784 -0.576360 H -2.192142 2.734680 -0.190425 O -3.846472 -2.015644 1.221136 H -3.324957 -0.957812 -1.662722
(OH + phen. rad.) 15	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8543838 ZPE (hartree): 0.1944450 $\langle S^2 \rangle$: 0 Rotational constants (GHz): 1.2582 0.3001 0.2495	35.931 52.044 104.09 125.05 172.7 187.24 212.11 269.08 375.12 402.05 425.73 455.02 485.59 523.83 526.39 542.01 596.76 635.46 640.67 684.41 693.33 731.04 745.11 772.58 781.98 790.63 837.69 876.12 911.8 921.96 963.11 970.13 975.83 980.55 994.95 1041.7 1063.6 1136.2 1149.8 1172.7 1176.5 1189.1 1227.9 1272.8 1278.3 1290.6 1348 1383.9 1395.2 1405.3 1458.6 1472.6 1504.7 1539.5 1605.1 1640.2 1655.9 1675.4 2207.8 3137.4 3156.1 3157.2 3160.8 3161.5 3171.6 3174.7 3175.7 3179.4 3187.6	C 4.045740 -1.058927 -0.252777 C 3.155221 -2.049461 0.223167 C 1.840600 -1.738895 0.473145 C 1.348845 -0.424025 0.257215 C 2.252790 0.577740 -0.216626 C 3.603046 0.224760 -0.465551 H 3.516530 -3.057911 0.390709 H 1.157903 -2.498623 0.839711 H 5.080668 -1.317154 -0.446743 H 4.284881 0.987727 -0.826984 C -0.002424 -0.075183 0.504703 C -0.476849 1.208987 0.294163 C 0.447484 2.200834 -0.151757 C 1.758439 1.895381 -0.405011 H 0.089871 3.214053 -0.301913 H 2.440080 2.665171 -0.752127 C -4.261795 -1.058915 -0.369809 C -3.116570 -0.410524 -0.261011 C -2.999674 0.909225 0.337692 C -1.867169 1.610817 0.545422 H -0.660828 -0.835715 0.908683 H -3.936285 1.388588 0.604896 H -1.993219 2.626123 0.911272 O -5.261131 -1.641324 -0.464453 H -2.256657 -0.912541 -0.689671
(OH + phen. rad.) 15-16_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7586416 ZPE (hartree): 0.1919670	-203.33 45.508 88.638 117.88 163.77 219.32 259.59 266.52 357 404.33 422.07 458.61 468.39 498.42 522.86 552.22 613.12 640.59 655.33 673.91 725.77 749.08 756.07 783.81 803.35 860.06	C -3.451062 -0.845670 0.218803 C -2.504942 -1.876317 0.172797 C -1.160327 -1.568530 0.007087 C -0.731230 -0.242812 -0.104501 C -1.686703 0.809121 -0.078735

		875.1 893.7 923.22 930.78 952.35 953.72	C	-3.047083	0.471015	0.090833
	$\langle S^2 \rangle$: 0	961 987.38 989.24 1058.1 1078.7 1107.5	H	-2.818171	-2.910277	0.259631
		1132.1 1157.9 1183.5 1218.6 1237.1	H	-0.433748	-2.372820	-0.052797
	Rotational constants (GHz):	1244.2 1266.9 1283.6 1296.5 1323 1342	H	-4.501860	-1.079412	0.349088
	0.9847	1350.2 1403.7 1443.8 1472.4 1499.2	H	-3.781133	1.269529	0.124351
	0.5644	1548.2 1558.2 1609.4 1642.1 2009.3	C	0.708688	0.098487	-0.348447
	0.3722	2859.6 2915.5 3155.5 3156.2 3160.5	C	1.056665	1.547766	-0.205941
		3174.2 3180.3 3188.5 3188.8 3245.9	C	0.053857	2.532493	-0.239869
			C	-1.272407	2.182708	-0.208951
			H	0.341949	3.579105	-0.227820
			H	-2.038349	2.949712	-0.204978
			C	2.416857	-1.669457	-0.041660
			C	1.815575	-0.564701	0.635410
			C	2.936452	0.474266	0.565073
			C	2.426085	1.663435	0.102143
			H	1.022139	-0.251917	-1.351179
			H	3.901503	0.308062	1.016273
			H	2.981776	2.593362	0.074691
			O	2.318691	-2.672450	-0.626838
			H	1.413810	-0.776562	1.643184
(OH + phen. rad.) 16	Theory: B3LYP/6-311G(d,p)	69.635 80.322 130.51 158.56 227.47	C	-3.679890	-0.776357	0.129622
		247.02 344.21 395.21 410.69 443.98	C	-2.810443	-1.861175	0.208126
	Energy (hartree): -614.7959041	484.16 506.78 531.83 539.13 564.99	C	-1.435154	-1.661428	0.082586
		620.19 654.71 691.43 729.68 735.65	C	-0.912803	-0.386481	-0.108404
	ZPE (hartree): 0.1953070	750.07 764.21 801.94 819.38 854.19	C	-1.791607	0.721119	-0.188088
		878.49 884.69 900.73 920.13 949.72	C	-3.171228	0.502145	-0.070014
	$\langle S^2 \rangle$: 0	958.1 981.72 992.06 1000 1031.1 1051.6	H	-3.198486	-2.862092	0.359079
		1065.1 1073.5 1132.5 1160 1185.4	H	-0.769627	-2.516796	0.123581
	Rotational constants (GHz):	1200.3 1207.3 1229 1237.1 1241.1	H	-4.749493	-0.926262	0.222214
	1.2868	1269.9 1307 1321 1331.8 1348.7 1425.7	H	-3.845588	1.350589	-0.125341
	0.4509	1481.5 1506.4 1594.4 1630.3 1643.1	C	0.557905	-0.118545	-0.361900
	0.3570	1669 1919.9 2946 3130.5 3150.5 3156.7	C	0.972430	1.281405	0.062297
		3159.5 3165.2 3176.2 3177.6 3189.5	C	0.049240	2.361262	-0.211024
		3194.1	C	-1.263157	2.074822	-0.351359
			H	0.399355	3.387864	-0.213961
			H	-1.981077	2.873968	-0.504947
			C	3.000601	-0.887021	-0.211166
			C	1.625194	-1.028594	0.285879

			C 2.676816 -0.067069 0.986264 C 2.141772 1.299102 0.727543 H 0.682073 -0.179315 -1.455595 H 3.132039 -0.300032 1.945125 H 2.646837 2.191479 1.076403 O 3.823869 -1.222258 -1.008613 H 1.334970 -1.960440 0.760182
(OH + phen. rad.) 16-17_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7389947 ZPE (hartree): 0.1923240 $\langle S^2 \rangle$: 0 Rotational constants (GHz): 1.3281 0.4377 0.3591	-605.54 60.847 74.413 115.92 153.35 232.59 250.56 308.12 380.15 400.67 416.34 436.49 455.41 504.13 531.49 552.73 564.7 625.22 667.32 709.33 743.53 749.15 771.63 794.87 813.22 834.09 861.82 877.67 902.26 929.2 953.22 959.92 987.56 994.45 1015 1059.6 1083.8 1121.9 1155.7 1179 1184.1 1214.2 1226.5 1234.7 1241.8 1262.4 1298.6 1307.8 1316.4 1331.6 1364 1427.4 1480.9 1505.9 1594.4 1627.8 1644.4 1664.7 2000.8 2771.8 3025 3154.4 3157.8 3166.4 3176.5 3179.8 3189.2 3214.4 3229.4	C 3.750445 -0.622204 -0.012266 C 2.948508 -1.751426 -0.162141 C 1.558601 -1.633640 -0.122779 C 0.954212 -0.394817 0.059391 C 1.762952 0.757034 0.195990 C 3.158193 0.623193 0.164056 H 3.402735 -2.725026 -0.309105 H 0.941216 -2.516935 -0.238918 H 4.830463 -0.711502 -0.038410 H 3.777037 1.509122 0.265273 C -0.547502 -0.232292 0.220767 C -1.027713 1.156041 -0.170209 C -0.174366 2.287245 0.115900 C 1.145305 2.076345 0.311879 H -0.581930 3.292203 0.098355 H 1.806031 2.919737 0.487673 C -3.346431 -0.701028 0.255340 C -1.487081 -1.123780 -0.550607 C -2.645753 -0.330237 -0.990023 C -2.218696 1.114823 -0.794409 H -0.708151 -0.306416 1.323602 H -3.216201 -0.549090 -1.897085 H -2.827178 1.950910 -1.110247 O -3.614486 -1.001522 1.352259 H -1.492178 -2.202371 -0.524543
(OH + phen. rad.) 17	Theory: B3LYP/6-311G(d,p) Energy (hartree): -501.4849628 ZPE (hartree): 0.1859080	99.433 111.53 226.13 247.33 273.21 411.69 417.34 437.09 497.97 516.51 554.3 578.65 604.26 665.18 696.2 725.88 749.52 753.92 805.14 830.02 834.34 859.73 879.04 893.3 945.44 951.22 954.69 976.82 988.6 1010.6 1028.6	C 3.277367 -0.161124 -0.219613 C 2.693765 -1.424280 -0.148878 C 1.318752 -1.544983 0.052949 C 1.094598 0.871154 0.072278 C 2.482078 0.973486 -0.109370 H 3.304894 -2.314185 -0.248815

	<S^2>: 0	1061.2 1101.5 1128.9 1158.5 1174.1	H	0.872410	-2.531054	0.118009
		1183.9 1189.5 1229 1239.2 1269.8	H	4.346836	-0.061613	-0.366778
	Rotational constants (GHz):	1304.3 1322.1 1336.5 1389 1421.2	H	2.932467	1.958705	-0.175874
	1.7442	1480.1 1505.4 1548 1590.2 1619 1639.7	C	-0.960472	-0.489106	0.500922
	0.6857	1655.1 2903.5 3154.7 3157.6 3165.3	C	-1.743990	0.724120	0.057315
	0.5033	3174.4 3176.3 3188.4 3188.9 3202.6	C	-1.095363	2.006522	0.059619
		3222.4	C	0.256632	2.067071	0.102829
			H	-1.686616	2.910973	-0.040183
			H	0.759883	3.028054	0.076179
			C	-1.862362	-1.638211	0.133649
			C	-3.035979	-1.135891	-0.309761
			C	-2.972576	0.319360	-0.360722
			H	-1.635112	-2.679690	0.312700
			H	-3.907667	-1.717652	-0.581992
			H	-3.775103	0.962596	-0.698685
			H	-1.004979	-0.465357	1.609276
			C	0.513048	-0.416583	0.168144
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	109.25 183.83 216.07 308.96 315.33	C	2.968237	-0.793968	-0.382212
18		448.74 464.08 474.28 493.5 499.62	C	1.961590	-1.808449	-0.158445
	Energy (hartree): -538.3059580	560.83 569.31 630.49 641.76 660.87	C	0.794641	-1.374810	0.412546
		696.14 702.82 755.73 770.22 800.86	C	0.700502	0.021714	0.652276
	ZPE (hartree): 0.1696910	805.22 823.02 891.5 894.71 897.7 908.79	C	1.472831	1.046989	0.171619
		969 972.46 974.99 994.85 1004.9 1042.4	C	2.756844	0.573249	-0.271607
	<S^2>: 0	1108.3 1164.3 1171.4 1203.5 1210.6	H	2.138526	-2.819168	-0.507422
		1215.2 1243.8 1311.3 1341.2 1358.1	H	3.934568	-1.126632	-0.747078
	Rotational constants (GHz):	1401 1424 1449.7 1463.3 1485.7 1501.8	H	3.540348	1.255615	-0.584062
	1.4012	1604.7 1609.5 1659.2 1725.7 3152.4	C	-0.700502	0.021716	0.652276
	0.7556	3156.7 3156.8 3170 3173.1 3173.5	C	-1.472829	1.046992	0.171616
	0.5143	3183.7 3184.7	C	-0.695137	2.254538	-0.061292
			C	0.695142	2.254537	-0.061289
			H	-1.200263	3.174559	-0.338785
			H	1.200271	3.174558	-0.338780
			C	-0.794644	-1.374809	0.412551
			C	-1.961595	-1.808448	-0.158434
			C	-2.968238	-0.793964	-0.382211
			C	-2.756841	0.573253	-0.271614
			H	-2.138534	-2.819167	-0.507409
			H	-3.934570	-1.126627	-0.747077

			H	-3.540343	1.255620	-0.584071
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	71.343 101.53 171.06 218.64 224.12	C	-3.604389	-0.277498	-0.007956
19		258.37 324.22 357.35 410.56 419.69	C	-2.874973	-1.485428	0.038622
	Energy (hartree): -613.5563657	434.03 502.14 514.65 529.61 538.32	C	-1.500233	-1.482061	0.061758
		598.39 617.53 658.6 687.81 731.71	C	-0.778336	-0.256868	0.034286
	ZPE (hartree): 0.1717820	752.74 767.42 824.28 838.2 846.18	C	-1.523598	0.968973	-0.016091
		855.97 892.79 915.46 951.06 975 987.08	C	-2.938980	0.924072	-0.031834
	$<S^2>$: 0	1015.6 1034.3 1057.2 1090.6 1167	H	-3.406807	-2.430015	0.057005
		1169.1 1184 1191.5 1231.1 1241.3	H	-0.945173	-2.407526	0.080658
	Rotational constants (GHz):	1296.8 1330.4 1353.7 1376.5 1392.1	H	-4.688086	-0.301591	-0.024019
	1.2445	1408.2 1455.6 1484.1 1512.1 1546.4	H	-3.489027	1.858446	-0.067722
	0.5363	1585.2 1619.4 1633.9 1654.3 3136.9	C	0.647430	-0.183095	0.108603
	0.3767	3155.3 3161.4 3163.8 3174 3180.7	C	1.298836	1.060274	0.038432
		3188.4 3237	C	0.534076	2.259707	-0.008511
			C	-0.831022	2.209900	-0.034187
			H	1.049783	3.213144	-0.040151
			H	-1.409901	3.126692	-0.070788
			C	1.550748	-1.376975	0.059651
			C	2.932543	-1.070859	0.357787
			C	3.575613	0.031037	-0.142229
			C	2.733886	1.140803	-0.064785
			H	4.653758	0.150731	-0.182942
			H	3.189605	2.115817	0.092542
			O	1.214530	-2.512199	-0.275734
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-340.21 83.538 96.428 160.23 219.75	C	-3.567081	-0.210837	-0.121310
19-20_TS		245.87 280.53 337.37 410.74 418.99	C	-2.853552	-1.421730	-0.232250
	Energy (hartree): -613.5506484	448.82 482.5 518.08 528.41 547.26	C	-1.478742	-1.443757	-0.185906
		565.17 643.23 676.52 692.49 702.33	C	-0.732232	-0.244481	-0.041178
	ZPE (hartree): 0.1702240	710.28 765.59 775.59 798.51 834.48	C	-1.462025	0.986356	0.064648
		837.5 869.08 882.5 890.29 960.19 969.84	C	-2.878366	0.967581	0.024529
	$<S^2>$: 0	984.27 1003.5 1018.7 1058.8 1130.1	H	-3.394854	-2.353660	-0.350483
		1151.6 1174.3 1185.7 1221.8 1240.1	H	-0.955494	-2.384416	-0.244254
	Rotational constants (GHz):	1275.2 1306.9 1324.5 1372.2 1385.8	H	-4.650638	-0.213794	-0.148994
	1.2039	1437.8 1449.9 1482.7 1497.8 1542.3	H	-3.408800	1.909840	0.113408
	0.5532	1579.9 1632.6 1652.7 1763.2 3160.9	C	0.706884	-0.174607	-0.060018
	0.3869	3164.8 3173.4 3177.3 3182.8 3188.9	C	1.366228	1.067723	0.014423
		3198.5 3248.5	C	0.600696	2.259877	0.154740
			C	-0.761868	2.217227	0.182617

			H	1.123401	3.206515	0.232323
			H	-1.335923	3.132837	0.277062
			C	1.510761	-1.519155	0.163368
			C	2.686623	-1.135956	-0.464782
			C	3.489402	-0.033535	-0.240466
			C	2.800163	1.138724	-0.052124
			H	4.556318	-0.065716	-0.430573
			H	3.306811	2.095159	-0.079424
			O	1.024730	-2.505918	0.674149
(OH + phen. rad.) 20	Theory: B3LYP/6-311G(d,p) Energy (hartree): -613.6551991 ZPE (hartree): 0.1734490 $<S^2>$: 0 Rotational constants (GHz): 0.9591 0.5874 0.3643	58.133 114.64 115.04 168.71 253.29 253.59 287.86 418.11 428.46 430.38 500.82 515.38 527.24 559.3 560.77 606.26 646.08 667.98 679.69 702.32 731.5 756.12 776.01 796.59 828.66 868.03 869.99 905.59 954.45 967.33 975.37 990.22 1032.5 1054.3 1093 1143.4 1169.4 1183.1 1196.3 1235.1 1237.5 1289 1357 1368.8 1376.6 1403.9 1449.2 1468.6 1484.4 1535.5 1561.3 1597.2 1629.1 1659.7 2205.9 3158.8 3162 3168.1 3179.5 3180.9 3190.7 3212 3238.6	C	-3.385131	0.949135	-0.000297
			C	-2.375481	1.935583	-0.000598
			C	-1.048605	1.574103	-0.000595
			C	-0.659327	0.210599	-0.000303
			C	-1.685697	-0.793242	0.000066
			C	-3.042173	-0.381900	0.000036
			H	-2.648576	2.984804	-0.000790
			H	-0.293380	2.351471	-0.000865
			H	-4.427938	1.245034	-0.000311
			H	-3.813743	-1.144944	0.000308
			C	0.687375	-0.241765	-0.000129
			C	1.003156	-1.610578	0.000519
			C	-0.024992	-2.581209	0.000896
			C	-1.333879	-2.174200	0.000749
			H	0.225858	-3.636315	0.001156
			H	-2.133375	-2.907381	0.000947
			C	2.205976	1.772113	0.002501
			C	1.972925	0.467326	-0.001539
			C	3.033231	-0.545967	-0.001512
			C	2.443925	-1.769015	-0.000520
			H	4.089160	-0.321589	-0.002542
			H	2.964999	-2.716348	-0.000583
			O	2.411146	2.909922	0.000879
(OH + phen. rad.) 21	Theory: B3LYP/6-311G(d,p) Energy (hartree): -500.1783046 ZPE (hartree): 0.1608530	108.4 140.99 198.84 242.64 280.57 390.18 413.75 436.89 470.52 493.9 517.42 541.34 592.44 655.57 680.16 703.3 730.66 761.04 789.15 826.52 830.79 869.87 880.29 903.61 953.64 969.97 974.08 1000.3 1034.5 1039.7	C	3.280558	-0.137421	-0.050114
			C	2.697676	-1.428811	-0.005071
			C	1.333475	-1.581274	0.017301
			C	0.482863	-0.447220	0.004299
			C	1.068572	0.867715	-0.009937
			C	2.485323	0.980504	-0.046780

	<S^2>: 0 Rotational constants (GHz): 1.9177 0.6747 0.5007	1100.6 1120 1159.7 1172 1181 1206.4 1243.7 1285.1 1339.2 1354.8 1378.7 1423.6 1427.9 1471.9 1474.4 1549.1 1592.2 1598 1659.1 3159.8 3161.5 3168.7 3173.4 3177.8 3181.9 3190.5 3224.4	H	3.340100	-2.302049	0.017670
			H	0.882398	-2.566010	0.059222
			H	4.359728	-0.038193	-0.073988
			H	2.929272	1.970359	-0.067561
			C	-0.927870	-0.524956	-0.011391
			C	-1.725981	0.633250	-0.032901
			C	-1.152311	1.903765	0.069699
			C	0.230290	2.008963	0.041719
			H	-1.769219	2.791437	0.161705
			H	0.695583	2.988521	0.073858
			C	-1.868466	-1.587420	0.273415
			C	-3.169384	-1.185837	-0.162056
			C	-3.134499	0.186008	-0.093369
			H	-4.052318	-1.806759	-0.200828
			H	-3.987018	0.839102	0.061042
(OH + phen. rad.) 22	Theory: B3LYP/6-311G(d,p) Energy (hartree): -613.6734647 ZPE (hartree): 0.1762760 <S^2>: 0 Rotational constants (GHz): 1.2348 0.6349 0.4193	89.085 196.72 211.36 300.44 323.46 344.17 436.41 453.87 488.21 505.19 553.8 574.59 579.8 605 616.81 650.25 681.49 701.48 727.14 766.37 767.52 800.45 801.9 832.95 834.89 891.75 899.78 968.34 969.19 980.78 1012.1 1012.2 1033.7 1050.2 1062.9 1159.3 1186.4 1192.1 1234 1237.7 1242.9 1262.6 1338.8 1386.4 1389.3 1434.5 1449.9 1474.4 1499.5 1521.5 1531.1 1619.2 1660.6 1676.7 1706.8 3159.7 3166.8 3166.9 3176.8 3182.8 3183.1 3205.8 3206.2	C	3.313387	-0.426707	0.000544
			C	2.471238	-1.571723	0.000192
			C	1.115900	-1.316744	-0.000464
			C	0.691464	0.008809	-0.000606
			C	1.472378	1.157863	-0.000126
			C	2.862681	0.896646	0.000402
			H	2.889727	-2.569645	0.000515
			H	4.383920	-0.599593	0.000916
			H	3.586382	1.704063	0.000660
			C	-0.691491	0.008805	-0.000552
			C	-1.472456	1.157840	-0.000211
			C	-0.690754	2.379213	-0.000178
			C	0.690632	2.379238	-0.000094
			H	-1.207720	3.333267	0.000129
			H	1.207646	3.333274	0.000027
			C	-1.115849	-1.316864	-0.000314
			C	-2.471156	-1.571786	0.000346
			C	-3.313321	-0.426764	0.000527
			C	-2.862688	0.896611	0.000257
			H	-2.889579	-2.569750	0.000714
			H	-4.383853	-0.599654	0.000931
			H	-3.586375	1.704040	0.000560
			O	0.000007	-2.157828	-0.000351

(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	98.06 128.08 224.81 238.53 243.77	C	-3.652209	-0.521029	-0.000061
23		379.92 411.63 434.74 451.22 462.99	C	-2.780344	-1.609549	-0.000121
	Energy (hartree): -538.3291898	472.49 519.62 559.77 579.08 593.46	C	-1.543697	-1.593938	-0.000080
		666.02 677.87 727.1 754.62 775.23	C	-0.712133	-0.469091	0.000037
	ZPE (hartree): 0.1686020	779.58 804.9 846.72 884.54 885.41	C	-1.510405	0.732539	0.000088
		939.47 965.01 979.17 980.3 998.13	C	-2.934627	0.674127	0.000042
	$<S^2>$: 0	1051.2 1080.6 1133.1 1144.9 1172.3	H	-4.733499	-0.554236	-0.000111
		1177.1 1222.5 1229.6 1250.6 1299.4	H	-3.482373	1.611391	0.000098
	Rotational constants (GHz):	1325.1 1363.6 1398.7 1435.4 1443.1	C	0.721801	-0.407118	0.000028
	1.7335	1474.1 1496.1 1542.1 1573 1639.4	C	1.352052	0.868231	-0.000058
	0.5554	1656.3 2038.3 3158.7 3160.8 3164	C	0.542975	2.050723	-0.000005
	0.4206	3166.9 3177.6 3179.1 3189.8 3202.3	C	-0.816267	1.988808	0.000093
			H	1.042490	3.013780	-0.000034
			H	-1.400741	2.902427	0.000196
			C	2.894379	-1.482500	0.000084
			C	3.522060	-0.221639	-0.000062
			C	2.764164	0.929635	-0.000129
			H	3.496442	-2.383946	0.000202
			H	4.604391	-0.159227	-0.000135
			H	3.245745	1.901861	-0.000250
			C	1.518997	-1.571494	0.000115
			H	1.027068	-2.538270	0.000213
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	43.105 49.322 63.584 133.01 158.54	C	-1.839523	1.982776	0.000130
24		166.75 199.47 254.75 270.42 355.98	C	-0.541242	2.370737	0.000142
	Energy (hartree): -614.7827439	393.02 427.32 442.52 484.23 502.24	C	0.537904	1.411279	0.000118
		545.56 584.02 585.06 616.59 680.44	C	0.172844	0.021080	0.000391
	ZPE (hartree): 0.1933940	710.83 718.78 747.31 755.53 791.91	C	-1.126976	-0.388676	0.000521
		851.28 872.7 904.94 923.76 926.1 949.11	C	-2.200071	0.590199	0.000163
	$<S^2>$: 0	955.42 972.34 983.07 990.11 1001.3	C	1.850562	1.879277	-0.000110
		1067.3 1147.1 1167.7 1192.8 1205.8	C	3.071080	1.154714	-0.000200
	Rotational constants (GHz):	1211.8 1247.9 1275 1305 1355.6 1381.4	C	3.260284	-0.189362	-0.000136
	1.0790	1406.9 1425.6 1437.4 1455.3 1482.9	C	4.090110	-1.164729	-0.000328
	0.3361	1514.3 1571.2 1591.1 1637.5 1675.5	C	-1.479072	-1.862905	0.001423
	0.2567	1701.6 2201 2991.8 3000.7 3053.8	C	-2.941871	-2.176561	-0.000413
		3147.1 3159.7 3161.4 3169.3 3174.1	C	-3.881371	-1.211344	-0.001075
		3178.3 3186	C	-3.511856	0.178191	-0.000449
			O	4.718280	-2.161748	-0.000380
			H	-2.635631	2.719932	0.000028

			H -0.287945 3.425511 0.000073 H 1.962329 2.959899 -0.000249 H 3.955543 1.797409 -0.000239 H 0.976102 -0.706119 0.000547 H -1.009956 -2.352786 -0.863654 H -3.226525 -3.223362 -0.000962 H -4.934134 -1.470284 -0.002174 H -4.297848 0.926461 -0.000727 H -1.012988 -2.350742 0.869334
(OH + phen. rad.) 25	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7739696 ZPE (hartree): 0.1939700 $<S^2>$: 0 Rotational constants (GHz): 1.1832 0.4775 0.3658	59.119 85.932 105.51 165.73 209.73 253.9 269.94 352.29 419.76 446.03 479.37 489.79 502.52 507.43 537.31 586.1 610.55 645.91 703.68 720.5 741.27 753.51 763.57 783.97 829.76 845.88 884.41 889.84 910 932.68 953.36 978.28 982.98 992.21 997.97 1023.7 1045.7 1063.9 1104.7 1165.3 1184.7 1198.9 1213.5 1223.7 1238.5 1256.2 1275.5 1354 1365.4 1411.8 1435.1 1444.2 1456.5 1549.9 1601.2 1628 1661.5 1688.9 1915.3 2966.9 2970.8 3125.7 3134.1 3154.2 3158.9 3167.4 3179.6 3181 3207.5	C 1.152462 2.152640 0.327886 C -0.167602 2.408361 0.179129 C -1.061507 1.331714 -0.165936 C -0.505552 -0.010330 -0.303662 C 0.811687 -0.283028 -0.138107 C 1.714594 0.826142 0.164323 C -2.405442 1.336247 -0.383706 C -2.919968 -0.026764 -0.693296 C -1.626003 -0.950439 -0.600111 C -2.745736 -1.038286 0.376750 C 1.365901 -1.693068 -0.237051 C 2.864205 -1.780595 -0.175299 C 3.634088 -0.706308 0.067590 C 3.061842 0.605329 0.261797 O -3.222933 -1.625510 1.296135 H 1.838645 2.956189 0.575498 H -0.559663 3.411288 0.306041 H -3.056229 2.197489 -0.312320 H -3.695101 -0.175973 -1.440586 H -1.479864 -1.799071 -1.263111 H 0.943261 -2.311480 0.569514 H 3.310830 -2.759494 -0.314501 H 4.712400 -0.812379 0.121142 H 3.723773 1.439384 0.468664 H 1.007588 -2.171558 -1.161263
(OH + phen. rad.) 25-26_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7372959	-399.15 57.034 86.398 101.52 166.77 207.55 241.96 265.01 326.4 408.15 422.9 456.54 472.2 498.88 502.45 538.11 580.51 607.18 624.28 654.41 704.99	C 3.696918 -0.569714 0.261297 C 3.009319 -1.686136 -0.049920 C 1.532980 -1.676894 -0.326098 C 0.889032 -0.312442 -0.189864

	ZPE (hartree): 0.1914670 <S^{2}>: 0 Rotational constants (GHz): 1.2356 0.4462 0.3638	727.57 747.03 749.61 799.36 810.18 854.6 860.1 868.12 924.86 959.31 963.2 968.5 983.2 990.48 1020 1054.9 1116.2 1160.7 1185.5 1199.4 1206.5 1208.8 1219.3 1242.7 1272.3 1323.4 1356.9 1378.7 1416.2 1434.2 1451.9 1465.9 1524.8 1575.8 1597.9 1628.4 1669.3 2051.7 2917.3 2930.6 3005 3148.5 3158 3165.7 3177.4 3179.6 3228.8 3242.8	C	1.693179	0.836513	0.136652
			C	3.047640	0.710733	0.353391
			H	3.522151	-2.640797	-0.114722
			H	1.353565	-2.083353	-1.336981
			H	4.764311	-0.626756	0.448461
			H	3.635138	1.587569	0.601766
			C	-0.463800	-0.143001	-0.392511
			C	-1.082782	1.183022	-0.268564
			C	-0.264647	2.319561	0.057302
			C	1.064335	2.138688	0.247762
			H	-0.717416	3.300736	0.147405
			H	1.700223	2.981840	0.497879
			C	-3.225496	-0.829716	0.510214
			C	-1.484634	-1.058993	-0.763721
			C	-2.785765	-0.335925	-0.805649
			C	-2.424250	1.108829	-0.510989
			H	-1.396606	-2.117930	-0.946093
			H	-3.520801	-0.514924	-1.597523
			H	-3.159315	1.898047	-0.457898
			O	-3.303313	-1.186441	1.607639
			H	1.033079	-2.400047	0.340771
(OH + phen. rad.) 26	Theory: B3LYP/6-311G(d,p) Energy (hartree): -501.4662592 ZPE (hartree): 0.1851260 <S^{2}>: 0 Rotational constants (GHz): 1.7570 0.6768 0.4901	55.922 138.4 170.31 242.98 245.61 315.59 430.29 457.88 467.62 502.29 503.91 578.93 603.15 627.53 644.18 704.52 723.91 746.01 764.76 780.77 831.86 838.59 858.07 916.54 921.76 929.05 940.05 967.25 993.05 995.66 1015.1 1046.8 1105.3 1112.8 1167.6 1192.4 1195.2 1211.3 1239.2 1274.6 1347.4 1352.2 1386.5 1404.5 1418.4 1430.1 1434.6 1481.8 1553.3 1578.7 1618.8 1640.5 1681.7 2996.6 3008.1 3156.7 3158.4 3166.3 3177.7 3184.4 3194.4 3209.9 3223.3	C	-3.292770	-0.065498	-0.005776
			C	-2.815887	-1.322488	-0.002802
			C	-1.346538	-1.605371	0.007755
			C	-0.438162	-0.395967	0.002447
			C	-1.031538	0.940701	0.001988
			C	-2.398750	1.063913	-0.001560
			H	-3.488623	-2.173514	-0.005741
			H	-1.104934	-2.247518	-0.850300
			H	-4.361373	0.118309	-0.011692
			H	-2.830668	2.059841	-0.002885
			C	0.924360	-0.501765	-0.000017
			C	1.778135	0.694276	-0.000333
			C	1.178557	1.989343	0.001310
			C	-0.174894	2.106591	0.002319
			H	1.808345	2.873214	0.001551
			H	-0.649972	3.081305	0.002819
			C	1.812274	-1.650304	-0.002046

			C	3.096765	-1.177336	-0.002915
			C	3.087476	0.271718	-0.001761
			H	1.511662	-2.688187	-0.002643
			H	3.965899	0.902837	-0.002174
			H	3.992295	-1.784970	-0.004235
			H	-1.116802	-2.228197	0.883633
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	39.128 61.092 66.936 119.13 146.07	C	3.991890	-1.088923	0.175886
27		190.78 240.84 246.22 277.34 384.54	C	2.971352	-2.171081	0.041377
	Energy (hartree): -614.7114382	394.83 419.26 434.8 460.28 500.39	C	1.575197	-1.703661	-0.132486
		538.01 549.62 596.66 625.36 673.84	C	1.212352	-0.383187	-0.146104
	ZPE (hartree): 0.1904790	689.08 724.33 746.85 763.91 786.01	C	2.270212	0.624043	-0.041761
		806.72 815.67 868.29 883.57 908.17	C	3.644050	0.209731	0.126889
	<S^2>: 0	934.8 967.17 971.22 979.03 997.81	H	3.216993	-2.827862	-0.810721
		1037.5 1042.5 1117.3 1141.1 1168.5	H	0.785683	-2.442092	-0.232036
	Rotational constants (GHz):	1180 1195.4 1235.9 1258.1 1276.6	H	5.025054	-1.384570	0.319117
	1.2099	1301.1 1342.1 1351.2 1369.4 1391.5	H	4.401040	0.982293	0.226072
	0.3108	1411.8 1437.6 1481 1515.3 1560.1	C	-0.196664	-0.074067	-0.200837
	0.2483	1589.1 1647.5 1664.1 2187.6 2879.7	C	-0.525446	1.296519	-0.022413
		2964.2 2971.1 3124.1 3131.6 3150.5	C	0.500040	2.261489	-0.100255
		3156 3167.9 3174.6 3181.1	C	1.868215	1.942358	-0.079906
			H	0.225250	3.311710	-0.179464
			H	2.603466	2.740193	-0.064814
			C	-4.219066	-1.112556	0.010370
			C	-3.122618	-0.388313	-0.015771
			C	-3.044123	1.044345	0.139220
			C	-1.901678	1.771143	0.125554
			H	-2.159780	-0.902212	-0.180568
			H	-3.978531	1.581879	0.270479
			H	-2.012319	2.845174	0.251159
			O	-5.157977	-1.801536	0.027534
			H	3.014685	-2.859266	0.901928
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-234.97 41.519 47.681 93.959 139.56	C	3.483968	-0.516972	0.273290
27-29_TS		169.78 225.61 262.54 283.87 387.87	C	2.778417	-1.575428	-0.522956
	Energy (hartree): -614.6881833	407.49 438.78 442.9 451.95 469.47	C	1.382190	-1.211408	-0.909395
		500.13 565.18 594.59 618.96 639.97	C	0.790566	-0.027428	-0.563058
	ZPE (hartree): 0.1896220	678.97 703.37 723.35 747.69 773.02	C	1.563426	0.993251	0.156206
		798.02 803.67 829.32 889.24 894.92	C	2.910449	0.659367	0.573892
	<S^2>: 0	920.22 948.87 956.16 969.6 979 992.67	H	3.357661	-1.805006	-1.434771

	Rotational constants (GHz): 0.9842 0.5121 0.3792	1041.9 1110.8 1118.2 1159.4 1169.9 1186.6 1202.2 1243.5 1269.8 1302.4 1343.1 1363.1 1367.2 1396.2 1401.5 1432.1 1437 1518.3 1564.1 1586.4 1650.3 1675.8 2157.8 2930 2945.3 3142.4 3144.7 3152.5 3156.2 3163.8 3165.2 3168.8 3177.9	H 0.793259 -1.951072 -1.442158 H 4.492089 -0.735788 0.609996 H 3.458617 1.397646 1.152649 C -0.598249 0.237250 -0.838888 C -1.219261 1.337611 -0.232978 C -0.424551 2.395476 0.217322 C 0.956136 2.196113 0.440255 H -0.863420 3.372558 0.397829 H 1.533362 2.988206 0.906776 C -2.050483 -1.832795 0.572581 C -2.436285 -1.088563 -0.464812 C -3.287470 0.123014 -0.248076 C -2.677674 1.311541 -0.156249 H -2.421256 -1.595210 -1.424698 H -4.363695 0.006855 -0.186889 H -3.239316 2.222991 0.025028 O -1.569437 -2.422011 1.448238 H 2.781114 -2.531269 0.027533
(OH + phen. rad.) 28	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7633035 ZPE (hartree): 0.1939070 $<S^2>$: 0 Rotational constants (GHz): 1.1327 0.5410 0.4233	64.278 92.146 141.92 154.43 209.66 256.97 268.16 344.34 383.72 427.09 447.41 474.79 502.17 512.93 581.24 612.84 619.78 664.01 700.33 708.03 757.47 770.26 795.92 803.59 832.48 839.66 859.53 891.78 915.05 918.15 938.37 950.66 965.43 985.43 997.35 1015.6 1024.8 1073.3 1108.3 1115.7 1170 1196.3 1206 1224.4 1253.1 1282.6 1312.2 1366.1 1372.2 1375.5 1423.3 1431.6 1455.9 1559.3 1593 1648.2 1660.2 1710.7 1907.1 2952.6 2958.9 3118.3 3146.9 3149.1 3160.3 3168.7 3176.8 3195.5 3215.5	C 3.516314 -0.164123 -0.100667 C 2.850622 -1.431984 -0.546541 C 1.352675 -1.353508 -0.532124 C 0.672070 -0.245798 -0.180384 C 1.375040 0.995587 0.178501 C 2.826979 0.939066 0.222473 H 3.201025 -1.699027 -1.556970 H 0.815272 -2.255282 -0.810931 H 4.600766 -0.160026 -0.055031 H 3.351705 1.840657 0.524224 C -0.812014 -0.187422 -0.049841 C -1.463621 1.156396 -0.089003 C -0.738350 2.262261 0.204891 C 0.684328 2.154786 0.399317 H -1.208222 3.238879 0.242522 H 1.239991 3.052658 0.649159 C -1.481024 -1.259037 0.772097 C -1.900599 -1.193871 -0.638057 C -3.084032 -0.302685 -0.847697 C -2.832416 0.981959 -0.517913

			H	-1.673960	-2.004380	-1.327333
			H	-4.035096	-0.696566	-1.181379
			H	-3.553502	1.787518	-0.568886
			O	-1.465104	-1.867707	1.794103
			H	3.187023	-2.272544	0.081496
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	-416.18 68.129 85.138 110.79 169.64	C	3.495006	-0.232471	0.025053
28-29_TS		217.5 224.45 273.31 313.73 406.64	C	2.825175	-1.499462	-0.427082
	Energy (hartree): -614.7406244	425.65 449.68 481.11 483.29 500.39	C	1.335963	-1.355598	-0.569671
		546.57 607.06 633.48 667.53 697.06	C	0.672733	-0.193688	-0.289242
	ZPE (hartree): 0.1916760	718.41 726.75 737.24 784.33 801.14	C	1.387696	1.014607	0.131541
		809.6 841.01 892.05 914.83 925.1 935.69	C	2.829688	0.906466	0.270158
	<S^2>: 0	950.66 961.14 967.56 995.52 1024.2	H	3.277867	-1.824941	-1.379755
		1076 1108.9 1144.5 1166.3 1177.4	H	0.786949	-2.223370	-0.924041
	Rotational constants (GHz):	1200.2 1216 1236.9 1248.6 1300.9	H	4.573578	-0.261168	0.150789
	1.0975	1332.1 1363.6 1368.1 1418.9 1434.6	H	3.371456	1.792623	0.588720
	0.5478	1443 1468.7 1521.9 1569.2 1601.6	C	-0.753753	-0.023007	-0.346970
	0.4156	1630.4 1688.7 2083.8 2912.1 2927.3	C	-1.411024	1.222090	-0.123913
		2938.5 3137.8 3138.9 3152.4 3160.1	C	-0.690015	2.340266	0.229644
		3187.8 3200.2 3234.2	C	0.718315	2.198850	0.365213
			H	-1.169013	3.296344	0.401112
			H	1.302192	3.066058	0.658789
			C	-1.616058	-1.617098	0.618304
			C	-1.781303	-1.060720	-0.698506
			C	-3.087611	-0.268093	-0.667811
			C	-2.831444	1.017523	-0.341619
			H	-1.637145	-1.748674	-1.545174
			H	-4.045537	-0.733829	-0.845949
			H	-3.583544	1.790732	-0.247499
			O	-1.564657	-1.942360	1.727208
			H	3.080263	-2.312884	0.274748
(OH + phen. rad.)	Theory: B3LYP/6-311G(d,p)	81.93 126 193.14 248.38 269.46 305.23	C	3.312116	0.004286	-0.000061
29		423.66 448.91 449.86 452.31 509.98	C	2.793706	-1.395810	0.000122
	Energy (hartree): -501.4633775	570.66 614.17 647.93 669.9 706.8 738.62	C	1.307222	-1.502660	0.000039
		746.57 783.98 819.74 834.77 841.67	C	0.466246	-0.436101	-0.000020
	ZPE (hartree): 0.1849290	866.44 867.05 903.59 914.67 950.97	C	1.041541	0.922972	-0.000011
		958.85 969.2 997.86 1023.2 1042.5	C	2.485361	1.060879	-0.000117
	<S^2>: 0	1082.2 1097.1 1163.4 1184.7 1189.5	H	3.200513	-1.945393	-0.865219
		1245.2 1277.7 1285 1311.1 1363.3	H	4.387797	0.145075	-0.000166

	Rotational constants (GHz): 1.8571 0.6467 0.4811	1370.7 1408.5 1422.7 1426.8 1435.9 1471.2 1550.6 1589.2 1615.9 1649.3 1702.1 2956 2958.1 3151.9 3155.2 3159.8 3171.9 3175 3193.8 3207 3225.3	H 2.888126 2.069140 -0.000266 C -0.984577 -0.541609 -0.000069 C -1.799727 0.678191 -0.000023 C -1.204042 1.905626 0.000092 C 0.221096 2.022087 0.000062 H -1.804127 2.810738 0.000190 H 0.665346 3.011756 0.000073 C -1.855257 -1.605048 -0.000061 C -3.212223 -1.091992 -0.000021 C -3.187504 0.276249 0.000008 H -1.599896 -2.656447 -0.000041 H -4.035484 0.945937 0.000027 H -4.098892 -1.712129 -0.000001 H 0.892513 -2.506010 0.000048 H 3.200361 -1.945097 0.865726
(OH + phen. rad.) CO	Theory: B3LYP/6-311G(d,p) Energy (hartree): -113.3462354 ZPE (hartree): 0.0050570 $<S^2>$: 0 Rotational constants (GHz): 0.0000 58.0386 58.0386	2219.8	C 0.000000 0.000000 -0.643976 O 0.000000 0.000000 0.482982
(OH + phen. rad.) H_2	Theory: B3LYP/6-311G(d,p) Energy (hartree): -1.1795710 ZPE (hartree): 0.0100680 $<S^2>$: 0 Rotational constants (GHz): 0.0000	4419.2	H 0.000000 0.000000 0.372089 H 0.000000 0.000000 -0.372089

	1810.9604 1810.9604		

Phenol Decomposition

(phenol decomposition) 1	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.5518584 ZPE (hartree): 0.1042880 <S2>: 0 Rotational constants (GHz): 5.6732 2.6198 1.7922	231.11 343.1 406.16 421.01 515.95 536.52 633.33 698.69 760.75 819.49 829.88 884.5 961.03 983.43 1012.5 1044 1093.9 1176.9 1190.2 1198.9 1287.8 1349.3 1370.8 1502.6 1530.9 1638.5 1651.1 3145.8 3166.3 3174.9 3189.5 3196.3 3832.3	C 0.262528 1.196840 0.000000 C 0.940106 -0.024237 0.000000 C 0.220131 -1.220983 0.000000 C -1.169604 -1.188144 0.000000 C -1.854719 0.027350 0.000000 C -1.130582 1.216503 0.000000 H 0.822889 2.127667 -0.000002 H 0.764725 -2.157365 0.000001 H -1.721658 -2.121490 0.000000 H -2.937892 0.046135 0.000000 H -1.648034 2.169390 0.000000 O 2.304457 -0.110650 -0.000002 H 2.677150 0.776884 0.000015
(phenol decomposition) 1-2_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4397479 ZPE (hartree): 0.0975920 <S2>: 0 Rotational constants (GHz): 5.2485 2.8124 1.8811	-2137.9 216.2 363.03 458.6 519.82 528.3 615.15 632.85 751.22 777.45 828.34 870.91 958.66 988.09 1000.4 1005 1076.7 1123.7 1172.7 1181.7 1260.3 1369.9 1395.3 1455 1525.9 1539.6 1623.8 1795.6 3083.1 3160.7 3170 3192 3198	C -0.381382 -1.152132 0.188160 C -0.978504 0.168574 0.102438 C -0.182972 1.336418 0.191674 C 1.170250 1.155658 -0.001067 C 1.776784 -0.125907 -0.160496 C 1.027862 -1.268854 -0.035030 H -0.807479 -1.787289 0.969487 H -0.636169 2.318621 0.240443 H 1.806468 2.032792 -0.067834 H 2.845049 -0.182011 -0.329632 H 1.501832 -2.244605 -0.040780 O -2.207788 0.048968 -0.254904 H -1.639632 -1.211792 -0.446533
(phenol decomposition) 2	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.5228322 ZPE (hartree): 0.1028520 <S2>: 0	57.582 270.88 444.9 455.77 494.28 541.32 578.76 724.53 743.22 814.61 944.53 945.74 953.71 997.66 998.32 1026.7 1159.5 1192 1193.3 1242.5 1334.2 1398.5 1408.2 1443.5 1609 1693.5 1746 3014.6 3033.3 3153.5 3158.7 3183.5 3190.6	C -0.279752 -1.276846 -0.000037 C -1.084957 0.025390 -0.000060 C -0.316995 1.279178 -0.000065 C 1.032611 1.276405 0.000022 C 1.815611 0.047965 0.000055 C 1.212030 -1.149036 -0.000018 H -0.610393 -1.863881 0.866875

	Rotational constants (GHz): 5.1956 2.6861 1.7897		H H H H O H	-0.892680 1.570093 2.896854 1.796382 -2.302639 -0.610430	2.197527 2.219966 0.124526 -2.063850 0.003929 -1.864053	-0.000133 0.000019 0.000094 -0.000066 0.000080 -0.866805
(phenol decomposition) 2-3_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4515928 ZPE (hartree): 0.0989570 <S2>: 0 Rotational constants (GHz): 5.4986 2.6124 1.7879	-831.85 139.1 383.1 431.04 452.67 518.34 590.36 650.59 702.69 799.29 807.31 876.23 937.5 978.6 993.61 1010.8 1053.2 1151.5 1171.2 1229.8 1260.8 1335.4 1399.8 1431.8 1529.5 1550.3 1678.5 2486.7 3141.4 3157.7 3181.1 3193.7 3213.3	C C C C C C H H H H H O H	0.323919 1.126063 0.314285 -1.072173 -1.831509 -1.137117 0.831719 0.863591 -1.582117 -2.912285 -1.667226 2.362005 -0.770531	-1.196617 0.017010 1.225433 1.240756 0.074276 -1.170715 -2.154528 2.160352 2.199025 0.092688 -2.086744 -0.005375 -1.308654	-0.054912 -0.001521 0.025276 -0.005019 -0.048141 -0.016177 -0.046469 0.060478 0.006477 -0.069690 -0.265447 -0.021713 1.091327
(phenol decomposition) 2-5_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4674869 ZPE (hartree): 0.0996560 <S2>: 0 Rotational constants (GHz): 4.7460 2.4746 1.6660	-525.88 153.64 260.44 353.97 390.69 458.63 530.7 590.75 653.53 720.3 806.82 839.43 849.01 966.7 983.3 987.06 1027.5 1087.9 1149.2 1227.3 1277.9 1407.8 1430.7 1506.5 1544.7 1617.9 2012.3 3108.8 3118.5 3131.6 3158.3 3182.4 3209.6	C C C C C C H H H H H O H	-0.095474 1.299323 0.468810 -0.943506 -1.813952 -1.332026 0.266463 0.975375 -1.380132 -2.871879 -1.927384 2.387307 0.340042	1.485648 -0.185324 -1.274231 -1.288984 -0.225474 1.088349 1.087265 -2.202503 -2.282739 -0.434516 1.764229 0.254512 2.432269	0.246975 -0.083292 0.007583 0.104051 0.015473 -0.193394 1.191324 -0.247579 0.133422 -0.091117 -0.805636 -0.089443 -0.049244
(phenol decomposition) 3	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4580883 ZPE (hartree): 0.1000090	76.561 157.69 396.33 422.03 455 509.98 579.16 668.21 712.16 790.33 875.9 932.93 945.28 966.04 1010.2 1027.2 1080.8 1113.9 1168.6 1261.5 1299.9 1320.6 1382 1401.4 1490.6 1560.5	C C C C C C	0.328924 1.144850 0.332755 -1.068775 -1.824106 -1.135413	-1.194828 -0.013274 1.205457 1.264052 0.119982 -1.175162	0.000018 0.000002 0.000009 -0.000005 -0.000018 0.000000

	<S2>: 0 Rotational constants (GHz): 5.4578 2.5726 1.7665	1680.1 2952.9 2955.2 3155.1 3172.2 3178.1 3200.4	H H H H H O H	0.830742 0.898420 -1.552165 -2.906510 -1.501927 2.383001 -1.501985	-2.157065 2.132965 2.235937 0.142844 -1.773152 -0.005724 -1.773104	-0.000014 0.000024 0.000003 0.000016 -0.855911 -0.000010 0.855922
(phenol decomposition) 3-4_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4496481 ZPE (hartree): 0.1003000 <S2>: 0 Rotational constants (GHz): 5.6311 2.5030 1.8764	-287.46 226.24 253.61 422.36 456.54 559.82 597.44 707.71 732.08 838.91 875.79 902.84 938.39 954.2 1008 1022.4 1097.9 1135.6 1147.4 1224.4 1316 1339 1372.8 1410 1419.3 1636.1 1782.9 2971.3 3023.4 3139.3 3151.2 3162.9 3201.2	C C C C C C H H H H H O H	0.282734 1.173004 0.329564 -1.043914 -1.791188 -1.155801 0.723464 0.808054 -1.441578 -2.796290 -1.217239 2.358908 -1.714068	-1.035162 -0.009749 1.052747 1.226990 0.148816 -1.166856 -1.780087 1.799673 2.235791 0.201458 -1.822517 -0.030064 -1.694530	0.365921 -0.115393 0.396871 -0.015818 -0.304123 -0.003023 1.023732 1.027167 -0.067000 -0.702748 -0.888642 -0.389926 0.780286
(phenol decomposition) 4	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4658303 ZPE (hartree): 0.1020570 <S2>: 0 Rotational constants (GHz): 5.3738 2.5327 2.1530	144.87 212.94 393.7 516.96 543.69 667.6 688.27 755.58 769.19 870.43 902.25 936.18 952.02 985.33 1002.1 1026 1059 1078.7 1130.2 1181.7 1235 1266.1 1326.4 1360.8 1488.7 1661.9 1922.9 3009.1 3039.8 3136.3 3146.4 3182.3 3205.3	C C C C C C H H H H H O H	0.181850 1.221167 0.252395 -0.941165 -1.667139 -1.120175 0.500832 0.548486 -1.145700 -2.552559 -0.928425 2.229461 -1.819913	-0.803398 -0.021067 0.786274 1.217991 0.191522 -1.154968 -1.415059 1.326216 2.262985 0.287303 -1.807397 -0.032476 -1.692357	0.645329 -0.040082 0.733444 -0.060909 -0.507378 -0.085831 1.483767 1.628208 -0.258719 -1.124217 -0.945152 -0.682163 0.565989
(phenol decomposition) 4-6H_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4058001 ZPE (hartree): 0.0988110	-661.42 104.36 172.84 360.86 403.43 421 562.65 712.52 750.01 788.03 859.53 913.45 943.18 953.98 956.47 995.63 1077.1 1123.2 1147.7 1237.9 1263.3 1294 1314.2 1379.7 1483.1 1655.7 1993	C C C C C	-0.140599 1.418451 0.248537 -0.770367 -1.560722	-0.855978 0.250194 0.550974 1.248449 0.342931	0.833799 0.003089 0.871488 -0.024043 -0.600569

	<S2>: 0 Rotational constants (GHz): 4.9356 2.4669 2.2133	2890.7 2967.6 3007.9 3183.8 3219.4 3236.7	C	-1.205288	-1.072986	-0.210266
			H	0.339847	-1.625898	1.416024
			H	0.525323	1.085223	1.786107
			H	-0.780045	2.320308	-0.166842
			H	-2.362672	0.583128	-1.289150
			H	-0.876696	-1.636940	-1.104252
			O	2.162053	-0.236163	-0.756642
			H	-2.082259	-1.618024	0.170263
(phenol decomposition) 4-6L_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4199894 ZPE (hartree): 0.0993170 <S2>: 0 Rotational constants (GHz): 4.8713 2.5912 2.3348	-617.73 114.3 229.54 295.48 442.74 510.17 526.54 666.87 727.18 797.93 850.44 915.56 937.06 948.94 1006.5 1021.8 1049.7 1111.5 1144.1 1206.6 1243.5 1287.2 1302.9 1390.1 1478.3 1534.1 2033.5 2937.9 3101.8 3112.2 3186.9 3221.3 3262.2	C	0.118155	-0.714563	0.727448
			C	1.214901	-0.305799	-0.165507
			C	-0.028432	0.750541	1.002936
			C	-0.865872	1.220877	-0.059863
			C	-1.420735	0.194876	-0.772296
			C	-1.117434	-1.126016	-0.076173
			H	0.487126	-1.390013	1.498975
			H	0.566036	1.313943	1.701895
			H	-1.021248	2.270667	-0.278578
			H	-2.147055	0.299112	-1.565175
			H	-0.911166	-1.970207	-0.733885
			O	2.193659	0.096440	-0.647432
			H	-1.926459	-1.414519	0.616946
(phenol decomposition) 5	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4811995 ZPE (hartree): 0.0997070 <S2>: 0 Rotational constants (GHz): 3.7910 2.3611 1.5240	69.628 119.18 153.46 193.37 354.67 447.17 501.49 569.59 621.89 671.74 774.73 796.3 903.02 950.77 962.79 977.02 1032.8 1091.5 1163.6 1268 1330.2 1429.6 1442.6 1467.3 1659.5 1682.3 2201.2 3110.5 3134 3141.3 3154.7 3167.5 3222.8	C	0.989527	-1.619160	0.432418
			C	-1.573572	0.013732	-0.073248
			C	-0.977455	1.168793	0.166341
			C	0.435368	1.519737	0.092179
			C	1.528640	0.762869	-0.127471
			C	1.624099	-0.688011	-0.288048
			H	0.332147	-1.364330	1.255918
			H	-1.687872	1.963373	0.373709
			H	0.598380	2.587234	0.200127
			H	2.465791	1.302184	-0.239473
			H	2.327292	-1.023966	-1.049259
			O	-2.166248	-0.967174	-0.248738
			H	1.134600	-2.674864	0.235848
(phenol decomposition) 5-6_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -307.4046198	-689.11 88.637 129.68 312.71 418.06 487.33 549.36 612.02 665.95 738.71 797.07 814.48 934.07 960.68 992.32 1021.3 1057.7 1075.8 1104.2 1145.9	C	0.716887	-1.200525	0.630459
			C	-1.666880	0.238134	0.110571
			C	-0.436825	0.356567	0.861424
			C	0.539874	1.271269	0.195463

	ZPE (hartree): 0.0982440 <S2>: 0 Rotational constants (GHz): 4.6702 2.2791 2.0321	1220.6 1275.6 1353.2 1436.8 1490 1539 1986 3073.7 3143.5 3156.5 3164.6 3185.4 3193.1	C C H H H H H O H	1.490911 1.433944 1.129558 -0.620156 0.401640 2.154275 1.614532 -2.171476 0.224495	0.643091 -0.772442 -0.930381 0.408458 2.345224 1.195653 -1.399401 -0.333203 -2.170487	-0.565230 -0.501752 1.601561 1.929817 0.204950 -1.222611 -1.366530 -0.771057 0.635669
(phenol decomposition) 6	Theory: B3LYP/6-311G(d,p) Energy (hartree): -194.1537205 ZPE (hartree): 0.0921580 <S2>: 0 Rotational constants (GHz): 8.4748 8.2336 4.2860	348.77 524.1 681.52 712.62 816.85 818.72 917.45 924.4 954.19 955.65 970.72 1012.4 1112 1125.8 1130 1266.2 1315 1397.2 1415.1 1552.2 1638.7 3010.5 3031.8 3186.7 3196.8 3215.3 3222	C C C C C H H H H H H	-0.734343 0.734367 1.179323 -0.000015 -1.179329 -0.000024 -0.000024 1.347868 2.210197 -2.210212 -1.347821	0.989389 0.989370 -0.280935 -1.215664 -0.280906 -1.877472 -1.877546 1.881372 -0.607668 -0.607613 1.881405	0.000000 0.000000 -0.000004 -0.000001 -0.000004 0.876899 -0.876841 0.000005 -0.000006 -0.000006 0.000006

Appendix C

Details of Triplet OH Oxidation

Table C.1. High-pressure rate coefficients (in s^{-1}) of the elementary reactions in the triplet OH + phenanthrene radical reaction system.

Reaction	1500 K	2000 K	2500 K
$k_{2\rightarrow 1}$	1.3E+08	3.9E+09	2.9E+10
$k_{2\rightarrow 3}$	3.5E+09	1.3E+10	3.1E+10
$k_{2\rightarrow 6}$	1.1E+06	4.0E+07	3.7E+08
$k_{2\rightarrow 4}$	2.1E+08	2.6E+09	1.2E+10
$k_{3\rightarrow 2}$	8.2E+08	9.0E+09	3.9E+10
$k_{3\rightarrow 18}$	2.8E+05	3.2E+07	5.6E+08
$k_{3\rightarrow 20}$	1.8E+06	3.8E+08	9.7E+09
$k_{3\rightarrow 5}$	4.3E+07	1.4E+09	1.2E+10
$k_{3\rightarrow 4}$	7.1E+08	1.3E+10	7.2E+10
$k_{5\rightarrow 3}$	5.3E+07	1.6E+09	1.3E+10
$k_{5\rightarrow 22}$	3.8E+05	1.2E+08	3.6E+09
$k_{5\rightarrow 23}$	3.5E+04	7.5E+06	1.9E+08
$k_{5\rightarrow 4}$	1.5E+09	2.2E+10	1.2E+11
$k_{6\rightarrow 2}$	2.8E+07	2.1E+09	2.9E+10
$k_{6\rightarrow 12}$	9.0E+07	7.1E+09	1.0E+11
$k_{6\rightarrow 7}$	3.6E+08	1.8E+10	1.9E+11
$k_{6\rightarrow 4}$	1.1E+10	2.1E+11	1.4E+12
$k_{7\rightarrow 6}$	7.3E+06	3.7E+08	3.9E+09

$k_{7\rightarrow 11}$	1.8E+07	1.2E+09	1.6E+10
$k_{7\rightarrow 8}$	9.0E+05	6.3E+07	8.1E+08
$k_{7\rightarrow 4}$	2.6E+09	2.9E+10	1.3E+11
$k_{8\rightarrow 7}$	3.3E+12	3.7E+12	3.9E+12
$k_{8\rightarrow 9}$	7.0E+12	7.0E+12	7.0E+12
$k_{9\rightarrow 11}$	2.2E+08	5.5E+09	3.8E+10
$k_{9\rightarrow 8}$	1.4E+07	3.6E+08	2.5E+09
$k_{9\rightarrow 10}$	4.1E+12	1.0E+13	1.8E+13
$k_{11\rightarrow 9}$	7.8E+10	1.2E+11	1.5E+11
$k_{11\rightarrow 7}$	4.8E+10	8.0E+10	1.1E+11
$k_{12\rightarrow 13}$	1.6E+12	1.7E+12	1.8E+12
$k_{12\rightarrow 6}$	8.2E+10	1.0E+11	1.1E+11
$k_{13\rightarrow 12}$	5.5E+11	6.3E+11	6.9E+11
$k_{13\rightarrow 14}$	2.5E+11	4.0E+11	5.4E+11
$k_{14\rightarrow 13}$	1.5E+07	5.4E+08	4.8E+09
$k_{14\rightarrow 15}$	4.0E+10	2.0E+11	5.2E+11
$k_{15\rightarrow 14}$	3.0E+11	1.1E+12	2.4E+12
$k_{15\rightarrow 16}$	1.6E+08	2.0E+09	9.0E+09
$k_{16\rightarrow 15}$	2.6E+10	1.4E+11	3.9E+11
$k_{16\rightarrow 17}$	5.5E+12	1.4E+13	2.4E+13
$k_{18\rightarrow 19}$	3.5E+12	3.7E+12	3.7E+12
$k_{18\rightarrow 3}$	2.9E+12	2.9E+12	3.0E+12
$k_{19\rightarrow 18}$	1.2E+08	1.3E+09	5.3E+09
$k_{19\rightarrow 21}$	7.3E+12	1.1E+13	1.5E+13
$k_{19\rightarrow 20}$	1.1E+08	3.0E+09	2.2E+10
$k_{20\rightarrow 19}$	1.7E+11	4.0E+11	6.7E+11
$k_{20\rightarrow 3}$	9.1E+11	1.6E+12	2.3E+12
$k_{22\rightarrow 24}$	1.3E+11	3.1E+11	5.2E+11
$k_{22\rightarrow 5}$	8.5E+11	1.5E+12	2.1E+12

$k_{23\rightarrow24}$	3.4E+12	4.3E+12	4.9E+12
$k_{23\rightarrow5}$	4.2E+12	4.6E+12	5.0E+12
$k_{24\rightarrow22}$	1.8E+08	4.7E+09	3.2E+10
$k_{24\rightarrow23}$	9.0E+07	1.3E+09	6.7E+09
$k_{24\rightarrow25}$	9.8E+12	1.6E+13	2.1E+13
$k_{4\rightarrow26}$	4.0E+05	4.5E+07	7.8E+08
$k_{4\rightarrow28}$	6.8E+05	2.3E+08	7.7E+09
$k_{26\rightarrow4}$	4.4E+12	4.8E+12	5.1E+12
$k_{26\rightarrow7}$	3.5E+12	4.4E+12	5.1E+12
$k_{26\rightarrow29}$	6.0E+10	2.9E+11	7.5E+11
$k_{27\rightarrow26}$	4.8E+08	4.3E+09	1.7E+10
$k_{27\rightarrow29}$	1.5E+13	2.0E+13	2.4E+13
$k_{27\rightarrow28}$	1.0E+08	3.4E+09	3.0E+10
$k_{28\rightarrow4}$	6.7E+11	1.2E+12	1.8E+13
$k_{28\rightarrow27}$	6.7E+10	1.7E+11	3.2E+11

Table C.2. The total energies, zero-point energies, expectation values of S^2, vibrational frequencies, rotational constants, unsymmetrical hindered rotor MultiWell parameters, and Cartesian coordinate geometries for the geometries discussed in Chapter 5. These parameters for Figure 5.6 are reported in Appendix A.

Reaction Species	Information	Frequencies	Cartesian coordinates, (angstroms)			
			Atom	X	Y	Z
OH + phen. rad. (triplet) 2	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8030084 ZPE (hartree): 0.1925430 <S2>: 2.04 Rotational constants (GHz): 1.1930 0.5208 0.3625	36.69 89.63 182.62 201.53 246.25 272.06 312.60* 343.97 345.98 395.88 421.14 477.74 480.31 514.35 529.27 546.18 557.69 578.26 656.11 660.26 680.86 696.82 697.72 730.68 738.93 769.80 794.04 811.07 842.40 843.54 932.89 938.50 942.28 965.36 986.76 1041.96 1060.25 1087.58 1112.15 1127.92 1176.13 1179.48 1203.02 1215.56 1260.56 1280.63 1303.97 1323.60 1371.92 1421.58 1426.08 1447.33 1454.53 1492.87 1521.99 1539.63 1562.66 1580.55 1610.63 3150.94 3159.15 3171.56 3173.21 3174.99 3186.36 3187.98 3190.93 3268.80 3830.05	C	-3.679310	-0.334596	0.000060
			C	-2.923224	-1.508155	0.000320
			C	-1.511929	-1.450748	0.000335
			C	-0.817161	-0.248630	0.000066
			C	-1.602601	0.978341	-0.000149
			C	-3.035006	0.883993	-0.000160
			H	-3.411414	-2.475548	0.000457
			H	-0.969337	-2.380348	0.000508
			H	-4.762833	-0.379383	0.000027
			H	-3.603424	1.807866	-0.000315
			C	0.668507	-0.139189	0.000024
			C	1.266088	1.188630	0.000106
			C	0.468181	2.317627	-0.000064
			C	-0.985647	2.216491	-0.000268
			H	0.931947	3.296875	-0.000064
			H	-1.583195	3.120070	-0.000367
			C	1.551651	-1.211665	-0.000190
			C	2.971193	-1.038167	-0.000015
			C	3.526639	0.231642	0.000193
			C	2.694107	1.335010	0.000275
			H	3.603805	-1.920601	-0.000120
			H	4.603648	0.353540	0.000391
			H	3.106113	2.337350	0.000383
			O	1.087145	-2.497977	-0.000438
			H	1.838601	-3.099515	-0.000583
	*Vibration replaced by unsymmetrical hindered rotor (hrd 3 5 1). The same representation of the hindered rotor potential was also used in VariFlex		Multiwell hindered rotor parameters: Vhrd2 1 0.0 823.0 -42.0 -781.0 Ihrd1 1 0.0 2.235 -0.2313 0.2930 -1.208 0.354			

OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-1873 95.202 123.05 188.86 198.54	C	-3.555877	-0.274912	-0.228923
(triplet)		250.09 315.23 365.78 403.35 438.35	C	-2.873321	-1.432777	0.098580
2-3_TS	Energy (hartree): -614.7751785	464.39 480.92 495.21 515.3 537.98	C	-1.443732	-1.414142	0.382448
		547.75 573.95 615.59 664.21 679.21	C	-0.760146	-0.148586	0.223934
	ZPE (hartree): 0.1885290	692.56 705.89 747.59 759.53 799.27	C	-1.497400	1.057831	-0.027739
		806.44 822.5 849.44 870.01 912.71	C	-2.917207	0.966453	-0.249844
	$<S^2>$: 2.03	922.07 953.53 960.97 963.57 1024.8	H	-3.407427	-2.373282	0.174191
		1047.5 1085 1101.6 1130.2 1166.7	H	-1.152094	-2.001309	1.261027
	Rotational constants (GHz):	1177.7 1200.5 1231.1 1247 1290.7	H	-4.618017	-0.324975	-0.445905
	1.1903	1324.2 1334.3 1355.2 1369.9 1413.3	H	-3.472165	1.872913	-0.460305
	0.5483	1420.8 1434.4 1468.4 1484.9 1490.5	C	0.658911	-0.097081	0.193365
	0.3801	1521.6 1525.6 1551.6 1568.4 1639.5	C	1.350161	1.154351	0.145801
		3012.6 3155 3163 3170.5 3173.7 3179.6	C	0.599013	2.329309	0.086880
		3184.7 3186.3 3205	C	-0.800783	2.272603	-0.035631
			H	1.102804	3.289490	0.077589
			H	-1.360282	3.195394	-0.147151
			C	1.400735	-1.302598	-0.050987
			C	2.827304	-1.236171	-0.195984
			C	3.493726	-0.019134	-0.101421
			C	2.781495	1.161326	0.065785
			H	3.352844	-2.166449	-0.370384
			H	4.574272	0.008411	-0.180523
			H	3.301086	2.112687	0.097884
			O	0.808942	-2.439623	-0.207286
			H	-0.369841	-2.194713	-0.185728
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-1894.6 80.043 97.899 182.94 191.09	C	-3.649032	-0.453150	-0.045691
(triplet)		219.82 247.32 341.32 368.44 396.29	C	-2.854346	-1.614768	0.007211
2-4_TS	Energy (hartree): -614.7316583	433.83 443.34 486.05 518.51 533.04	C	-1.480569	-1.513703	0.068948
		545.18 560.53 597.84 658.45 686.29	C	-0.843201	-0.250170	0.061431
	ZPE (hartree): 0.1882720	710.3 743.04 769.55 793.2 803.55 811.75	C	-1.652200	0.932287	0.016581
		827.64 854.99 882.38 936.86 959.09	C	-3.058451	0.791814	-0.035591
	$<S^2>$: 2.02	968.15 987.2 996.54 1019.8 1056.4	H	-3.325025	-2.591115	0.010841
		1061.3 1137.1 1142 1160.2 1173.2	H	-0.871073	-2.406834	0.117460
	Rotational constants (GHz):	1183.4 1204.8 1234.8 1248.4 1277.8	H	-4.729188	-0.540525	-0.085205
	1.2031	1305.8 1351.5 1355.5 1376.2 1431.9	H	-3.669633	1.687523	-0.070230
	0.5214	1447.2 1451.8 1480.1 1508.9 1539	C	0.589253	-0.109568	0.119668
	0.3665	1562.2 1595.3 1639.2 1678.2 2998.3	C	1.174011	1.202099	0.051561
			C	0.336158	2.337236	0.014154

		3152.5 3157.5 3159.7 3172.5 3179.7 3181 3185.2 3201	C	-1.033153	2.217446	0.013814
			H	0.793525	3.319867	-0.045220
			H	-1.662463	3.099469	-0.017461
			C	1.504687	-1.171775	0.159143
			C	2.972992	-1.014308	0.272927
			C	3.478189	0.267940	-0.110668
			C	2.593123	1.325025	-0.147762
			H	3.466530	-1.560329	1.086034
			H	4.538362	0.434682	-0.262424
			H	2.983129	2.324537	-0.318368
			O	1.408685	-2.404493	-0.324775
			H	2.741583	-2.209756	-0.491570
OH + phen. rad. (triplet) 3	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8229711 ZPE (hartree): 0.1936790 $<S^2>$: 2.04 Rotational constants (GHz): 1.1924 0.5252 0.3654	56.139 95.893 126.82 188.24 229.9 231.7 303.07 354.69 396.7 452.39 466.4 485.55 515.38 519.67 542.04 549.82 585.1 650.81 656.98 683.08 703.86 720.02 761.79 801.83 817.35 833.8 844.57 890.93 926.69 941.68 967.28 969.99 975.87 976.75 1029.4 1093.3 1115.1 1153.2 1174.7 1176.3 1208.2 1211.8 1216.7 1226.6 1275 1312.4 1346.2 1376.3 1380.4 1415.1 1421.2 1442.2 1479.6 1500.8 1535.2 1543.7 1555.3 1587.5 1618.7 2996.2 3001.1 3156.1 3160.5 3166.3 3173.6 3178 3181.8 3186.8 3197.1	C	-3.652050	-0.239668	-0.000071
			C	-2.983539	-1.437258	-0.000130
			C	-1.490792	-1.532359	0.000031
			C	-0.755987	-0.203952	0.000026
			C	-1.510039	0.994902	0.000066
			C	-2.953295	0.968652	0.000064
			H	-3.534526	-2.371466	-0.000267
			H	-1.156502	-2.136861	0.853320
			H	-4.737160	-0.226641	-0.000144
			H	-3.484469	1.912921	0.000127
			C	0.659544	-0.131227	0.000002
			C	1.302380	1.141041	0.000000
			C	0.524580	2.317174	0.000042
			C	-0.846237	2.242340	0.000079
			H	1.022786	3.280570	0.000045
			H	-1.441664	3.149195	0.000114
			C	1.530245	-1.338574	-0.000016
			C	2.967453	-1.134287	-0.000044
			C	3.545207	0.124373	-0.000062
			C	2.732340	1.246536	-0.000040
			H	3.562946	-2.039424	-0.000046
			H	4.623938	0.233052	-0.000087
			H	3.169968	2.238873	-0.000048
			O	1.089016	-2.501170	0.000046
			H	-1.156301	-2.137012	-0.853059

OH + phen. rad. (triplet) 3-5_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7548471 ZPE (hartree): 0.1891340 $<S^2>$: 2.05 Rotational constants (GHz): 1.1987 0.5207 0.3637	-2078.4 64.63 88.149 159.32 189.89 242.55 260.93 355.89 359.43 396 447.89 480.55 487.19 513.25 522.41 544.85 552.37 619.89 653.73 666.84 684.94 696.76 735.35 760.52 804.56 810.96 825.29 834.71 873.48 910.27 919.65 940.51 962.34 976.43 976.99 1030.5 1093.9 1109.5 1141.5 1154.2 1169.7 1202.7 1213.2 1229.4 1252.6 1263.9 1327.6 1337.9 1365 1382.3 1419 1427.7 1447.9 1488.5 1522.6 1554.4 1567.4 1577.7 1584.8 2141.3 3160.2 3163.6 3166.3 3178.5 3182.2 3183.9 3200.4 3209.8 3251.7	C	3.656686	-0.238173	-0.058565
			C	2.959808	-1.482248	0.007909
			C	1.469825	-1.463426	0.038296
			C	0.750905	-0.218567	0.012629
			C	1.513361	1.000979	-0.002259
			C	2.975183	0.936827	-0.048679
			H	3.452692	-2.432597	-0.141427
			H	0.934747	-2.393265	-0.057164
			H	4.739300	-0.246106	-0.114657
			H	3.513048	1.877498	-0.084529
			C	-0.676419	-0.140951	-0.002667
			C	-1.304395	1.148102	0.006873
			C	-0.526689	2.315379	0.016183
			C	0.863742	2.231382	0.005559
			H	-1.018288	3.281146	0.026838
			H	1.459247	3.138220	-0.003099
			C	-1.551401	-1.339693	-0.024102
			C	-2.994802	-1.133482	-0.014828
			C	-3.554383	0.126690	0.001761
			C	-2.733268	1.249542	0.012301
			H	-3.594108	-2.035383	-0.026135
			H	-4.632308	0.247238	0.006293
			H	-3.171334	2.241525	0.026819
			O	-1.124691	-2.507292	-0.052540
			H	2.225613	-1.574104	1.084912
OH + phen. rad. (triplet) 3-18_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7320235 ZPE (hartree): 0.1900330 $<S^2>$: 2.08 Rotational constants (GHz): 1.1041 0.5640 0.4141	-125.66 85.357 106.13 138.26 176.32 188.35 244.36 292.34 342.23 413.81 453.3 473.57 492 501.03 520.04 554.48 596.65 629.76 667.31 675.82 690.04 713.39 745.07 769.75 781.89 814.76 836.63 899.08 916.21 927.08 932.04 940.63 959.82 968.71 978.93 1009.3 1036.9 1084 1109.5 1116.2 1182.5 1191 1208.9 1214.6 1237.9 1247.3 1288 1316.2 1353.5 1392.3 1396 1418.3 1440.3 1450.5 1503.2 1547.4 1565.6 1585.3 1871 2928.2 2934.3 3096.5	C	3.514721	-0.186648	-0.236063
			C	2.868922	-1.370999	-0.429279
			C	1.378973	-1.489590	-0.326497
			C	0.667723	-0.181508	-0.095220
			C	1.384229	1.010286	0.115599
			C	2.806386	1.000590	0.048011
			H	3.427993	-2.275443	-0.642226
			H	0.980487	-1.975165	-1.233637
			H	4.597319	-0.149897	-0.300107
			H	3.343249	1.928278	0.207652
			C	-0.786322	-0.143490	0.016852
			C	-1.453545	1.171392	0.065498
			C	-0.696881	2.309605	0.327423

		3156.3 3162.1 3174.1 3181.2 3185.9 3193 3212.1	C	0.685731	2.234230	0.378661
			H	-1.194602	3.268102	0.431894
			H	1.270045	3.129640	0.557256
			C	-1.463996	-1.370062	0.621174
			C	-1.984417	-1.135492	-0.709224
			C	-3.113932	-0.173399	-0.796658
			C	-2.821899	1.066850	-0.333289
			H	-1.822695	-1.884319	-1.484223
			H	-4.076951	-0.496764	-1.170174
			H	-3.523707	1.889587	-0.289562
			O	-1.254961	-2.211034	1.444842
			H	1.124400	-2.196327	0.482462
OH + phen. rad. (triplet) 3-20_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7202542 ZPE (hartree): 0.1895270 $\langle S^2 \rangle$: 2.03 Rotational constants (GHz): 1.0303 0.4042 0.3041	-92.144 34.206 53.515 78.298 124.59 174.87 179.05 223.87 283.88 360.79 411.47 423.01 465.15 475.59 494.81 499.92 544.27 579.36 588.23 649.03 671.01 678.95 700.74 739.68 756.1 781.69 792.89 838.47 906.59 916.68 933.41 950.31 960.5 969.4 992.01 1003 1081.2 1132.1 1140 1173.6 1194.4 1199.8 1215.7 1228.9 1239.4 1287.3 1330.4 1377.7 1385.7 1423.5 1425.7 1434.8 1444.9 1479.9 1535.9 1565.2 1597.5 1664.3 2209.5 2968.4 2973.5 3125 3143.3 3146.7 3150.8 3155.2 3170.9 3173.7 3182.6	C	3.793925	-0.898453	0.028479
			C	2.933721	-1.922081	-0.255352
			C	1.455631	-1.714836	-0.379949
			C	1.006231	-0.282853	-0.161439
			C	1.956555	0.747406	0.134343
			C	3.342650	0.421224	0.224097
			H	3.310943	-2.928626	-0.399375
			H	1.115995	-2.054185	-1.370269
			H	4.856635	-1.103670	0.107337
			H	4.051535	1.209700	0.449935
			C	-0.304480	0.095933	-0.230757
			C	-0.825429	1.369118	-0.041488
			C	0.134976	2.369319	0.249298
			C	1.479434	2.064055	0.332724
			H	-0.200046	3.390122	0.408226
			H	2.195699	2.847176	0.557150
			C	-3.168044	-1.500543	0.242379
			C	-3.104734	-0.585398	-0.699353
			C	-3.256462	0.866088	-0.408662
			C	-2.241126	1.701018	-0.131226
			H	-2.984226	-0.947047	-1.716676
			H	-4.263010	1.274185	-0.453303
			H	-2.486472	2.746835	0.037871
			O	-3.217600	-2.305262	1.079303
			H	0.926663	-2.372378	0.326115

OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	50.644 83.207 146.27 172.97 242.58	C	3.648109	-0.199969	0.000375
(triplet)		257.17 270.87 355.75 393.2 420.4 463.34	C	2.952694	-1.523939	0.000329
5	Energy (hartree): -614.8211650	483.52 503.18 520.86 544.5 554.53	C	1.461539	-1.436104	-0.000127
		600.01 666.05 666.28 701.12 722.67	C	0.758657	-0.231556	-0.000238
	ZPE (hartree): 0.1935570	749.75 775.29 800.54 812.75 824.82	C	1.515536	1.006409	-0.000059
		833.22 887.49 912.84 937.5 948.57	C	2.960986	0.953801	0.000001
	<S^2>: 2.08	972.92 982.84 990.39 1003.9 1087.6	H	3.283423	-2.126257	-0.864106
		1096.4 1143.9 1166.2 1182.7 1188.7	H	0.906837	-2.360816	-0.000180
	Rotational constants (GHz):	1214.9 1224.5 1259.9 1287.7 1327.9	H	4.733180	-0.193337	0.000651
	1.1925	1356.2 1365.4 1388.2 1419.8 1435.2	H	3.491040	1.901664	-0.000112
	0.5174	1440.1 1457.6 1489.6 1525 1554.3	C	-0.688581	-0.149230	-0.000173
	0.3616	1564.9 1568.3 1667.3 2921.1 2932.9	C	-1.311394	1.134064	-0.000123
		3147.4 3158.5 3164.7 3170.8 3178.3	C	-0.519977	2.315583	-0.000269
		3182.1 3199.9 3241.6	C	0.856196	2.239001	-0.000130
			H	-1.018897	3.277853	-0.000574
			H	1.448981	3.148131	0.000031
			C	-1.573507	-1.343230	-0.000205
			C	-3.014946	-1.126761	0.000418
			C	-3.563586	0.130192	0.000445
			C	-2.725666	1.250406	0.000222
			H	-3.618711	-2.025897	0.000581
			H	-4.639985	0.262420	0.000705
			H	-3.156403	2.245724	0.000035
			O	-1.156102	-2.514424	-0.000596
			H	3.282991	-2.126103	0.864948
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-93.655 30.421 59.647 90.357 126.73	C	-3.814112	-0.810559	0.036944
(triplet)		161.84 204.89 247.1 254.62 351.72	C	-2.914880	-1.970564	-0.277838
5-22_TS	Energy (hartree): -614.7119508	390.81 424.45 452.37 471.19 484.5 496.4	C	-1.468267	-1.605317	-0.365606
		545.47 590.01 600.74 654.29 673.8 692.1	C	-1.008065	-0.301449	-0.165897
	ZPE (hartree): 0.1892440	703.68 734.34 749.55 774.98 791.44	C	-1.942654	0.766036	0.137869
		828.35 891.74 896.98 925.2 935.93	C	-3.352967	0.436080	0.224497
	<S^2>: 2.06	946.33 991.71 992.67 996.95 1050.7	H	-3.060054	-2.764575	0.475661
		1131.8 1138.1 1171.5 1185.7 1193.9	H	-0.751305	-2.387054	-0.588059
	Rotational constants (GHz):	1222.6 1242.3 1260.6 1304.2 1332.9	H	-4.877941	-1.012383	0.111420
	1.0376	1362.3 1379.4 1410.3 1423.8 1432.5	H	-4.044273	1.242660	0.451054
	0.3975	1441.8 1483.3 1524.9 1574.4 1668.3	C	0.338884	0.082172	-0.235284
	0.3010	1672.4 2211.4 2919.9 2931.3 3123.6	C	0.849554	1.346917	-0.042900
			C	-0.101938	2.358727	0.251235

		3145.2 3146.3 3148.2 3154.7 3167.8 3171.8 3177.2	C	-1.460054	2.058988	0.336104
			H	0.240655	3.375889	0.412174
			H	-2.166017	2.851210	0.563436
			C	3.196096	-1.514985	0.240160
			C	3.138038	-0.600325	-0.702315
			C	3.285254	0.852029	-0.413580
			C	2.270902	1.683104	-0.133328
			H	3.026371	-0.962510	-1.720248
			H	4.290618	1.263107	-0.462599
			H	2.512952	2.729576	0.035711
			O	3.247285	-2.321627	1.074814
			H	-3.244034	-2.448034	-1.217430
OH + phen. rad. (triplet) 5-23_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7180410 ZPE (hartree): 0.1895390 $<S^2>$: 2.04 Rotational constants (GHz): 1.1045 0.5497 0.4104	-281.17 71.135 88.18 151.4 157.86 228.31 243.68 251.92 330.35 407.74 422.94 457.8 474.94 488.94 531.49 570.28 588.14 643.5 669.29 684.49 701.5 720.1 735.88 763.49 777.41 795.4 838.78 864.16 891.1 905.55 931.73 946.83 950.37 973.31 991.36 992.45 1039 1062.7 1100.9 1123.5 1180.4 1182.9 1202.2 1225.6 1237.8 1272.3 1290 1309.1 1340.8 1381.1 1411.7 1431.3 1443.2 1450 1472.4 1519.7 1609.9 1620.1 1863.7 2903.1 2926.4 3116.6 3148.7 3162.7 3168.5 3173.9 3182.3 3193.3 3210.4	C	3.522501	-0.149545	-0.196441
			C	2.843677	-1.449862	-0.494587
			C	1.352811	-1.382996	-0.388626
			C	0.678804	-0.226539	-0.106609
			C	1.391124	0.999892	0.120125
			C	2.820382	0.973380	0.090223
			H	3.140918	-1.807785	-1.497483
			H	0.805870	-2.309672	-0.523517
			H	4.606670	-0.126166	-0.218387
			H	3.349151	1.899147	0.297606
			C	-0.798705	-0.178155	0.045423
			C	-1.460170	1.136115	0.032482
			C	-0.678033	2.304561	0.333167
			C	0.678641	2.228976	0.379543
			H	-1.186851	3.253095	0.462713
			H	1.265164	3.120371	0.575302
			C	-1.492187	-1.330493	0.671498
			C	-2.120994	-1.187049	-0.639651
			C	-3.149769	-0.167731	-0.839668
			C	-2.791979	1.089453	-0.403991
			H	-2.016931	-2.032105	-1.318107
			H	-4.101800	-0.426108	-1.284880
			H	-3.445017	1.952058	-0.424310
			O	-1.302610	-2.155626	1.517060
			H	3.227085	-2.237864	0.177254

OH + phen. rad. (triplet) 6	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8098318 ZPE (hartree): 0.1931510 $\langle S^2 \rangle$: 2.04 Rotational constants (GHz): 1.1772 0.5230 0.3629	-32.05 54.049 90.856 195.84 227.16 248.22 324.69 352.57 388.61 403.74 470.25 476.86 511.1 514.47 527.42 552.22 570.42 627.01 655.59 703.51 706.48 749.21 781.87 783.97 788.37 826.58 892.55 929.55 941.66 943.39 958.39 967.94 969.86 1000.6 1006.1 1067.3 1089.8 1122.8 1159.1 1173.5 1193.2 1209 1213 1241.3 1286.8 1304.2 1338.3 1359 1394.4 1398.5 1443.7 1446 1463.5 1487.8 1515.6 1563.7 1578.8 1595.2 1604.8 2975 2980.2 3150 3159.9 3162.9 3169.7 3175.4 3182.8 3190.6 3246.6	C	3.665428	-0.359307	0.000016
			C	2.928375	-1.530996	0.000152
			C	1.531239	-1.483634	0.000201
			C	0.829255	-0.255893	0.000065
			C	1.609280	0.952773	-0.000031
			C	2.997801	0.876260	-0.000068
			H	3.425693	-2.493826	0.000242
			H	0.959611	-2.397717	0.000335
			H	4.749218	-0.386527	-0.000010
			H	3.572469	1.796393	-0.000166
			C	-0.615894	-0.167112	0.000042
			C	-1.235362	1.200420	0.000076
			C	-0.409307	2.340054	-0.000027
			C	0.954513	2.243709	-0.000086
			H	-0.884568	3.315638	-0.000059
			H	1.573302	3.133465	-0.000151
			C	-1.491648	-1.330625	-0.000028
			C	-3.009992	-1.140868	0.000341
			C	-3.494121	0.264652	0.000064
			C	-2.633325	1.333640	0.000049
			H	-3.399298	-1.695555	-0.866410
			H	-4.565213	0.438522	-0.000118
			H	-3.040871	2.340196	-0.000075
			O	-1.093630	-2.501755	-0.000737
			H	-3.398759	-1.694995	0.867709
OH + phen. rad. (triplet) 6-7_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7401798 ZPE (hartree): 0.1887330 $\langle S^2 \rangle$: 2.04 Rotational constants (GHz): 1.1790 0.5245 0.3669	-2153.5 55.139 93.462 160.65 203.37 233.03 245.42 328.08 364.62 388.12 404.57 470.26 477.06 510.25 517.64 533.68 553.51 590.92 623.15 665.04 689.42 717.94 741.92 773.37 783.41 792.2 825.62 834.31 851.94 879.48 936.05 946.94 983.81 986.36 990.95 1010 1036.8 1065 1146.2 1165.1 1174.8 1187.2 1214.6 1223 1242.1 1297.8 1316.6 1336.5 1347.9 1355.5 1383.3 1433.1 1453.9 1488.6 1551.3 1583.1 1604.4 1610.3 1644.5 2145.6 3156.3	C	3.654610	-0.359302	0.098988
			C	2.894561	-1.534321	0.175789
			C	1.514379	-1.492773	0.144041
			C	0.812705	-0.255952	0.024064
			C	1.609258	0.944962	-0.036553
			C	3.003940	0.864888	-0.003938
			H	3.393097	-2.492891	0.268455
			H	0.947343	-2.407899	0.200818
			H	4.737112	-0.402787	0.127240
			H	3.579357	1.783356	-0.058661
			C	-0.606047	-0.150050	-0.025928
			C	-1.240978	1.170503	-0.033352
			C	-0.390974	2.336785	-0.135173

		3159.5 3169.4 3174.6 3178.2 3188.3 3195.4 3208.2 3245.4	C	0.952976	2.226465	-0.140454
			H	-0.867055	3.309805	-0.191512
			H	1.575554	3.112413	-0.211322
			C	-1.504349	-1.338686	-0.136738
			C	-2.939492	-1.153627	0.094458
			C	-3.517485	0.206638	0.241985
			C	-2.597927	1.331795	0.086193
			H	-3.582669	-1.998494	-0.114389
			H	-4.588873	0.331135	0.170171
			H	-3.016384	2.331597	0.069129
			O	-1.105513	-2.462627	-0.451110
			H	-3.204443	-0.649173	1.228661
OH + phen. rad. (triplet) 6-12_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7325362 ZPE (hartree): 0.1917660 $<S^2>$: 2.01 Rotational constants (GHz): 1.0945 0.4984 0.3491	-216.67 57.938 75.503 127.18 168.67 185.65 240.56 251.66 316.4 381.68 412.42 438.68 446.39 475.75 506.24 519.29 542.77 609.12 637.63 651.87 711.92 733.76 762.43 770.22 774.88 822.69 830.16 879.73 911.81 923.66 956.09 964.24 974.09 990.93 1002.1 1011.3 1044.3 1139.5 1168.8 1172.6 1178.2 1213 1222.9 1237.3 1272.9 1293.4 1344.8 1358.9 1394.5 1429.5 1444.6 1448.7 1492.5 1518 1575.9 1625.5 1649.3 1690.4 1762.8 2986.7 3057.6 3150.3 3155.8 3159.8 3171.3 3172.8 3176.8 3187.4 3213.4	C	-3.669809	-0.559174	0.070798
			C	-2.818536	-1.680888	0.197306
			C	-1.453351	-1.528167	0.205179
			C	-0.878385	-0.235014	0.091002
			C	-1.741152	0.912084	-0.040088
			C	-3.142498	0.704371	-0.049919
			H	-3.249517	-2.671893	0.282343
			H	-0.795348	-2.382919	0.286021
			H	-4.744568	-0.700925	0.062920
			H	-3.795391	1.564494	-0.157259
			C	0.492960	0.039844	0.085185
			C	1.093950	1.268544	0.008051
			C	0.202693	2.379305	-0.139215
			C	-1.156097	2.202473	-0.155484
			H	0.627983	3.374782	-0.220640
			H	-1.811873	3.061052	-0.252217
			C	1.975406	-1.490557	-0.575869
			C	3.085254	-0.965175	0.381999
			C	3.435964	0.479807	0.207389
			C	2.539372	1.463629	0.055606
			H	2.778756	-1.194262	1.412296
			H	4.491037	0.733012	0.215186
			H	2.889791	2.485621	-0.051476
			O	1.483506	-2.576483	-0.473454
			H	3.946459	-1.603588	0.158828

OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	33.295 95.313 130.66 155.4 219.14	C	-3.678786	-0.320952	0.000078
(triplet)		246.03 293.69 358.09 394.63 404.77	C	-2.928831	-1.511304	0.000158
7	Energy (hartree): -614.8160156	482.73 493.94 520.8 523.3 541.72 557.28	C	-1.551151	-1.486437	0.000147
		606.18 652.32 668.87 696.2 705.34	C	-0.833722	-0.255591	0.000034
	ZPE (hartree): 0.1935900	745.93 770.96 783.85 794.52 831.36	C	-1.612241	0.952612	-0.000026
		841.86 890.89 912.58 948.9 968.14	C	-3.020867	0.889540	-0.000005
		984.56 1010 1015 1015.1 1056.9 1087.2	H	-3.440483	-2.467490	0.000217
	$\langle S^2 \rangle$: 2.05	1157 1163 1170.9 1184.6 1218.9 1231.4	H	-0.993036	-2.407955	0.000216
		1252.9 1300.8 1340.7 1363.3 1371	H	-4.762208	-0.357343	0.000100
	Rotational constants (GHz):	1394.5 1407.5 1434.3 1447 1467.2	H	-3.580514	1.819201	-0.000047
	1.1964	1485.1 1515.6 1540.3 1562.7 1634	C	0.600329	-0.160829	-0.000004
	0.5180	1639.6 2891.2 2909.4 3156.6 3159.6	C	1.225915	1.127859	-0.000043
	0.3623	3165.3 3169.8 3178.1 3184.1 3186.7	C	0.400313	2.307063	-0.000152
		3255.6	C	-0.951885	2.219458	-0.000131
			H	0.890364	3.274486	-0.000188
			H	-1.560079	3.118222	-0.000161
			C	1.498627	-1.349068	-0.000146
			C	2.923594	-1.145963	-0.000113
			C	3.594532	0.178258	0.000390
			C	2.611542	1.298998	0.000038
			H	3.514559	-2.054982	-0.000414
			H	4.277187	0.257915	0.866687
			H	3.001779	2.311240	-0.000147
			O	1.088767	-2.526656	-0.000304
			H	4.278087	0.258105	-0.865178
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-308.05 89.758 97.469 150.28 183.54	C	3.540835	-0.310234	-0.248887
(triplet)		200.37 241.92 290.84 361.91 405.79	C	2.777623	-1.490486	-0.385994
7-8_TS	Energy (hartree): -614.7346679	409.15 458.1 483.5 508.41 531.47 555.18	C	1.400543	-1.442273	-0.283503
		564.93 621.05 662.81 675.35 694.12	C	0.728680	-0.226016	-0.068329
	ZPE (hartree): 0.1905920	727.04 758.73 780.18 785.6 834.27	C	1.499608	0.982321	0.079796
		860.84 867.74 884.38 900.86 950.11	C	2.918523	0.890458	-0.015982
	$\langle S^2 \rangle$: 2.02	954.66 964.01 985.24 1001.2 1004.7	H	3.273384	-2.437639	-0.563032
		1049.5 1089.1 1112.1 1136.6 1156.2	H	0.829871	-2.360030	-0.362880
	Rotational constants (GHz):	1177.9 1192.1 1220.6 1239.5 1284.4	H	4.621606	-0.357126	-0.321518
	1.1206	1298.9 1321.9 1338 1356.3 1403.4	H	3.501726	1.798179	0.097596
	0.5566	1441.3 1475.5 1481.8 1522.5 1554	C	-0.721592	-0.140653	0.076292
	0.4095	1568.8 1626 1845.7 2936.9 3009.9	C	-1.340578	1.177772	0.162632
			C	-0.561090	2.299327	0.315682

		3114.3 3160.7 3167 3172.5 3181.2 3187.1 3193.4 3199.5	C	0.855988	2.209984	0.313349
			H	-1.037006	3.270537	0.397160
			H	1.452618	3.104157	0.448097
			C	-1.479219	-1.354942	0.584130
			C	-2.022046	-1.099263	-0.718314
			C	-3.146169	-0.089188	-0.861853
			C	-2.761643	1.116352	-0.063538
			H	-1.836983	-1.820869	-1.512465
			H	-3.267180	0.173304	-1.926272
			H	-3.419511	1.967127	0.058812
			O	-1.269132	-2.243962	1.364589
			H	-4.102256	-0.524895	-0.545097
OH + phen. rad. (triplet) 7-11_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7356253 ZPE (hartree): 0.1900770 $<S^2>$: 2.07 Rotational constants (GHz): 1.0635 0.5022 0.3450	-436.2 40.733 80.615 140.08 152.24 173.82 207 239.27 286.25 342.27 375.16 411.37 450.56 475.58 505.87 514.43 517.09 592.17 607.56 627.37 650.51 691.53 722.09 758.04 765.65 774.51 820.89 844.41 881.25 905.93 958.46 972.47 973.91 986 998.66 1035.5 1051.6 1131.1 1138.2 1166 1174.7 1194.9 1226 1229.5 1271.6 1316.6 1334.6 1344.5 1375.1 1393.7 1427.4 1440.7 1458.3 1472.8 1515 1557.1 1615.6 1634.1 2074.5 2952.9 3066.7 3152.6 3155.9 3159.5 3167.9 3169.3 3173.3 3186 3226.9	C	-3.671478	-0.560003	0.039567
			C	-2.819969	-1.682278	0.004677
			C	-1.452066	-1.528818	-0.025960
			C	-0.865765	-0.232398	-0.021996
			C	-1.741604	0.914123	0.012689
			C	-3.135742	0.711861	0.042467
			H	-3.247188	-2.678872	-0.000111
			H	-0.805389	-2.393678	-0.057864
			H	-4.746515	-0.697491	0.062580
			H	-3.787310	1.579714	0.067269
			C	0.514260	0.024179	-0.047962
			C	1.098946	1.296444	-0.033767
			C	0.178807	2.416857	-0.004909
			C	-1.166140	2.224812	0.019129
			H	0.593143	3.420031	-0.002636
			H	-1.835801	3.078365	0.044825
			C	2.042206	-1.710498	0.044539
			C	3.031792	-0.913754	0.478827
			C	3.458481	0.369213	-0.188828
			C	2.479789	1.502498	-0.062997
			H	3.380636	-1.143316	1.481092
			H	4.421979	0.662061	0.236047
			H	2.866237	2.515907	-0.080880
			O	1.474722	-2.689575	-0.253349
			H	3.653337	0.180445	-1.256384

OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	62.94 89.83 142.8 173.09 196.02 231.9	C	3.533389	-0.330415	-0.190396
(triplet)		259.85 333.77 371.11 397.97 429.05	C	2.777712	-1.481987	-0.500026
8	Energy (hartree): -614.7368323	455.46 508.86 512.4 543.41 577.09	C	1.392820	-1.424839	-0.476509
		580.49 625.2 671.67 677.89 695.16	C	0.721343	-0.235695	-0.169294
	ZPE (hartree): 0.1910780	715.69 762.49 772.36 786.55 828.62	C	1.481819	0.955459	0.130096
		846.46 859.92 863.92 915.7 938.29	C	2.905994	0.851263	0.117814
	$\langle S^2 \rangle$: 2.02	941.49 972.93 980.34 999.9 1028.2	H	3.278762	-2.409872	-0.748500
		1045.4 1070.4 1089.4 1133.7 1151.7	H	0.821688	-2.320897	-0.696450
	Rotational constants (GHz):	1164.6 1187.7 1208.7 1233 1281.4	H	4.616504	-0.382123	-0.197400
	1.1248	1301.8 1317.5 1334.1 1346.2 1393.4	H	3.488647	1.736295	0.350599
	0.5484	1437.9 1471.8 1473.9 1516.8 1547.4	C	-0.736590	-0.149175	-0.048823
	0.4233	1577.4 1613.4 1899.5 2948.2 3027.7	C	-1.363054	1.188304	-0.001114
		3106.7 3157.8 3161.6 3168.8 3176.4	C	-0.595701	2.291544	0.263728
		3186.1 3191.7 3202.7	C	0.829592	2.169385	0.389616
			H	-1.056964	3.270264	0.334588
			H	1.420755	3.047379	0.620301
			C	-1.462094	-1.263095	0.759652
			C	-1.858490	-1.151080	-0.624768
			C	-3.079770	-0.264706	-0.907301
			C	-2.750564	1.074380	-0.322459
			H	-1.620527	-1.954235	-1.320327
			H	-3.221729	-0.192063	-1.997809
			H	-3.438008	1.909744	-0.347194
			O	-1.383389	-1.921938	1.748592
			H	-4.000451	-0.705038	-0.507832
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-353.18 73.369 95.015 150.63 174.84	C	3.521670	-0.330653	-0.188705
(triplet)		202.59 238.12 263.22 366.73 399.12	C	2.760693	-1.481727	-0.497445
8-9_TS	Energy (hartree): -614.7366875	432.43 452.72 491.86 512.06 531.79	C	1.379831	-1.420589	-0.477693
		571.73 580.27 593.48 661.85 677.05	C	0.709631	-0.224140	-0.174221
	ZPE (hartree): 0.1904050	696.86 726.39 766.13 778.45 783.92	C	1.476388	0.962973	0.127178
		822.85 855.08 862.27 872.27 922.16	C	2.899316	0.853237	0.116617
	$\langle S^2 \rangle$: 2.02	939.65 945.12 975.47 981.82 994.84	H	3.259948	-2.411529	-0.742593
		1033 1047.7 1073.8 1107.8 1140.6	H	0.805329	-2.314732	-0.695707
	Rotational constants (GHz):	1154.5 1167.7 1192.4 1210.6 1236.8	H	4.604528	-0.387495	-0.193936
	1.1155	1281.5 1302.8 1324.5 1334.6 1354.8	H	3.485393	1.735893	0.349993
	0.5543	1404.4 1438.9 1472.4 1477.4 1516	C	-0.738023	-0.125946	-0.068622
	0.4228	1542.6 1562.1 1620.5 1887.6 2940.3	C	-1.358645	1.200173	0.005123
			C	-0.586557	2.305357	0.278744

		3037.7 3079.2 3158.3 3162.7 3167.9 3176.4 3184.7 3191.4 3202.6	C	0.827950	2.181422	0.385723
			H	-1.050927	3.279868	0.380850
			H	1.425433	3.056829	0.610829
			C	-1.477792	-1.292020	0.755497
			C	-1.853335	-1.135603	-0.624609
			C	-3.080172	-0.248320	-0.885023
			C	-2.752037	1.083041	-0.282678
			H	-1.621805	-1.922577	-1.343630
			H	-3.223978	-0.159550	-1.974811
			H	-3.446779	1.912734	-0.281021
			O	-1.326726	-2.006602	1.695217
			H	-3.996835	-0.699852	-0.491026
OH + phen. rad. (triplet) 9	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7990052 ZPE (hartree): 0.1934860 $\langle S^2 \rangle$: 2.04 Rotational constants (GHz): 0.9537 0.5829 0.3776	44.999 70.277 109.88 142.36 207.12 218.83 266.38 324.81 354.75 412.5 425.61 464.81 480.59 516.95 520.28 554.7 611.46 621.28 671.23 674.28 747.53 759.06 770.37 801.86 817.91 828.41 869.32 879.47 941.72 959.24 975.26 979.8 994.91 1000.7 1023.9 1051.4 1076.2 1162 1166.8 1170.7 1181.9 1200.4 1222.3 1231.3 1276.7 1291.1 1313.8 1353.2 1372.3 1409.5 1414.2 1462 1471.7 1474.1 1546.6 1576 1615.5 1640.1 1911.6 2997.6 3007.9 3025.1 3158.3 3161.5 3171.2 3182.2 3186.6 3199 3207.6	C	3.458686	0.685099	0.076885
			C	2.538657	1.724510	0.325368
			C	1.186101	1.471991	0.356544
			C	0.686675	0.157816	0.142034
			C	1.628032	-0.901813	-0.107172
			C	3.005438	-0.600666	-0.135441
			H	2.900809	2.733042	0.490222
			H	0.491917	2.283914	0.532940
			H	4.520936	0.899151	0.052584
			H	3.710740	-1.403145	-0.325685
			C	-0.682783	-0.179258	0.172871
			C	-1.128451	-1.508082	-0.010902
			C	-0.175704	-2.544861	-0.268528
			C	1.151206	-2.236027	-0.314827
			H	-0.515540	-3.563607	-0.416683
			H	1.883813	-3.013583	-0.505872
			C	-2.012664	1.753603	-0.705343
			C	-1.878650	0.727828	0.427457
			C	-3.098476	-0.243772	0.447263
			C	-2.516873	-1.590847	0.130346
			H	-1.774671	1.292154	1.362819
			H	-3.592653	-0.228542	1.426293
			H	-3.104201	-2.495383	0.046001
			O	-1.704019	2.892554	-0.699680
			H	-3.856168	0.062447	-0.284505

OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-358.23 32.971 70.837 96.963 142.38	C	-3.465679	0.546289	-0.115590
(triplet)		145.81 218.42 230.92 270.25 324.25	C	-2.592669	1.590148	-0.510123
9-10_TS	Energy (hartree): -614.7807170	335.54 426.93 436.48 465.87 507.33	C	-1.237914	1.382258	-0.572896
		518.92 551.75 577.71 609.72 676.41	C	-0.677620	0.114607	-0.248275
	ZPE (hartree): 0.1899510	685.77 740.39 753.49 782.1 788.75	C	-1.567332	-0.947460	0.155704
		823.25 836.44 869.6 875.97 924.05	C	-2.959717	-0.688897	0.210097
	$\langle S^2 \rangle$: 2.02	953.43 960.35 966.58 989.22 990.33	H	-3.001845	2.562653	-0.759813
		1007.2 1041.9 1077.8 1150.4 1163.1	H	-0.580175	2.193773	-0.858206
	Rotational constants (GHz):	1174.7 1187.7 1198.2 1239.5 1266.2	H	-4.533222	0.728236	-0.069088
	0.9214	1287.7 1314.4 1343.3 1380.5 1394.1	H	-3.625182	-1.489991	0.515065
	0.5682	1437.5 1463.6 1470.1 1481.8 1530.5	C	0.702937	-0.168038	-0.303027
	0.3853	1579.7 1590.4 1646.4 2023.7 2956.5	C	1.202999	-1.450762	0.026284
		2974.4 3156.8 3159 3162.2 3170.4	C	0.317005	-2.478899	0.426479
		3180.6 3185.4 3196.6 3207.7	C	-1.033961	-2.220016	0.488230
			H	0.701108	-3.463457	0.668983
			H	-1.721899	-3.002507	0.791257
			C	2.099088	2.024140	0.940741
			C	1.831381	0.694329	-0.667105
			C	3.097218	-0.152606	-0.671319
			C	2.610599	-1.480490	-0.159930
			H	1.712380	1.498963	-1.385231
			H	3.534287	-0.232926	-1.678785
			H	3.241692	-2.346241	-0.010060
			O	1.304319	2.834358	1.103560
			H	3.880289	0.289008	-0.038235
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	110.85 125.78 193.9 238.18 244.12	C	-3.334790	-0.202582	0.000152
(triplet)		304.47 417.72 430.29 457.01 477.95	C	-2.705405	-1.476097	-0.000113
10	Energy (hartree): -501.4438129	519.96 527.96 546.73 602.27 610.47	C	-1.337744	-1.574329	-0.000275
		677.35 687.89 746.05 746.78 782.95	C	-0.518489	-0.412591	-0.000073
	ZPE (hartree): 0.1823430	793.18 811.62 864.88 877.86 921.34	C	-1.157104	0.885059	0.000059
		935.83 946.35 959.49 978.21 987.1	C	-2.579569	0.940504	0.000197
	$\langle S^2 \rangle$: 2.02	988.94 1032.9 1051.5 1119.5 1143.8	H	-3.314400	-2.373097	-0.000264
		1169 1178.1 1201.1 1240.7 1250 1281.6	H	-0.867727	-2.551079	-0.000607
	Rotational constants (GHz):	1299.3 1345 1373.5 1391.8 1449.3 1452	H	-4.417192	-0.140805	0.000282
	1.8126	1473.8 1490.8 1515.6 1561.8 1587.3	H	-3.059130	1.914005	0.000345
	0.6590	1646.7 2902 2918.4 3157.3 3162.5	C	0.899592	-0.457788	-0.000143
	0.4847	3166.3 3178.3 3179.4 3189.1 3206.9	C	1.660000	0.750134	-0.000259
		3210.6	C	1.024337	1.993335	-0.000105

			C	-0.370468	2.053583	0.000057
			H	1.608812	2.906873	-0.000200
			H	-0.868930	3.016836	0.000122
			C	1.794611	-1.559651	0.000217
			C	3.227519	-1.084527	0.000187
			C	3.055358	0.412301	-0.000040
			H	1.512337	-2.603426	0.000773
			H	3.794717	-1.448894	0.874680
			H	3.869529	1.124636	-0.000229
			H	3.794904	-1.449163	-0.874065
OH + phen. rad. (triplet) 11	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7442645 ZPE (hartree): 0.1912370 $<S^2>$: 2.05 Rotational constants (GHz): 1.1711 0.3097 0.2625	15.331* 33.452 71.425 114.55 138.64 186.3 219.19 256.81 306.1 347.17 410.34 450.69 487.74 500.22 514.97 515.13 537.64 580.03 627.6 628.81 647.38 697.52 737.03 758.24 766.23 769.74 818.59 865.91 872.88 919.93 953.79 953.81 970.24 991.12 1024.8 1043.7 1066.7 1134.3 1142 1164.5 1171.4 1191.7 1228.6 1233.9 1269.5 1311.1 1334.9 1345 1405.8 1412.9 1430 1452.4 1458.8 1474.5 1512.9 1558.7 1611.9 1633.1 2210.4 3005.7 3077.5 3152.3 3156.4 3158.7 3169.7 3173.8 3183 3185.9 3192.8	C	4.091637	-0.897813	-0.208227
			C	3.276232	-1.902432	0.353453
			C	1.944042	-1.663645	0.603673
			C	1.370856	-0.400144	0.299581
			C	2.203331	0.627218	-0.275103
			C	3.561366	0.340252	-0.514827
			H	3.704321	-2.870279	0.588553
			H	1.313374	-2.432488	1.034057
			H	5.138959	-1.100985	-0.399750
			H	4.190572	1.111581	-0.947436
			C	0.038558	-0.059001	0.514648
			C	-0.590165	1.154827	0.240363
			C	0.294495	2.154057	-0.339177
			C	1.608916	1.895983	-0.577369
			H	-0.127285	3.124841	-0.580237
			H	2.239082	2.665585	-1.010913
			C	-4.060416	-1.075429	-0.563189
			C	-4.015464	0.078543	0.055881
			C	-2.914891	0.445018	1.051420
			C	-1.939491	1.430351	0.485042
			H	-4.779734	0.801869	-0.200653
			H	-3.394697	0.860021	1.946324
			H	-2.319122	2.410833	0.213273
			O	-4.099012	-2.110113	-1.096291
			H	-2.387424	-0.456774	1.370107
	*Vibration replaced by unsymmetrical hindered rotor (hrd 4 4 1)	Multiwell hindered rotor parameters: Vhrd2 1 0.0 370.5 -41.19 -163.4 -108.8 Ihrd1 1 0.0 93.58 -11.83 16.98 -7.08				

OH + phen. rad. (triplet) 11-9_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7375177 ZPE (hartree): 0.1904390 $<S^2>$: 2.06 Rotational constants (GHz): 0.9529 0.4761 0.3236	-371.58 40.825 72.969 97.286 151.54 195.32 207.44 216.51 285.11 377.41 400.76 414.22 449.22 496.07 512.87 516.76 576.66 595.13 622.52 640.05 668.8 714.99 749.53 755.96 776.35 784.47 819.95 866.76 874.7 915.63 953.81 971.79 976.87 989.68 999.32 1037.9 1047.4 1112.3 1133.5 1162.1 1170.7 1184.1 1205.3 1227.3 1265.9 1300.1 1333.2 1347.5 1365.8 1400.5 1420.6 1442.8 1456.6 1474.5 1523 1559.5 1609.8 1633 2156.3 2979.8 3021.4 3149 3150 3154 3164.9 3170.1 3178.3 3180.1 3188.7	C	-3.558818	-1.144401	0.018332
			C	-2.509441	-2.079709	0.136147
			C	-1.198818	-1.659275	0.156496
			C	-0.876700	-0.278084	0.061760
			C	-1.951381	0.674995	-0.062882
			C	-3.279784	0.204763	-0.080772
			H	-2.739646	-3.136918	0.207566
			H	-0.390531	-2.377492	0.234614
			H	-4.586703	-1.488525	0.002393
			H	-4.088583	0.922831	-0.175192
			C	0.428966	0.226431	0.075358
			C	0.752531	1.583306	-0.022233
			C	-0.343857	2.516670	-0.149934
			C	-1.629945	2.068873	-0.166183
			H	-0.128033	3.577564	-0.230437
			H	-2.448577	2.775377	-0.259977
			C	2.863759	-1.635006	-0.024595
			C	2.485879	-0.477611	0.540049
			C	3.125414	0.842173	0.097880
			C	2.102278	1.937227	0.016287
			H	2.246074	-0.583048	1.594585
			H	3.930230	1.112934	0.791360
			H	2.432596	2.966362	-0.065763
			O	2.962722	-2.644128	-0.599372
			H	3.610908	0.701838	-0.878444
OH + phen. rad. (triplet) 12	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7366129 ZPE (hartree): 0.1920410 $<S^2>$: 2.01 Rotational constants (GHz): 1.0510 0.4183 0.3057	32.241 37.802 51.008 88.147 128.29 182.84 207.18 268.37 306.23 377.29 406.75 432.28 451.41 463.56 506.11 519.67 550.63 602.04 640.5 656.62 723.26 737.19 765.18 777.81 780.87 817.44 839.5 882.32 917.95 924.17 958.74 960.45 974.78 999.62 1004 1035.8 1045.4 1141.3 1162.4 1172.8 1179.9 1201.6 1236.9 1257.9 1265.2 1275.1 1351.9 1363.9 1396.6 1430.9 1445.6 1453.8 1494.1 1518.3 1579.6 1633.1 1652.6 1690.7 1911.5 3015.1	C	-3.788084	-0.910031	0.074230
			C	-2.833223	-1.953375	0.120535
			C	-1.489521	-1.671074	0.098674
			C	-1.045058	-0.324043	0.030318
			C	-2.011365	0.741268	-0.024735
			C	-3.387195	0.403029	0.002254
			H	-3.169087	-2.982728	0.172026
			H	-0.748613	-2.461104	0.127637
			H	-4.844522	-1.152713	0.093674
			H	-4.122452	1.200251	-0.036218
			C	0.292834	0.068335	0.002957
			C	0.793610	1.336297	-0.079363
			C	-0.201130	2.370137	-0.144663

		3069.7 3139.4 3153.4 3159.5 3164.9 3171.5 3175.4 3183.8 3194.6	C	-1.540447	2.080104	-0.112927
			H	0.131553	3.401025	-0.219061
			H	-2.267656	2.883529	-0.161360
			C	3.322216	-1.550190	-0.395643
			C	3.221631	-0.481345	0.715428
			C	3.271603	0.924228	0.191152
			C	2.215789	1.687587	-0.128731
			H	2.306538	-0.677007	1.284092
			H	4.260579	1.354451	0.069845
			H	2.419663	2.704748	-0.452738
			O	2.627153	-2.491008	-0.541921
			H	4.086802	-0.667963	1.360546
OH + phen. rad. (triplet) 12-13_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7356674 ZPE (hartree): 0.1917690 $\langle S^2 \rangle$: 2.02 Rotational constants (GHz): 1.1220 0.3989 0.3068	-100.73 31.556 40.594 85.133 115.2 181.64 195.82 263.9 279.34 380.57 399.05 427.63 439.82 486.97 504.09 518.78 553.96 600.34 641.14 657.64 718.85 735.64 762.68 773.43 780.13 800.95 833.28 879 916.41 939.13 958.27 959.22 971.72 996.52 1000.4 1029.3 1041.2 1141.4 1161.6 1172.7 1175.3 1199.9 1236.6 1255.3 1265.8 1276.8 1351.5 1363.3 1397.1 1433.8 1447.1 1465.7 1493.8 1517.8 1579.3 1630.5 1650.8 1683 1916.5 3024.6 3099.9 3137.4 3153.5 3159.5 3161.7 3171.4 3175.5 3183.8 3194.4	C	-3.851261	-0.855060	0.073261
			C	-2.930548	-1.923985	0.179627
			C	-1.578631	-1.682929	0.177317
			C	-1.088900	-0.354254	0.069636
			C	-2.021415	0.735920	-0.048416
			C	-3.407251	0.441135	-0.039517
			H	-3.298912	-2.940203	0.261127
			H	-0.866141	-2.495772	0.250850
			H	-4.914952	-1.064340	0.078285
			H	-4.115823	1.258648	-0.124686
			C	0.261432	-0.004345	0.057566
			C	0.802044	1.244381	-0.063187
			C	-0.160671	2.303308	-0.191520
			C	-1.508195	2.055485	-0.178583
			H	0.204997	3.320134	-0.297450
			H	-2.209048	2.877776	-0.274955
			C	3.487450	-1.639787	-0.207363
			C	3.217870	-0.566437	0.887903
			C	3.270981	0.816987	0.314011
			C	2.230631	1.566540	-0.085089
			H	2.229183	-0.792554	1.301440
			H	4.263751	1.245758	0.217484
			H	2.458289	2.567203	-0.443090
			O	2.741458	-2.013635	-1.038150
			H	3.975773	-0.689336	1.662318

OH + phen. rad. (triplet) 13	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7382593 ZPE (hartree): 0.1917650 $\langle S^2 \rangle$: 2.02 Rotational constants (GHz): 1.3348 0.3040 0.2545	22.213 30.16 69.977 101.91 125.24 176.08 188.97 224.97 253.13 378.81 389.84 423.84 438.5 501.7 518.42 524.95 589.98 617.32 643.96 678.11 725.54 735.45 763.86 775.97 779.27 815.16 833.93 870.72 876.9 921.17 957.49 958.75 970.07 998.14 1001.2 1038.1 1055 1142.2 1161.6 1172.7 1174.1 1198.4 1236.6 1252.3 1268 1287.4 1352.1 1362.9 1395.1 1422.2 1442.1 1450.1 1493.7 1517.9 1579.2 1631.7 1651.7 1688.5 1919.7 3003.3 3056.8 3137.3 3155 3160.2 3164 3170.9 3176.3 3183.1 3193.2	C 4.101758 -0.939407 0.184756 C 3.210466 -2.000067 -0.102291 C 1.867859 -1.759840 -0.260778 C 1.355614 -0.440446 -0.138850 C 2.259587 0.642293 0.151132 C 3.636931 0.348135 0.308000 H 3.594186 -3.009492 -0.196443 H 1.181177 -2.568815 -0.480298 H 5.158330 -1.148248 0.307734 H 4.321895 1.160440 0.528389 C 0.012551 -0.089856 -0.279788 C -0.545886 1.153409 -0.181134 C 0.390595 2.204706 0.104853 C 1.728657 1.955532 0.263834 H 0.011298 3.218128 0.193427 H 2.407868 2.773357 0.479263 C -4.112812 -1.437158 0.416116 C -3.001394 -0.828039 -0.444475 C -3.018121 0.669375 -0.473938 C -1.964117 1.488729 -0.345872 H -2.042526 -1.231691 -0.108462 H -4.001872 1.117740 -0.572367 H -2.168741 2.556133 -0.359035 O -5.102515 -0.926584 0.804992 H -3.171622 -1.259076 -1.441535
OH + phen. rad. (triplet) 13-14_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7269951 ZPE (hartree): 0.1866890 $\langle S^2 \rangle$: 2.01 Rotational constants (GHz): 1.0097 0.4044 0.2930	-1187.1 37.934 68.879 91.134 137.41 172.71 202.79 219.8 285.44 383.9 404.99 411.25 439.47 442.36 503.81 519.79 535.57 559.86 630.61 648.29 682.93 718.55 741.66 763.31 780.33 809.26 833.18 872.73 878.57 953.66 960.92 962.18 971.86 984.04 989.3 999.64 1037.1 1042.9 1145.1 1170.6 1174.9 1204.2 1214.1 1236.4 1253.2 1271.2 1302.8 1360 1366.7 1391.6 1414.2 1453.7 1482.3 1515.1 1526.8 1582.8 1621.6 1651.5 1681.6 1877.2 3015.1	C 3.685380 -1.253351 0.011980 C 2.623388 -2.175959 -0.140884 C 1.322012 -1.740926 -0.183658 C 1.023377 -0.356348 -0.077517 C 2.100840 0.586371 0.078585 C 3.429068 0.092294 0.119689 H 2.842811 -3.234348 -0.222605 H 0.506027 -2.445216 -0.297286 H 4.706611 -1.615291 0.045435 H 4.244376 0.798402 0.239043 C -0.265990 0.186097 -0.106395 C -0.587439 1.514979 -0.012826 C 0.499804 2.426223 0.145919

		3144.4 3157.7 3160.5 3170.6 3171.5 3176.9 3182.1 3192.6	C	1.793093	1.969704	0.187560
			H	0.289808	3.487825	0.228415
			H	2.610770	2.672778	0.305456
			C	-3.468239	-1.277041	0.535348
			C	-2.808901	-0.352175	-0.437236
			C	-3.010672	1.114417	-0.246720
			C	-1.984413	1.958730	-0.070421
			H	-1.590360	-0.487757	-0.238369
			H	-4.028658	1.493318	-0.256643
			H	-2.173209	3.021071	0.045212
			O	-3.822199	-2.393506	0.350084
			H	-2.938420	-0.700837	-1.469877
OH + phen. rad. (triplet) 14	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7983743 ZPE (hartree): 0.1929660 $<S^2>$: 2.04 Rotational constants (GHz): 1.2078 0.3042 0.2467	33.952 61.186 97.321 150.48 177.84 193.72 213.72 267.29 305.65 386.07 404.27 426.33 444.22 483.12 516.19 525.78 528.59 624.7 648.28 681.24 736.54 753.58 775.54 780.93 795.96 832.83 859.06 879.4 912.89 919.92 967.07 968.34 982.33 996.11 1000.6 1042.7 1066.6 1115.9 1157.1 1174.4 1180.6 1210.1 1226.5 1256.9 1280.5 1293.9 1305.5 1376.2 1392.6 1412.4 1453.8 1486.9 1490.5 1528.8 1541.2 1593.3 1633.6 1653.9 1836.3 3132.3 3136.6 3151.6 3161.5 3162.9 3167.4 3179.1 3180 3191.7 3198.2	C	4.021295	-1.140849	-0.157785
			C	3.064521	-2.124889	0.181737
			C	1.745428	-1.780323	0.348712
			C	1.318936	-0.435006	0.180056
			C	2.291549	0.559907	-0.156833
			C	3.641835	0.172164	-0.321115
			H	3.377859	-3.154625	0.309576
			H	1.009224	-2.533627	0.608104
			H	5.059126	-1.425953	-0.287103
			H	4.377126	0.927563	-0.577313
			C	-0.032545	-0.056130	0.339287
			C	-0.451116	1.264930	0.173497
			C	0.547890	2.249457	-0.126265
			C	1.859235	1.908640	-0.296443
			H	0.238284	3.283214	-0.235520
			H	2.593599	2.669893	-0.537643
			C	-4.589982	-0.847155	-0.108946
			C	-3.244933	-0.299338	-0.141183
			C	-3.013396	0.995317	0.281521
			C	-1.811962	1.711557	0.329084
			H	-0.742216	-0.815230	0.641354
			H	-3.903070	1.549071	0.572108
			H	-1.919432	2.779948	0.495769
			O	-4.963769	-1.927592	-0.448387
			H	-2.460878	-0.929209	-0.554176

OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-294.79 18.61 53.897 90.051 142.15	C	-3.845919	-1.090069	-0.015006
(triplet)		182.8 201.13 245.77 279.1 381.32 390.23	C	-2.850974	-2.079377	0.170780
14-15_TS	Energy (hartree): -614.7675257	426.55 441.91 481.66 502.56 527.69	C	-1.525070	-1.728143	0.226481
		561.07 602.05 632.94 652.59 688.23	C	-1.127203	-0.369787	0.099179
	ZPE (hartree): 0.1911440	716.65 761.3 780.97 784.06 803.12	C	-2.134339	0.628583	-0.090318
		833.08 872.59 907.05 922.36 964.99	C	-3.494724	0.231959	-0.142584
	<S^2>: 2.01	965.25 975.12 981.38 994.28 999.46	H	-3.142158	-3.119050	0.268205
		1041.7 1085.3 1145.1 1173.9 1175.2	H	-0.761176	-2.485702	0.366272
	Rotational constants (GHz):	1186.5 1230 1250.4 1273.4 1292.7	H	-4.889124	-1.382098	-0.057215
	1.0570	1297.9 1383.9 1398.2 1406.6 1440.1	H	-4.256052	0.991529	-0.286346
	0.3732	1469.6 1502.3 1540.7 1606.1 1640.3	C	0.231654	0.020140	0.152730
	0.2809	1658.1 1680.5 1779 3055.3 3079.9	C	0.618499	1.343868	0.023503
		3145.2 3158.2 3159.8 3164.7 3174	C	-0.400804	2.323760	-0.166871
		3176.8 3177.3 3189.5	C	-1.725867	1.980610	-0.221049
			H	-0.109685	3.363707	-0.270400
			H	-2.481634	2.745381	-0.366259
			C	3.578923	-1.248392	-0.562673
			C	3.344093	-0.290842	0.497953
			C	3.151026	1.142220	0.270648
			C	2.007250	1.817328	0.073000
			H	0.972590	-0.757880	0.293433
			H	4.072119	1.727853	0.285001
			H	2.111645	2.890386	-0.063761
			O	3.766948	-2.424150	-0.448277
			H	3.388612	-0.672080	1.522647
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	29.707 72.195 87.967 149.95 153.34	C	3.880848	0.979053	0.000041
(triplet)		186.16 214.75 282.93 303.92 399.04	C	2.918571	2.014719	0.000022
15	Energy (hartree): -614.7928575	400.46 432.54 467.05 491.67 517.33	C	1.578119	1.714172	0.000017
		535.97 541.8 632.01 647.39 679.99	C	1.137639	0.362301	0.000050
	ZPE (hartree): 0.1930990	740.58 766.43 776.33 787.89 794.96	C	2.115258	-0.683238	-0.000033
		828.26 867.75 886.44 925.92 934.85	C	3.486684	-0.340607	-0.000011
	<S^2>: 2.04	963.53 971.23 977.94 981.05 998.75	H	3.244422	3.048503	-0.000023
		1002.2 1042.6 1103.2 1154 1174.2	H	0.834688	2.503766	-0.000100
	Rotational constants (GHz):	1185.1 1219.2 1237.3 1277.8 1295.5	H	4.935750	1.229278	0.000154
	1.0784	1304.1 1374.4 1393 1412.9 1420.4 1457	H	4.226896	-1.133835	-0.000020
	0.3799	1487.9 1499.8 1528.9 1545.5 1590.6	C	-0.235171	0.034071	0.000189
	0.2810	1634.5 1652 1819.8 3089.8 3119.7	C	-0.675013	-1.291390	-0.000183
			C	0.326480	-2.323401	-0.000007

		3125.5 3147 3159.1 3161.7 3169.7 3177.1 3179.8 3191	C 1.659387 -2.032354 -0.000008 H 0.001821 -3.358571 -0.000018 H 2.392647 -2.831985 0.000029 C -3.039342 1.443868 0.000210 C -3.779339 0.202889 0.000279 C -3.303303 -1.099175 0.000175 C -2.044754 -1.725273 -0.000275 H -0.963592 0.838277 0.000464 H -4.110832 -1.827840 0.000278 H -2.130727 -2.808857 -0.000951 O -3.465568 2.560074 -0.000449 H -4.862923 0.326862 0.000982
OH + phen. rad. (triplet) 15-16_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7444708 ZPE (hartree): 0.1914450 $<S^2>$: 2.04 Rotational constants (GHz): 1.0179 0.5374 0.4153	-561.69 54.99 61.447 119.84 156.49 210.78 231.74 278.96 311.94 383.1 411.51 434.22 456.36 510.68 516.11 541.06 553.8 620.42 661.25 690.45 735.39 747.55 760.47 778.8 793.93 814.41 847.26 881.22 908.25 946.73 950.43 962.43 972.96 980.82 995.93 1019.8 1051 1082.9 1130.2 1148.9 1158.3 1179.1 1198.2 1228.8 1258.9 1282.9 1298.1 1332.4 1359.4 1373.2 1395.3 1453 1484.8 1532.1 1549.3 1590.3 1611.9 1643.9 1820.4 3054.7 3132.8 3151 3161.6 3164.4 3167 3178.8 3181.8 3185.6 3192	C 3.481404 -0.308610 0.105071 C 2.846393 -1.275001 -0.696071 C 1.511145 -1.133611 -1.021604 C 0.765806 -0.036418 -0.551776 C 1.410296 0.954665 0.247963 C 2.778735 0.786104 0.562892 H 3.405054 -2.131829 -1.054123 H 1.017720 -1.883766 -1.630284 H 4.528636 -0.425282 0.360044 H 3.271205 1.535212 1.173831 C -0.634469 0.129719 -0.878285 C -1.338111 1.275799 -0.375311 C -0.663731 2.252687 0.365643 C 0.677214 2.104893 0.668826 H -1.216750 3.101893 0.752446 H 1.187490 2.858040 1.258761 C -1.625250 -1.532069 1.117350 C -2.127412 -1.204773 -0.212497 C -3.180044 -0.171132 -0.382368 C -2.783220 1.113780 -0.441008 H -0.940630 -0.249776 -1.848187 H -4.224854 -0.463622 -0.431221 H -3.469658 1.952700 -0.461051 O -1.020354 -2.498881 1.468203 H -2.107914 -2.038728 -0.918784

OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	53.586 57.507 106.94 145.2 217.62	C	-3.436475	-0.706533	-0.147350
(triplet)		246.93 256.12 351.44 373.96 408 417.37	C	-2.578508	-1.721278	0.276008
16	Energy (hartree): -614.7763883	464.81 490.11 521.33 541.1 545.38	C	-1.236833	-1.434518	0.532820
		617.85 671.57 702.85 731.86 747.18	C	-0.732673	-0.149604	0.360793
	ZPE (hartree): 0.1932750	754.84 782.55 800.6 814.86 858.53	C	-1.596551	0.886965	-0.083224
		878.07 914.86 923.51 928.48 948.04	C	-2.949800	0.580752	-0.324133
	<S^2>: 2.04	955.01 956.08 987.62 1025.8 1061.1	H	-2.949863	-2.730560	0.410495
		1095.9 1120.8 1141.8 1183.6 1208	H	-0.582633	-2.229523	0.874399
	Rotational constants (GHz):	1219.1 1226.6 1228.8 1244.8 1288.1	H	-4.480678	-0.922610	-0.342857
	0.9803	1300.2 1306.5 1318.3 1345.7 1386.4	H	-3.612728	1.369310	-0.665087
	0.5741	1403.4 1464.8 1511.5 1533.1 1544.6	C	0.681872	0.226067	0.740265
	0.3891	1601.2 1631.6 1906.1 2912.5 3021.2	C	1.173439	1.513136	0.110036
		3157.1 3159.3 3165.4 3176.4 3179	C	0.277343	2.493190	-0.294820
		3189.4 3190.8 3217.4	C	-1.081119	2.213607	-0.332204
			H	0.641698	3.454748	-0.642371
			H	-1.780491	2.976600	-0.655294
			C	1.717790	-1.606403	-0.758313
			C	1.858900	-0.766627	0.517803
			C	3.029771	0.175692	0.270949
			C	2.592027	1.434789	0.002973
			H	0.671820	0.414883	1.828637
			H	4.053633	-0.170192	0.230502
			H	3.228980	2.263085	-0.283141
			O	2.059610	-2.726111	-0.917822
			H	2.018286	-1.452250	1.357675
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-411.43 31.69 46.835 101 127.45 187.08	C	-3.427767	0.713594	0.134111
(triplet)		239.07 247.65 254.03 298.02 406.34	C	-2.582442	1.690709	-0.396086
16-17_TS	Energy (hartree): -614.7587665	417.98 439.96 464.79 519.01 532.19	C	-1.249376	1.379076	-0.674511
		559.39 613.37 667.51 706.24 724.38	C	-0.741685	0.111095	-0.424295
	ZPE (hartree): 0.1900050	741.67 767.77 788.12 798.57 822.5 861.3	C	-1.590473	-0.888672	0.131888
		880.58 890.12 907.58 924.03 944.4	C	-2.938664	-0.556127	0.394852
	<S^2>: 2.03	949.37 980.87 982.23 1029.6 1057	H	-2.958154	2.687114	-0.597939
		1095.9 1112.9 1133.7 1179.6 1199.5	H	-0.604815	2.141422	-1.099186
	Rotational constants (GHz):	1209.6 1226.9 1229.6 1282.7 1298.1	H	-4.464383	0.949155	0.347231
	0.9335	1303.8 1333.9 1344.8 1379.3 1411.7	H	-3.589451	-1.311922	0.822365
	0.5596	1465.3 1510.1 1539.6 1583.8 1591.6	C	0.658166	-0.297934	-0.827712
	0.3895	1621.3 2003.7 2837.3 3157 3158.3 3162	C	1.174461	-1.535506	-0.118334
			C	0.315327	-2.455872	0.416724

		3166.4 3175.2 3179.7 3189.6 3194.6	C	-1.068392	-2.180457	0.466830
		3215.2	H	0.694779	-3.368688	0.865067
			H	-1.747771	-2.918346	0.878001
			C	1.624126	1.747752	1.047856
			C	1.836217	0.659075	-0.704333
			C	3.002879	-0.176843	-0.424653
			C	2.618317	-1.431022	-0.067835
			H	0.601479	-0.568528	-1.903233
			H	4.020842	0.189817	-0.438359
			H	3.278744	-2.225901	0.254516
			O	2.133981	2.777789	1.061269
			H	1.912711	1.530363	-1.345630
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	84.961 111.99 214.94 237.34 267.68	C	-3.290570	-0.148361	-0.221157
(triplet)		397.77 414.04 427.17 450.24 511.6	C	-2.704475	-1.416834	-0.135574
17	Energy (hartree): -501.4270572	519.22 535.88 604.27 615.51 667.11	C	-1.327660	-1.533645	0.068373
		700.16 707.71 732.88 735.86 776.08	C	-0.520231	-0.409498	0.180448
	ZPE (hartree): 0.1826870	807.24 826.47 861.85 870.46 885.83	C	-1.103853	0.892436	0.070747
		902.53 935.06 944.43 977.91 998.68	C	-2.506064	0.985388	-0.120404
	$<S^2>$: 2.04	1047.6 1056.7 1084.2 1095.3 1128.2	H	-3.316809	-2.307347	-0.217990
		1172.7 1183.4 1188.5 1221.2 1228.7	H	-0.886619	-2.520965	0.152522
	Rotational constants (GHz):	1264.9 1290.7 1297.8 1334.4 1350.1	H	-4.360196	-0.054858	-0.372785
	1.7804	1383.5 1426.4 1457.7 1471.1 1503.4	H	-2.956261	1.968993	-0.206542
	0.6743	1574.4 1610.5 1632.2 2817.5 3155.5	C	0.946891	-0.485764	0.553000
	0.5002	3157 3163.5 3174.1 3179.2 3188.4 3192	C	1.743216	0.735377	0.120365
		3212.7 3224.3	C	1.144546	1.947690	-0.007365
			C	-0.280702	2.051262	0.095429
			H	1.721114	2.827042	-0.276708
			H	-0.751676	3.025994	0.040037
			C	1.809768	-1.618032	0.044290
			C	3.056885	-1.107682	-0.335533
			C	3.072756	0.277827	-0.256122
			H	0.980765	-0.504526	1.663969
			H	3.891519	-1.714511	-0.663581
			H	3.895037	0.923164	-0.533519
			H	1.540077	-2.663970	0.075617
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	60.086 84.022 124.46 169.8 184.19	C	3.513305	-0.191742	-0.217251
(triplet)		188.63 259.84 301.4 352.95 414.84	C	2.868698	-1.371438	-0.440785
18	Energy (hartree): -614.7320620	452.86 479.68 494.46 496.46 531.89	C	1.376767	-1.488299	-0.363337

	ZPE (hartree): 0.1903560 <S^2>: 2.08 Rotational constants (GHz): 1.1044 0.5630 0.4166	553.79 597.49 628.57 666.8 675.67 691.9 717.24 745.74 769.11 784.86 812.84 831.77 905.8 914.31 920.72 932.54 939.84 960.51 968.79 978.61 1013.4 1029.6 1084.5 1106.1 1114.6 1182.4 1190.1 1207.7 1215.3 1230.7 1245.7 1290.1 1316.2 1353.3 1389 1395.2 1418.1 1439.9 1450.5 1502.5 1547.7 1561.6 1584.6 1880.9 2921.4 2932.8 3092 3156.1 3161.9 3174 3181.2 3186 3194.9 3214	C C C H H H H C C C C H H C C C C H H H O H	0.666279 1.380262 2.803443 3.429416 0.991708 4.596819 3.339978 -0.790930 -1.454419 -0.700551 0.681437 -1.195832 1.266707 -1.465668 -1.936664 -3.096728 -2.819650 -1.752430 -4.056923 -3.532383 -1.293877 1.110468	-0.183030 1.003810 0.992337 -2.272981 -1.954239 -0.156270 1.916378 -0.143845 1.176034 2.310415 2.227903 3.270022 3.118662 -1.358002 -1.131338 -0.199556 1.053890 -1.880464 -0.549916 1.867852 -2.166239 -2.211972	-0.115634 0.124718 0.076205 -0.661574 -1.286470 -0.264899 0.256608 -0.011480 0.037082 0.317685 0.391372 0.423588 0.588787 0.647870 -0.706630 -0.805343 -0.365366 -1.476491 -1.160357 -0.333338 1.509011 0.427424
OH + phen. rad. (triplet) 18-19_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7313571 ZPE (hartree): 0.1900000 <S^2>: 2.08 Rotational constants (GHz): 1.0928 0.5712 0.4166	-362.25 84.886 88.695 133.91 177.34 188.06 223.7 306.75 359.28 402.7 428.77 457.25 478.76 485.19 505.11 566.61 586.85 611.13 644.19 674.06 702.89 710.23 751.14 779.29 792.76 815.82 821.84 902.53 924.46 927.64 934.46 945.84 969.2 976.36 979.02 1021.2 1050.6 1089 1110.3 1124.4 1182.1 1194.7 1213.4 1220.7 1232.5 1249.1 1303 1321.7 1367 1390.7 1401.5 1422.3 1445.4 1460.1 1505.5 1558 1566.4 1584.7 1866.4 2917.1 2945.9 3045.6 3156.2 3162.9 3174 3180.5 3185.6 3196.7 3218.2	C C C C C C H H H H C C C C H H	3.498148 2.847789 1.354773 0.645672 1.369126 2.793005 3.404715 0.977871 4.582499 3.334396 -0.794637 -1.450840 -0.701268 0.678260 -1.193357 1.268431	-0.194869 -1.364523 -1.472551 -0.165128 1.014707 0.988501 -2.266041 -1.936003 -0.166915 1.904979 -0.102040 1.202200 2.336000 2.240890 3.295196 3.124512	-0.191690 -0.450237 -0.392006 -0.144288 0.133125 0.112828 -0.680390 -1.318449 -0.221788 0.316206 -0.071765 0.002840 0.301813 0.391891 0.423108 0.606789

			C	-1.482595	-1.396308	0.671485
			C	-1.891115	-1.106069	-0.684749
			C	-3.099361	-0.219375	-0.732046
			C	-2.831448	1.051461	-0.342032
			H	-1.700413	-1.816580	-1.493387
			H	-4.068221	-0.614250	-1.006331
			H	-3.562951	1.847267	-0.283354
			O	-1.216711	-2.256659	1.453862
			H	1.077657	-2.196283	0.395685
OH + phen. rad. (triplet) 19	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7770556 ZPE (hartree): 0.1920900 $<S^2>$: 2.04 Rotational constants (GHz): 0.9652 0.5543 0.3641	30.981 66.476 81.421 148.39 171.76 209.11 251.52 320.28 354.74 376.66 427.64 472.55 487.73 497.53 517.2 528.46 613.71 623.56 654.12 671.04 725.4 745.76 757.63 789.51 832.81 842.16 874.82 892.22 932.64 939.52 952.2 962.03 968.08 969.1 989.88 1041.4 1098.2 1116.1 1168.1 1172.2 1180.1 1207.3 1213.1 1224.3 1250.9 1253.5 1307 1337.6 1385.5 1398.1 1429.1 1442.4 1459.3 1496.8 1563.6 1575.1 1612.6 1625 1897.4 2944 2957.6 3003 3156.2 3161.5 3174.3 3179.9 3184.5 3197.1 3226.5	C	-3.447919	-0.899755	0.005219
			C	-2.534988	-1.891275	0.230840
			C	-1.064373	-1.617230	0.307877
			C	-0.683777	-0.162835	0.126654
			C	-1.684916	0.827852	-0.105867
			C	-3.058582	0.442129	-0.164453
			H	-2.859246	-2.918118	0.357904
			H	-0.671998	-1.982524	1.271452
			H	-4.502875	-1.149098	-0.044885
			H	-3.807379	1.205290	-0.341922
			C	0.634596	0.252672	0.184734
			C	1.003234	1.605677	0.021342
			C	0.026053	2.577379	-0.209846
			C	-1.298897	2.180337	-0.271055
			H	0.296153	3.619719	-0.337954
			H	-2.075018	2.917587	-0.447732
			C	2.173472	-1.592347	-0.689826
			C	1.888182	-0.559879	0.425590
			C	2.980645	0.492482	0.391629
			C	2.450924	1.706706	0.150658
			H	1.869914	-1.112774	1.374601
			H	4.025372	0.253849	0.531834
			H	3.008233	2.632076	0.077223
			O	2.619399	-2.675784	-0.552474
			H	-0.540271	-2.231213	-0.441715
OH + phen. rad. (triplet) 19-21_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7687497	-462.34 42.824 72.382 79.762 127.52 152.44 197.3 237.51 271.8 315.74 346.01 427.44 474.9 486.42 495.03 503.83 589.34 609.94 625.51 655.91 666.78	C	-3.477525	-0.986551	-0.034806
			C	-2.558417	-1.946849	0.289960
			C	-1.098064	-1.639399	0.427122
			C	-0.736857	-0.189963	0.184608

	ZPE (hartree): 0.1896950 <S^2>: 2.04 Rotational constants (GHz): 0.9814 0.5139 0.3572	725.41 746.16 760.8 797.43 834.03 840.34 868.84 927.46 932.54 937.05 946.59 955.28 966.18 982.68 997.75 1047.8 1098.7 1114.9 1170.8 1177.8 1203.5 1216.5 1233.9 1247.1 1273.3 1315.2 1338.2 1382.6 1397.1 1429.5 1444.9 1454.4 1496.1 1548.5 1561.5 1603.3 1618.8 1983.7 2938.2 2949.3 3144.2 3154.6 3160.5 3172.9 3178.1 3184.5 3202.2 3226.7	C -1.739517 0.764413 -0.155218 C -3.105729 0.350243 -0.259263 H -2.872387 -2.971258 0.457369 H -0.750663 -1.942397 1.429084 H -4.523779 -1.261352 -0.122583 H -3.856888 1.087619 -0.517073 C 0.575235 0.251180 0.280398 C 0.928874 1.604158 0.047912 C -0.049603 2.537105 -0.287524 C -1.367858 2.109589 -0.385571 H 0.205570 3.576308 -0.464008 H -2.145597 2.820718 -0.643757 C 2.296847 -1.614389 -0.890311 C 1.815862 -0.484194 0.585487 C 2.887228 0.530938 0.595589 C 2.370283 1.735776 0.250376 H 1.817904 -1.289687 1.314979 H 3.922473 0.310721 0.814033 H 2.923838 2.660424 0.152274 O 3.169443 -2.355691 -0.756508 H -0.520578 -2.277908 -0.260817
OH + phen. rad. (triplet) 20	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7311468 ZPE (hartree): 0.1902840 <S^2>: 2.03 Rotational constants (GHz): 1.1804 0.3129 0.2477	39.062 57.519 76.009 91.733 150.5 171.19 181.25 225.74 284.6 382.31 411.95 422.23 469.18 494.43 495.89 523.27 573.51 578.66 621.65 656.45 669.48 690.85 704.66 720.37 759.84 764.21 785.01 838.22 903.67 915.16 935.67 949.42 966.43 968.56 970.17 1068.6 1081.2 1137.7 1140.9 1170.9 1192.3 1200.8 1212.7 1240.2 1265.8 1283.7 1331.5 1345.6 1385.1 1426.2 1433.1 1447.9 1466.6 1489 1530.3 1567.3 1588.2 1656.1 2202.9 2966.6 2969.6 3120.9 3148.3 3152.2 3155 3170.6 3171.6 3173.7 3183.1	C -3.987286 -1.146325 -0.000496 C -3.058581 -2.148271 -0.000758 C -1.584716 -1.875775 0.000548 C -1.226576 -0.401457 0.000095 C -2.247799 0.604040 0.000408 C -3.618035 0.213717 0.000385 H -3.373189 -3.186081 -0.001601 H -1.118526 -2.362628 0.870541 H -5.042320 -1.400417 -0.001105 H -4.380779 0.983930 0.000697 C 0.060325 0.049853 -0.000360 C 0.525846 1.359415 -0.000327 C -0.515345 2.327422 0.000152 C -1.845195 1.960554 0.000482 H -0.243193 3.378756 0.000222 H -2.611889 2.728015 0.000763 C 4.196041 -1.135912 0.000289

			C	3.078642	-0.431450	0.000199
			C	3.031277	1.014862	-0.000348
			C	1.915296	1.780701	-0.000630
			H	2.159007	-1.011174	0.000614
			H	3.987862	1.526924	-0.000600
			H	2.064742	2.855738	-0.001033
			O	5.166419	-1.772175	0.000148
			H	-1.116428	-2.363913	-0.867516
OH + phen. rad. (triplet) 20-19_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7144440 ZPE (hartree): 0.1890860 $<S^2>$: 2.05 Rotational constants (GHz): 0.9625 0.4680 0.3256	-395.41 40.267 62.107 91.6 133.04 177.67 193.67 207.91 293.4 366.34 407.52 421.72 442.26 472.66 493.65 496.8 563.34 583.34 616.66 649.18 665.61 670.72 704.07 742.48 763.6 783.91 794.73 837.84 904.43 924.73 934.82 950.16 962.37 968.45 972.73 1003 1080.9 1098.9 1133.4 1173.3 1178.3 1197.6 1199.9 1221.4 1244.2 1287.2 1302 1328.5 1385.5 1401.2 1423.3 1431.4 1445.1 1479.1 1547.9 1564.4 1582.9 1644.1 2149.3 2952.2 2970.5 3099.8 3149.9 3153 3166.7 3168.8 3171.6 3180.4 3190	C	-3.579265	-1.049853	-0.035321
			C	-2.639828	-2.012680	0.206473
			C	-1.181523	-1.692720	0.328108
			C	-0.840692	-0.226390	0.137718
			C	-1.873807	0.735457	-0.109559
			C	-3.232470	0.306479	-0.190130
			H	-2.936912	-3.049496	0.321347
			H	-0.814387	-2.025906	1.312039
			H	-4.624045	-1.333815	-0.111418
			H	-4.003841	1.044858	-0.378109
			C	0.448625	0.239023	0.182734
			C	0.819625	1.571095	0.017482
			C	-0.200345	2.515580	-0.210101
			C	-1.516286	2.095987	-0.273064
			H	0.046405	3.565765	-0.334676
			H	-2.305244	2.818547	-0.453544
			C	2.926368	-1.587688	-0.154467
			C	2.497162	-0.526511	0.555613
			C	3.083391	0.828031	0.305444
			C	2.242987	1.852462	0.081708
			H	2.215680	-0.789564	1.575492
			H	4.158731	0.954266	0.330640
			H	2.612733	2.863142	-0.057006
			O	3.066751	-2.505305	-0.858635
			H	-0.606789	-2.294982	-0.391508
OH + phen. rad. (triplet) 21	Theory: B3LYP/6-311G(d,p) Energy (hartree): -501.4469783 ZPE (hartree): 0.1827130	80.459 137 177.99 232.41 233.92 328.23 425.05 458.68 479.42 486.81 499.14 541.08 596.28 617.99 657.01 659.88 713.22 731.33 737.18 760.95 806.35 837.71 838.01 873.57 902.84 915.63	C	3.307891	-0.069164	-0.000963
			C	2.800245	-1.342241	-0.001102
			C	1.326867	-1.617478	0.001255
			C	0.459737	-0.376618	0.000461
			C	1.047114	0.922409	0.000554

	$\langle S^2 \rangle$: 2.05 Rotational constants (GHz): 1.8046 0.6636 0.4866	942.07 947.22 963.82 976.31 1006 1052.3 1088.9 1110.1 1168.8 1174.9 1205 1208.7 1224.9 1232.3 1278.4 1326.8 1348.9 1385 1394.1 1427.4 1445.8 1457.2 1481.6 1493.7 1553 1603.2 1606.2 2938.6 2943 3152.9 3160.1 3170.9 3176.6 3184.5 3203.8 3212.2 3228.4	C	2.475745	1.060008	0.000351
			H	3.468912	-2.196210	-0.002531
			H	1.065864	-2.246600	-0.865765
			H	4.384114	0.071715	-0.002099
			H	2.904535	2.055191	0.000589
			C	-0.932480	-0.468613	0.000046
			C	-1.755871	0.700620	-0.000278
			C	-1.181326	1.960179	-0.000022
			C	0.214168	2.060513	0.000383
			H	-1.792118	2.856718	-0.000201
			H	0.679545	3.040593	0.000466
			C	-1.820667	-1.600411	0.000058
			C	-3.159610	-1.126216	-0.000273
			C	-3.148809	0.255100	-0.000682
			H	-1.524868	-2.640738	0.000703
			H	-4.040405	-1.752563	-0.000313
			H	-4.011911	0.906767	-0.001032
			H	1.068310	-2.243398	0.871452
OH + phen. rad. (triplet) 22	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7227593 ZPE (hartree): 0.1899800 $\langle S^2 \rangle$: 2.06 Rotational constants (GHz): 1.1919 0.3086 0.2455	33.856 57.689 88.632 100.87 130.27 171.9 224.69 230.91 251.24 381.17 386.62 425.9 460.49 470.63 497.18 526.05 584.61 591.55 622.72 660.02 686.73 692.91 701.1 722.89 747.41 754.7 781.41 827.33 887.51 898.55 924.85 936.23 950.24 967.94 991.84 1046 1069.8 1137.1 1141 1172.8 1184.9 1188.6 1237 1256.5 1263.2 1311.4 1333.6 1346.5 1363.1 1409.1 1430.9 1441.3 1472.7 1483.6 1522.2 1569.4 1656.3 1669.7 2204.8 2919.9 2931.1 3124 3146.2 3150.8 3154.8 3168.5 3170.2 3172.4 3173.8	C	-4.013832	-1.054710	-0.000065
			C	-3.036985	-2.194433	-0.000030
			C	-1.605896	-1.763565	-0.000088
			C	-1.226158	-0.419314	-0.000015
			C	-2.232654	0.626017	0.000084
			C	-3.627736	0.231235	0.000010
			H	-3.234921	-2.849931	0.866172
			H	-0.838745	-2.529428	-0.000278
			H	-5.069781	-1.305101	-0.000144
			H	-4.372292	1.022046	-0.000008
			C	0.097059	0.038189	-0.000027
			C	0.552959	1.338166	-0.000026
			C	-0.479479	2.320128	0.000144
			C	-1.823564	1.959423	0.000185
			H	-0.198966	3.368473	0.000309
			H	-2.580252	2.737367	0.000300
			C	4.223822	-1.154634	0.000478
			C	3.106453	-0.451005	-0.000063
			C	3.061300	0.996581	-0.000223
			C	1.949056	1.762619	-0.000233

			H H H O H	2.186310 4.019138 2.097337 5.195129 -3.234932	-1.029522 1.506625 2.837604 -1.789531 -2.850056	0.000072 -0.000463 -0.000466 -0.000016 -0.866131
OH + phen. rad. (triplet) 22-24_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7058198 ZPE (hartree): 0.1888420 $\langle S^2 \rangle$: 2.07 Rotational constants (GHz): 0.9687 0.4597 0.3214	-406.82 39.56 73.735 102.11 131.65 169.67 202.77 243.81 260.07 364.33 391.6 417.95 442.53 463.67 476.57 497.01 572.77 591.66 623.2 651.62 667.32 695.22 703.56 728.52 748.01 785.98 799.78 826.82 892.67 896.43 926.17 935.85 953.71 974.32 991.12 992.03 1053.1 1099.7 1132 1168.7 1176.4 1185.5 1212.3 1238.2 1259.9 1293.8 1311.1 1332.3 1361 1399 1407.6 1433.8 1442.1 1480.7 1533.7 1563.9 1648.2 1671.8 2148.8 2915.7 2928.9 3101.5 3142.2 3153 3165.7 3167.2 3169.4 3170.8 3190.3	C C C C C C H H H H C C C C H H C C C C H H H O H	-3.609110 -2.614571 -1.197125 -0.838696 -1.863570 -3.247728 -2.869145 -0.417023 -4.657035 -4.005473 0.487256 0.844206 -0.170119 -1.501043 0.082760 -2.282998 2.963530 2.514240 3.108828 2.272945 2.216919 4.183774 2.640130 3.118006 -2.730214	-0.961371 -2.061356 -1.589600 -0.246700 0.757002 0.323080 -2.599127 -2.328095 -1.240028 1.083301 0.225730 1.552183 2.509941 2.095936 3.558757 2.830867 -1.603334 -0.533492 0.819434 1.840753 -0.786548 0.944420 2.853026 -2.531415 -2.834473	-0.016523 0.215576 0.263848 0.113803 -0.106656 -0.162758 1.146179 0.411292 -0.065285 -0.330473 0.149094 0.000811 -0.211482 -0.261624 -0.328973 -0.424544 -0.128858 0.556618 0.312248 0.077315 1.574633 0.355672 -0.055701 -0.815866 -0.564353
OH + phen. rad. (triplet) 23	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7201553 ZPE (hartree): 0.1902950 $\langle S^2 \rangle$: 2.04	61.298 80.531 137.07 145.46 206.94 219.27 243.82 307.46 376.43 422.01 427.53 467.49 489.98 509.89 559.88 582.6 601.89 634.13 666.25 692.94 713.67 723.67 747.67 771.54 778.33 804.02 831.23 882.87 892.62 904.18 920.12 933.08 943.23 968.2 986.35 1000.1 1013.9 1062 1085 1126.4 1179.2	C C C C C C H H	3.519686 2.854362 1.359675 0.679616 1.378139 2.804759 3.185990 0.817610	-0.167285 -1.447598 -1.384871 -0.248151 0.969912 0.942312 -1.744283 -2.299296	-0.135051 -0.535523 -0.480065 -0.156309 0.157243 0.181052 -1.547572 -0.699520

	Rotational constants (GHz): 1.1127 0.5413 0.4235	1182.4 1202.7 1210.8 1235.8 1271.8 1283.5 1305.4 1332.9 1378.7 1404.8 1420.2 1435.8 1450.4 1462.9 1526.6 1608.3 1620.9 1907.5 2903.5 2929.2 3116.5 3148.3 3157 3160.8 3174.3 3179.6 3196.6 3222.6	H H C C C C H H C C C C H H H O H	4.603719 3.326353 -0.804937 -1.465534 -0.701716 0.649298 -1.207163 1.227114 -1.503720 -1.921855 -3.061458 -2.768697 -1.694612 -3.998718 -3.457435 -1.515162 3.212723	-0.144981 1.855859 -0.203349 1.127251 2.287602 2.196193 3.239225 3.076888 -1.249523 -1.202079 -0.300294 1.005015 -2.065928 -0.665071 1.834102 -1.845164 -2.276020	-0.112071 0.451494 -0.038086 -0.084949 0.275119 0.411787 0.397311 0.671287 0.791128 -0.627269 -0.933899 -0.584385 -1.248519 -1.329030 -0.686951 1.819839 0.100102
OH + phen. rad. (triplet) 23-24_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7157547 ZPE (hartree): 0.1892960 $\langle S^2 \rangle$: 2.03 Rotational constants (GHz): 1.0939 0.5618 0.4132	-577.67 75.255 92.178 140.85 149.4 219.03 237.04 255.46 342.94 400.34 417.72 428.66 448.39 481.91 496.44 543.11 583.27 619.95 660.33 692.77 708.9 718.36 729.62 773.97 789.65 799.72 819.81 881.16 901.05 916.4 928 941.86 966.69 976.72 977.95 1003.2 1039.4 1083.5 1110.4 1119.7 1180.4 1182.3 1193.9 1214.1 1239.1 1284.8 1292.3 1315.5 1381.7 1387.6 1400.5 1434.1 1443.6 1459.9 1489.5 1512.2 1593.1 1635.2 1896.7 2899.7 2920.7 3009.8 3148.3 3162.2 3167.1 3172.9 3181.7 3197.8 3223.6	C C C C C C H H H H C C C C H H C C C C H	3.498837 2.811444 1.319953 0.648573 1.372486 2.808664 3.160401 0.764531 4.583145 3.344766 -0.817785 -1.450226 -0.677285 0.681966 -1.168916 1.279072 -1.538541 -1.885644 -3.117059 -2.826737 -1.693160	-0.178171 -1.461367 -1.363340 -0.191292 1.008491 0.950432 -1.816982 -2.272432 -0.177536 1.862391 -0.096966 1.197524 2.352706 2.244255 3.310475 3.120402 -1.407867 -1.097886 -0.237828 1.054346 -1.796743	-0.105662 -0.457560 -0.444652 -0.166869 0.135713 0.164618 -1.444666 -0.647735 -0.075490 0.410476 -0.116600 -0.043837 0.277763 0.376505 0.405560 0.605922 0.660874 -0.702698 -0.695650 -0.348366 -1.523927

			H	-4.096165	-0.651069	-0.892557
			H	-3.557702	1.848927	-0.268957
			O	-1.340693	-2.225178	1.500309
			H	3.137695	-2.264234	0.227415
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	37.498 68.838 100.2 131 203.23 226.63	C	3.473889	0.588423	0.019856
(triplet)		241.98 297.31 345.89 408.27 437.46	C	2.589121	1.769142	0.285429
24	Energy (hartree): -614.7676352	443.83 478.23 493.55 505.26 529.33	C	1.134205	1.435162	0.335847
		617.1 631.26 668.76 705.14 717.61	C	0.646063	0.138984	0.140849
	ZPE (hartree): 0.1920620	732.46 743.25 795.34 829.59 838.01	C	1.566732	-0.947072	-0.110143
		866.77 898.89 902.9 925.43 940.99 961.2	C	2.986959	-0.648881	-0.160058
	$<S^2>$: 2.04	971.3 982.54 993.71 1019.2 1080 1124.5	H	2.896935	2.260521	1.225015
		1159.5 1176.4 1183.6 1188.1 1217.7	H	0.441854	2.249114	0.515132
	Rotational constants (GHz):	1243.1 1250.7 1281.7 1331.5 1356.8	H	4.543654	0.765342	-0.024476
	0.9557	1375.7 1393.5 1424.4 1439 1442 1487	H	3.664701	-1.475711	-0.350530
	0.5683	1565.5 1578.2 1623.4 1676 1895.5	C	-0.730896	-0.201137	0.185256
	0.3702	2921.4 2932.3 3001.8 3147.9 3159.8	C	-1.175248	-1.515134	0.010955
		3170.3 3182.5 3184.4 3197.1 3224.4	C	-0.267774	-2.554641	-0.233167
			C	1.091101	-2.247627	-0.292922
			H	-0.610799	-3.573513	-0.369949
			H	1.809613	-3.039099	-0.480720
			C	-2.076734	1.717249	-0.703020
			C	-1.933557	0.686799	0.436581
			C	-3.083077	-0.297379	0.414112
			C	-2.631570	-1.536351	0.158341
			H	-1.869561	1.244436	1.380957
			H	-4.111299	0.000203	0.564905
			H	-3.239490	-2.428882	0.081584
			O	-1.978711	2.890686	-0.623969
			H	2.768790	2.546868	-0.477674
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-471.73 44.624 66.044 98.328 119.15	C	3.505233	-0.863406	0.047322
(triplet)		164.05 215.48 237.58 264.17 295.83	C	2.558110	-1.960977	-0.340768
24-25_TS	Energy (hartree): -614.7581842	341.97 429.05 449.82 471.07 498.41	C	1.135838	-1.516342	-0.446493
		508.32 585.29 611.36 623.53 673.25	C	0.730313	-0.198306	-0.200340
	ZPE (hartree): 0.1892020	682.65 718.78 729.9 748.77 800.68	C	1.706345	0.799744	0.171816
		821.98 838.78 858.66 896.72 911.74	C	3.095600	0.393943	0.278349
	$<S^2>$: 2.06	923.2 926.05 937.5 971.59 991.09 1019.2	H	2.884632	-2.415593	-1.292814
		1021.2 1079.3 1110.6 1160.9 1179.1	H	0.396589	-2.261362	-0.718650
	Rotational constants (GHz):	1183.5 1226.7 1246.4 1257.5 1269.9	H	4.555586	-1.120426	0.138672

	0.9832 0.5060 0.3566	1344 1356.3 1390.7 1401.3 1420.4 1437.5 1443.2 1463.1 1509.1 1577.4 1586.2 1672.6 1990.2 2914.9 2927.3 3146.6 3152.5 3158.6 3169 3171 3181.5 3200.8 3226.4	H	3.818505	1.154639	0.558074
			C	-0.613392	0.235535	-0.298773
			C	-0.980882	1.567710	-0.057450
			C	-0.020520	2.522376	0.311950
			C	1.308239	2.117968	0.419905
			H	-0.301963	3.551396	0.503680
			H	2.066229	2.842248	0.700755
			C	-2.270162	-1.625963	0.903888
			C	-1.852987	-0.520935	-0.626066
			C	-2.920163	0.468765	-0.652020
			C	-2.416569	1.683011	-0.281837
			H	-1.841048	-1.344657	-1.333750
			H	-3.949628	0.245111	-0.892451
			H	-2.982321	2.601086	-0.188849
			O	-3.134497	-2.384597	0.846116
			H	2.639377	-2.794394	0.379507
OH + phen. rad. (triplet) 25	Theory: B3LYP/6-311G(d,p) Energy (hartree): -501.4375494 ZPE (hartree): 0.1822590 $<S^2>$: 2.06 Rotational constants (GHz): 1.7848 0.6620 0.4843	98.528 112.21 197.15 240.34 246.02 284.6 420.62 444.47 458.22 496.44 497.48 536.95 604.52 612.92 677.2 677.96 693.49 720.06 731.97 761.11 806.09 816.33 822.37 846.52 899.68 900.34 923.83 933.93 964.07 983 989.76 1027.3 1079.2 1114.5 1173.1 1179.6 1186.4 1210.1 1226.7 1254.6 1274.3 1351.3 1357.4 1375.5 1410.9 1420 1438.9 1450.2 1464 1504.8 1556 1574.4 1661.1 2913.6 2926.6 3145.6 3159 3168.3 3174.9 3179.6 3202.3 3213.2 3231.3	C	-3.282937	-0.025102	-0.000244
			C	-2.767299	-1.436064	0.000401
			C	-1.274969	-1.522790	0.000060
			C	-0.445320	-0.392894	0.000007
			C	-1.025291	0.936775	-0.000070
			C	-2.468833	1.044899	-0.000344
			H	-3.177099	-1.984062	0.867251
			H	-0.827747	-2.510159	0.000224
			H	-4.359604	0.111182	-0.000523
			H	-2.894957	2.043988	-0.000729
			C	0.964817	-0.474693	0.000012
			C	1.773204	0.694530	0.000121
			C	1.185383	1.974748	0.000184
			C	-0.202564	2.070944	0.000051
			H	1.800688	2.867314	0.000390
			H	-0.672316	3.049186	0.000065
			C	1.869640	-1.637533	-0.000131
			C	3.158247	-1.171746	-0.000295
			C	3.131068	0.263573	0.000188
			H	1.564444	-2.674068	-0.000765
			H	4.054231	-1.775948	-0.000415
			H	3.999151	0.909907	0.000274

			H	-3.177668	-1.985213	-0.865414
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-1870.9 53.585 95.543 148.88 212.89	C	-3.643727	-0.379426	0.015789
(triplet)		241.57 260.58 344.41 366.55 397.83	C	-2.859028	-1.554014	0.050157
2-4_TS	Energy (hartree): -614.7528586	418.06 441.45 484.88 499.27 526.04	C	-1.486516	-1.491610	0.044336
		535.52 536.41 554.38 609.84 662.19	C	-0.803286	-0.241217	0.010437
	ZPE (hartree): 0.1865760	674.8 703.61 716.84 757.58 777.77 803.1	C	-1.612750	0.951170	-0.017424
		810.72 835.34 846.39 853.74 889.42	C	-3.027036	0.844709	-0.016481
	<S2>: 2.02	963.94 970.13 983.24 987.74 1015.6	H	-3.346405	-2.522076	0.079353
		1027.7 1057.4 1106.9 1133.8 1166.3	H	-0.905576	-2.398791	0.062503
	Rotational constants (GHz):	1184.9 1187.6 1226.8 1240.4 1256.6	H	-4.725556	-0.449329	0.014978
	1.1820	1302.6 1355.4 1364.1 1390.9 1396.3	H	-3.612515	1.757649	-0.041043
	0.5277	1430.1 1453.1 1484.6 1513.3 1534	C	0.628418	-0.108813	0.013337
	0.3655	1566.9 1583.8 1615.4 1649.3 3161	C	1.200233	1.188171	0.000055
		3163.3 3171.2 3173.1 3180.4 3186.3	C	0.369016	2.337782	-0.033911
		3188 3210.4 3255.7	C	-0.994675	2.223903	-0.042635
			H	0.837412	3.315541	-0.062699
			H	-1.620502	3.109317	-0.069376
			C	1.558578	-1.248808	0.046651
			C	3.003929	-0.991571	0.067610
			C	3.504271	0.282561	0.039644
			C	2.622010	1.369320	0.007164
			H	3.641615	-1.862718	0.139908
			H	4.574532	0.454827	0.052688
			H	3.008174	2.382215	-0.000181
			O	1.184856	-2.459270	-0.041998
			H	1.913366	-3.205410	-0.948524
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-738.81 65.528 100.65 166.38 215.61	C	3.620619	-0.281443	-0.067476
(triplet)		243.94 255.82 300.14 351.84 378.43	C	2.884402	-1.476369	-0.039604
3-4_TS	Energy (hartree): -614.7662894	399.85 441.07 463.21 491.89 529.18	C	1.496774	-1.463889	0.054548
		533.4 545.13 552.24 567.65 647.86	C	0.775760	-0.224130	0.000077
	ZPE (hartree): 0.1865960	678.47 700.79 716.83 765.65 770.47	C	1.542884	0.982614	-0.011745
		811.06 830.24 846.37 849.26 893.16	C	2.960484	0.925033	-0.037393
	<S2>: 2.04	903.45 976.14 982.1 987.71 990.68	H	3.401113	-2.429028	-0.056654
		1031.9 1047.9 1064.3 1102.2 1147.6	H	0.937030	-2.381066	-0.033543
	Rotational constants (GHz):	1167.6 1175.4 1186.4 1222.5 1230.8	H	4.703326	-0.311827	-0.112248
	1.1913	1247.6 1295.3 1344.9 1366.5 1392.7	H	3.515359	1.856968	-0.047853
	0.5290	1404.5 1445.5 1460.3 1491.5 1528.7	C	-0.659606	-0.139202	-0.008896
	0.3686	1539 1557.6 1573.5 1630.9 1636.1	C	-1.273994	1.136536	0.007688

		3161.3 3164.2 3167.8 3176.2 3179.8	C	-0.475991	2.318876	0.011983
		3183.2 3189.8 3199 3241.4	C	0.882951	2.243197	-0.005245
			H	-0.974812	3.281759	0.024558
			H	1.485151	3.145455	-0.010513
			C	-1.546530	-1.328627	-0.050288
			C	-2.982462	-1.102484	-0.012864
			C	-3.533395	0.159744	0.019926
			C	-2.693389	1.269859	0.023564
			H	-3.591878	-1.998022	-0.028965
			H	-4.609319	0.291876	0.038317
			H	-3.113366	2.269532	0.041930
			O	-1.135415	-2.500434	-0.132033
			H	1.339684	-1.840473	1.935594
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-684.34 59.076 93.494 160.23 205.62	C	3.609759	-0.237891	-0.070788
(triplet)		243.57 266.91 310.53 346.81 366.92	C	2.878787	-1.454360	-0.018865
5-4_TS	Energy (hartree): -614.7671123	399.27 423.32 466.33 491.76 513.74	C	1.487643	-1.440378	-0.052583
		531.37 550.66 558.57 568.18 640.56	C	0.762854	-0.221448	-0.026487
	ZPE (hartree): 0.1864370	677.45 705.06 716.11 762.75 790.52	C	1.520420	1.000833	-0.020782
		810.61 825.02 844.94 848.91 893.18	C	2.936905	0.954855	-0.057107
	<S2>: 2.07	909.64 971.18 982.85 986.76 988.29	H	3.397655	-2.394703	-0.160202
		1024.9 1032.4 1055.7 1101.2 1145.7	H	0.939285	-2.367851	-0.071650
	Rotational constants (GHz):	1166.4 1177.8 1183.5 1224.2 1233.7	H	4.692825	-0.260530	-0.099249
	1.1898	1250.2 1302.1 1339.4 1374.7 1382.5	H	3.482000	1.892623	-0.079341
	0.5241	1405.8 1445.4 1457.3 1486.5 1526.6	C	-0.676862	-0.147415	-0.013997
	0.3658	1545 1562.7 1569.1 1622.3 1635.4	C	-1.302332	1.126580	0.016265
		3160.7 3163.8 3167.3 3177.5 3179.5	C	-0.511531	2.316418	0.026747
		3182.7 3191.4 3199.7 3253.3	C	0.847881	2.252771	0.006378
			H	-1.019004	3.274498	0.049473
			H	1.441371	3.160853	0.011238
			C	-1.557353	-1.345357	-0.028992
			C	-2.996713	-1.130249	-0.003854
			C	-3.551879	0.125458	0.028253
			C	-2.716906	1.245391	0.037353
			H	-3.599117	-2.030442	-0.013868
			H	-4.628471	0.253007	0.045557
			H	-3.147240	2.240544	0.061291
			O	-1.136505	-2.514646	-0.064116
			H	3.148680	-1.922094	1.840438

OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-1205.1 56.915 93.004 155.11 211.52	C	3.646329	-0.386586	0.020533
(triplet)		246.02 258.51 344.25 358.61 396.37	C	2.876850	-1.560616	0.021755
6-4_TS	Energy (hartree): -614.7563972	407.85 421.05 460.71 495.87 524.91	C	1.498686	-1.501267	0.012823
		530.91 547.05 550.05 565.03 647.46	C	0.814355	-0.254313	-0.005383
	ZPE (hartree): 0.1867300	676.46 717.52 753.88 756.82 785.68	C	1.613173	0.939169	0.004011
		804.2 815.15 841.03 845.73 892.31	C	3.016213	0.842825	0.013806
	<S2>: 2.02	914.01 975.95 984.3 987.58 1016.8	H	3.367709	-2.527034	0.034481
		1033.6 1047.1 1059.4 1076.7 1145.7	H	0.912926	-2.406177	0.015989
	Rotational constants (GHz):	1156.6 1175.5 1186.2 1224 1237.4	H	4.728955	-0.444063	0.030225
	1.1868	1253.2 1302.6 1345.8 1362.8 1398.2	H	3.600165	1.757012	0.017863
	0.5275	1401.7 1445.1 1453 1468.9 1514.4	C	-0.621996	-0.135776	-0.027322
	0.3672	1557.1 1563.4 1584.9 1635.2 1646.4	C	-1.208100	1.181066	-0.012636
		3161.3 3163.6 3167.7 3174.4 3178.3	C	-0.364166	2.343877	0.001566
		3182 3188.5 3188.8 3247	C	0.983137	2.228199	0.006118
			H	-0.837844	3.319378	0.008072
			H	1.614695	3.109942	0.014515
			C	-1.527361	-1.298130	-0.052521
			C	-2.971752	-1.045033	0.056665
			C	-3.472801	0.232818	-0.061946
			C	-2.591369	1.344195	-0.037276
			H	-3.599548	-1.911457	-0.115836
			H	-4.541875	0.400833	-0.128232
			H	-2.999303	2.348608	-0.058856
			O	-1.147773	-2.477603	-0.155384
			H	-3.210878	-1.408787	1.783698
OH + phen. rad.	Theory: B3LYP/6-311G(d,p)	-597.8 59.731 95.901 158.37 217.59	C	3.669081	-0.329530	0.049402
(triplet)		233.63 246.62 325.72 360.11 394.46	C	2.915552	-1.519627	0.049807
7-4_TS	Energy (hartree): -614.7678718	406.97 415.79 492.71 499.27 513.81	C	1.539570	-1.489611	0.023156
		530.04 545.52 552.85 566.78 641.24	C	0.830703	-0.255468	-0.003926
	ZPE (hartree): 0.1866600	678.38 710.92 718.06 760.48 785.16	C	1.608661	0.951619	-0.003109
		809.77 820.34 846.98 850.21 876.36	C	3.020549	0.882406	0.023075
	<S2>: 2.05	896.71 975.34 987.49 988.24 1009.2	H	3.425078	-2.476483	0.071316
		1021.2 1036.4 1062.8 1084.7 1149.3	H	0.974891	-2.407375	0.020771
	Rotational constants (GHz):	1166.3 1174.8 1188.7 1224.9 1235	H	4.752212	-0.371156	0.069942
	1.1990	1251.4 1302.9 1346 1373.5 1386.5	H	3.584487	1.809189	0.022784
	0.5212	1405.8 1450.6 1461.8 1489.7 1520.1	C	-0.606243	-0.155855	-0.028137
	0.3654	1541.9 1548.7 1577.2 1636.5 1648.9	C	-1.211600	1.127100	-0.041692
			C	-0.400253	2.304304	-0.048065

		3160.2 3162.6 3172.4 3173.1 3180.3	C	0.955950	2.217450	-0.029432
		3186.4 3187.6 3201.8 3253.6	H	-0.891728	3.270790	-0.064464
			H	1.565281	3.115042	-0.031847
			C	-1.506009	-1.339228	-0.055061
			C	-2.939554	-1.104008	-0.059969
			C	-3.487956	0.172113	0.006626
			C	-2.622585	1.277910	-0.051104
			H	-3.557179	-1.993203	-0.088334
			H	-4.554872	0.315214	-0.114353
			H	-3.033475	2.280876	-0.070620
			O	-1.107494	-2.516628	-0.086550
			H	-3.999940	0.152664	1.887783

Larger Ring Structures, from Section 5.3

4 ring, radical	Theory: B3LYP/6-311G(d,p)	53.311 82.753 147.83 172.01 174.09	C-2.374755		-0.952442	0.000001
		237.78 285.51 293.59 384.31 398.32	C	-1.477127	-2.062758	-0.000251
	Energy (hartree): -692.6531683	441.78 482.61 488.91 489.84 515.74	C	-0.129629	-1.877251	-0.000328
		537.03 558.48 572.51 580.88 591.31	C	0.434283	-0.566372	-0.000151
	ZPE (hartree): 0.2272140	671.35 688.85 693.93 739.11 750.87	C	-0.411291	0.563381	-0.000077
		763.82 778.24 801.97 828.91 841.21	C	-1.849373	0.374034	-0.000019
	<S2>: 0.758	857.15 878.42 886.61 888.79 900.35	H	-1.892887	-3.064864	-0.000446
		950.86 964.3 973.89 981.88 994.42	H	0.544719	-2.726047	-0.000597
	Rotational constants (GHz):	1030.3 1055.4 1062.1 1089.4 1158.2	C	1.865508	-0.390865	-0.000047
	1.2819	1169.2 1181.8 1188.7 1192.6 1217.1	C	2.432505	0.922664	-0.000108
	0.2646	1246.6 1251.5 1282.2 1310.1 1343.7	C	1.540688	2.035648	-0.000119
	0.2193	1373.1 1384.1 1392.6 1418.6 1447.4	C	0.188556	1.862416	-0.000102
		1460.4 1468.1 1508.8 1516.7 1555.1	H	1.960356	3.036314	-0.000160
		1587.8 1629.2 1645 1651.3 1659 3159.1	H	-0.443527	2.740311	-0.000135
		3160 3162.7 3163.4 3169.6 3170.5	C	2.790370	-1.435065	0.000158
		3181.3 3182.6 3185.2 3193 3208.3	C	4.144214	-1.328489	0.000273
			C	4.682069	-0.015303	0.000200
			C	3.840466	1.075320	-0.000008
			H	4.796275	-2.194974	0.000517
			H	5.758189	0.120677	0.000269
			H	4.252454	2.078696	-0.000126
			C	-3.775318	-1.150568	0.000197
			C	-4.643516	-0.083147	0.000224
			C	-4.132396	1.227950	0.000102

			C	-2.771711	1.448139	0.000023
			H	-4.813101	2.071847	0.000008
			H	-2.413725	2.469115	0.000091
			H	-4.155033	-2.166971	0.000320
			H	-5.714966	-0.247850	0.000451
4 ring, singlet	Theory: B3LYP/6-311G(d,p)	53.633 71.518 118.35 170.52 187.34	C	-2.510623	0.916211	-0.138141
		226.31 246.23 274.01 314.75 339.4	C	-1.559989	1.951101	-0.358596
	Energy (hartree): -768.5757850	393.71 429.91 437.71 468.62 488.65	C	-0.219893	1.703311	-0.329024
		503.29 519.3 536.15 543.36 565.18	C	0.305216	0.389642	-0.085799
	ZPE (hartree): 0.2449080	567.37 579.62 629.33 636.29 692.77	C	-0.616918	-0.683983	-0.000195
		694.82 747.66 766.54 768.92 773.57	C	-2.042577	-0.419312	0.029514
	<S2>: 0	816.48 821.61 837.21 850.2 876.07	H	-1.919270	2.952699	-0.570161
		883.57 889.67 895.86 956.32 968.65	H	0.454144	2.510254	-0.578365
	Rotational constants (GHz):	976.49 993.29 1004.9 1030.4 1040.5	C	1.733421	0.119335	-0.011587
	0.9857	1060 1096.6 1139 1172.2 1183.8 1189.4	C	2.183370	-1.234501	-0.103004
	0.2491	1199.7 1204.4 1219.4 1254.9 1257.2	C	1.215221	-2.281533	-0.102036
	0.2006	1282.1 1307.7 1321.1 1361.5 1379	C	-0.115224	-2.021693	-0.002996
		1387.7 1389.6 1439.2 1457.8 1465.6	H	1.567515	-3.305894	-0.158789
		1480.5 1523.2 1553.4 1556.2 1605.9	H	-0.807290	-2.851999	0.021935
		1635.4 1647.5 1657.4 1659.3 3160.5	C	2.742361	1.111974	0.177044
		3165.3 3165.7 3168.9 3171.1 3183	C	4.085954	0.790426	0.108481
		3186.3 3196.6 3197.9 3210.4 3214.6	C	4.498206	-0.532699	-0.091519
		3809.4	C	3.560612	-1.537899	-0.164693
			H	4.803988	1.588625	0.251198
			H	5.556509	-0.761226	-0.143739
			H	3.863686	-2.574572	-0.257937
			O	2.464352	2.426384	0.456683
			H	1.601186	2.486513	0.879782
			C	-3.899286	1.186798	-0.112808
			C	-4.812777	0.177391	0.080461
			C	-4.359527	-1.144277	0.254803
			C	-3.012674	-1.433592	0.226042
			H	-5.075807	-1.942042	0.416060
			H	-2.702840	-2.458851	0.376972
			H	-4.231240	2.210964	-0.247541
			H	-5.874626	0.394243	0.101437
4 ring, triplet	Theory: B3LYP/6-311G(d,p)	52.587 75.686 110.78 167.37 190.04	C	2.535060	-0.870680	-0.272135
		207.01 229.75 260.65 318.89 334.88	C	1.593508	-1.872069	-0.654418

	Energy (hartree): -768.4902935	377.16 411.1 430.55 471.77 479.17	C	0.201774	-1.646491	-0.560123
		494.91 504.26 524.38 530.1 544.84	C	-0.320607	-0.418038	-0.197852
	ZPE (hartree): 0.2404780	556.54 566.1 605.14 619.97 673.91	C	0.620786	0.719157	-0.082535
		688.21 707.29 723.9 738.11 765.07	C	2.059049	0.429937	0.074289
	<S2>: 2.03	767.03 776.77 798.17 805.72 863.21	H	1.956457	-2.845725	-0.961931
		870.65 873.25 888.71 905.67 933.26	H	-0.459200	-2.460572	-0.834535
	Rotational constants (GHz):	938.42 962.79 976.17 1006.6 1023.2	C	-1.756670	-0.138157	-0.037427
	0.9821	1051.5 1066.2 1077 1101.6 1125 1169.8	C	-2.215956	1.207270	-0.220175
	0.2456	1178.7 1197 1209.2 1224 1241.3 1273.5	C	-1.259267	2.245037	-0.378306
	0.2023	1299.3 1306.1 1317 1329.5 1352.3	C	0.128471	1.989608	-0.242079
		1371.9 1405.7 1426.8 1457.6 1472.2	H	-1.606883	3.260483	-0.525746
		1488.6 1503.4 1517.3 1563.7 1571	H	0.812150	2.829301	-0.284543
		1588.6 1594.6 1627.7 3160.1 3167.3	C	-2.706714	-1.104312	0.314292
		3168.3 3169.9 3173.6 3180 3184.2	C	-4.089039	-0.801876	0.350780
		3184.5 3188.9 3192.5 3202.2 3728.4	C	-4.522941	0.479917	0.080084
			C	-3.594450	1.488743	-0.189153
			H	-4.775320	-1.601771	0.598363
			H	-5.582648	0.706911	0.096071
			H	-3.927098	2.505105	-0.366679
			O	-2.390573	-2.381112	0.658271
			H	-1.435816	-2.441477	0.801214
			C	3.916990	-1.131948	-0.208882
			C	4.815022	-0.154951	0.213129
			C	4.344887	1.097134	0.592843
			C	2.972902	1.378167	0.527392
			H	5.032720	1.857758	0.943373
			H	2.620951	2.352033	0.846974
			H	4.276984	-2.115432	-0.492331
			H	5.875453	-0.376398	0.255263
5 ring, radical	Theory: B3LYP/6-311G(d,p)	39.208 66.614 110.59 124.79 135.32	C	1.133920	1.310146	-0.000001
		194.61 222.39 233.7 273.01 284.89	C	0.117701	2.322500	0.000037
	Energy (hartree): -846.3253384	322.32 396.32 402.14 434.26 453.19	C	-1.198432	1.998401	0.000027
		476.07 498.99 500.64 506.69 517.88	C	-1.628996	0.629916	-0.000011
	ZPE (hartree): 0.2736350	542.65 553.03 578.43 595.12 631.75	C	-0.678580	-0.407796	-0.000019
		644.9 648.88 702 726.62 728.32 748.59	C	0.742738	-0.077449	-0.000011
	<S2>: 0.759	755.83 771.3 794.3 800.05 818.3 828.05	H	0.427623	3.362166	0.000082
		831.12 855.3 879.4 885.02 889.47 896.22	H	-1.957553	2.772260	0.000055
	Rotational constants (GHz):	906.73 940 960.06 969.01 973.7 985.24	C	-3.033258	0.316092	-0.000019

	1.0189	996.23 1019.8 1032.8 1056.9 1080.9	C	-3.469789	-1.047820	0.000015
	0.1424	1154.6 1165.4 1171.4 1182.3 1191.1	C	-2.474200	-2.065730	-0.000004
	0.1249	1195.5 1220.9 1239.3 1251.4 1283.8	C	-1.144439	-1.757481	-0.000028
		1295.1 1306.9 1342.2 1354.2 1376.6	H	-2.791479	-3.103369	-0.000014
		1385.6 1396.9 1415.7 1421.2 1447.3	H	-0.428267	-2.568256	-0.000067
		1461.2 1463.9 1502.4 1508.9 1523.8	C	-4.056768	1.265687	-0.000052
		1570.5 1592.1 1621 1634.5 1647.7	C	-5.392886	1.026910	-0.000008
		1657.5 1668.7 3155.4 3157.4 3158.6	C	-5.800098	-0.333566	0.000025
		3161.5 3162.2 3162.8 3169.7 3175.4	C	-4.857021	-1.336641	0.000048
		3181.3 3181.9 3182.5 3188.1 3205.8	H	-6.126877	1.825167	-0.000050
			H	-6.857892	-0.573554	0.000061
			H	-5.169801	-2.375279	0.000073
			C	2.485113	1.650302	-0.000017
			C	3.494960	0.679424	-0.000026
			C	3.112927	-0.705588	-0.000020
			C	1.749754	-1.041172	-0.000020
			H	1.498596	-2.094491	-0.000030
			H	2.761977	2.700172	-0.000035
			C	4.881966	1.009886	-0.000006
			C	5.836367	0.029018	0.000029
			C	5.459533	-1.341935	0.000034
			C	4.137725	-1.697172	0.000002
			H	5.167826	2.056587	-0.000024
			H	6.888055	0.292428	0.000061
			H	6.228625	-2.106039	0.000054
			H	3.849746	-2.743385	-0.000015
5 ring, singlet	Theory: B3LYP/6-311G(d,p)	37.377 57.217 93.359 112.36 139.38	C	-1.317330	1.230031	-0.205496
		187.77 196.82 229.63 257.22 275.66	C	-0.265240	2.182578	-0.374671
	Energy (hartree): -922.2476004	284.18 331.62 350.58 386.69 412.41	C	1.041324	1.815747	-0.320524
		435.66 462.34 473.33 476.33 506.56	C	1.446978	0.447812	-0.101901
	ZPE (hartree): 0.2911610	515.33 532.49 537.77 552.76 558.16	C	0.439711	-0.543603	-0.078542
		564.04 601.51 634.56 635.7 671.8 681.59	C	-0.968230	-0.160012	-0.070423
	<S2>: 0	718.03 739.59 755.9 768.37 772.43	H	-0.529133	3.216659	-0.569410
		793.81 804.58 814.47 834.63 836.01	H	1.791919	2.563658	-0.532738
	Rotational constants (GHz):	843.54 856.47 891.41 895.13 896.25	C	2.842392	0.059080	0.002405
	0.8303	908.54 935.46 965.12 969.62 975.48	C	3.182905	-1.325502	-0.119564
	0.1329	996.17 1003.6 1026.7 1028 1033.7	C	2.133532	-2.285593	-0.181050
	0.1154	1093.6 1145.1 1162.2 1168.9 1187.2	C	0.825425	-1.915741	-0.113335

		1194.4 1197.1 1201.9 1220.9 1236	H	2.399733	-3.333908	-0.262820
		1258.7 1285.6 1298 1309.4 1311.4	H	0.065818	-2.684933	-0.137982
		1351.1 1362 1381.3 1386.3 1396.2	C	3.925171	0.958766	0.249765
		1419.9 1439.9 1454.2 1466.5 1475.3	C	5.238007	0.528801	0.205003
		1511.3 1520.2 1549.2 1583.7 1596	C	5.546203	-0.818549	-0.026567
		1626.1 1639.2 1654.2 1658 1668.6	C	4.532897	-1.739880	-0.155304
		3157.4 3159 3163.6 3166.1 3166.8 3169	H	6.015217	1.259294	0.393158
		3176.3 3183 3185.9 3188.5 3196.4	H	6.583440	-1.131746	-0.058240
		3208.9 3209.3 3809.9	H	4.752234	-2.794894	-0.273776
			C	-2.655226	1.621000	-0.197586
			C	-3.694589	0.694694	-0.051085
			C	-3.356200	-0.694881	0.092444
			C	-2.006683	-1.079907	0.075994
			H	-1.791551	-2.133296	0.202041
			H	-2.895498	2.674249	-0.305992
			O	3.748075	2.282572	0.565925
			H	2.882022	2.401318	0.970093
			C	-5.069318	1.073663	-0.034714
			C	-6.052978	0.134695	0.116415
			C	-5.719629	-1.240399	0.260405
			C	-4.411390	-1.641628	0.249376
			H	-5.321172	2.123314	-0.144194
			H	-7.094878	0.434170	0.127734
			H	-6.511975	-1.970763	0.379159
			H	-4.157171	-2.690737	0.359292
5 ring, triplet	Theory: B3LYP/6-311G(d,p)	35.826 55.276 87.413 107.86 137.34	C	-1.301213	1.239551	-0.223950
		187.27 191.56 226.65 254.16 265.07	C	-0.278018	2.170511	-0.409231
	Energy (hartree): -922.1787271	277.82 312.75 352.3 367.53 412.31	C	1.077857	1.806417	-0.352143
		432.15 444.66 455.79 476.83 493.96	C	1.472783	0.486440	-0.132417
	ZPE (hartree): 0.2871860	516.81 526.97 533.76 539.82 545.34	C	0.427835	-0.529263	-0.094329
		547.42 600.45 620.85 625.58 661.73	C	-0.953065	-0.147533	-0.058609
	<S2>: 2.03	677.52 710.43 720.31 733.28 737.31	H	-0.536262	3.208511	-0.589201
		763.09 773.36 785.35 792.88 800.2	H	1.810971	2.573054	-0.561702
	Rotational constants (GHz):	810.15 823.73 828.69 843.88 869.4	C	2.870626	0.068076	-0.011883
	0.8333	889.71 894.17 916.66 922.45 946.43	C	3.193972	-1.313627	-0.159121
	0.1315	963.2 967.92 972.6 1000.3 1027.4 1039.9	C	2.126250	-2.268710	-0.262019
	0.1146	1056.8 1091.8 1118.2 1146.7 1171.5	C	0.820811	-1.897233	-0.178203
		1182.3 1183.6 1192.3 1206.5 1216.3	H	2.387669	-3.315086	-0.375363

		1241.1 1256.6 1269.5 1283.1 1287	H	0.059336	-2.663847	-0.230844
		1314.7 1323 1355.1 1365.1 1389.4	C	3.946598	0.946333	0.280786
		1414.1 1426.5 1459.7 1461.6 1466.6	C	5.266238	0.499751	0.273780
		1478.3 1497.1 1516.1 1518.9 1558.3	C	5.560226	-0.837263	0.026458
		1574 1579.1 1601.6 1617.7 1636.5	C	4.529805	-1.744690	-0.162261
		3159.9 3162.8 3165.1 3167.5 3169	H	6.044195	1.221205	0.490968
		3170.4 3176.5 3183.7 3186.9 3191.1	H	6.592077	-1.168926	0.018719
		3198.2 3201.4 3204.8 3762.5	H	4.741328	-2.798916	-0.300273
			C	-2.670980	1.624209	-0.225799
			C	-3.729203	0.688993	-0.055457
			C	-3.388073	-0.692381	0.124242
			C	-2.005606	-1.069985	0.122249
			H	-1.785969	-2.116052	0.291838
			H	-2.914344	2.671454	-0.371895
			O	3.776146	2.261441	0.608791
			H	2.867167	2.398301	0.903506
			C	-5.080517	1.059730	-0.052486
			C	-6.093431	0.103260	0.125138
			C	-5.763666	-1.230255	0.300195
			C	-4.413077	-1.624914	0.298932
			H	-5.341520	2.103954	-0.188445
			H	-7.131733	0.414370	0.125117
			H	-6.540436	-1.973168	0.438831
			H	-4.158581	-2.670880	0.435198
6 ring, radical	Theory: B3LYP/6-311G(d,p)	30.41 53.238 75.078 93.219 120.48	C	0.115700	1.488411	-0.000254
		159.96 164.69 202.16 212.01 218.69	C	1.201977	2.428983	-0.000080
	Energy (hartree): -999.9939385	261.58 299.72 326.53 344.43 393.07	C	2.490935	2.016234	0.000195
		400.37 429.91 437.23 471.38 477.91	C	2.829957	0.618467	0.000039
	ZPE (hartree): 0.3198720	491.84 501.24 506.26 517.93 524.93 547	C	1.814835	-0.353714	-0.000307
		566.34 587.85 593.94 620.61 638.57	C	0.414658	0.069471	-0.000190
	<S2>: 0.759	642.99 694.1 706.26 720.94 745.48	H	0.963557	3.487303	-0.000055
		748.89 752.24 766.12 774.08 779.17	H	3.301476	2.736013	0.000501
	Rotational constants (GHz):	798.09 821.99 824.31 827.71 847.59	C	4.209333	0.214451	0.000138
	0.8428	848.14 861.85 880.48 883.4 887.18	C	4.556788	-1.175715	-0.000195
	0.0842	908.96 913.53 915.68 932.15 959.38	C	3.497701	-2.125665	-0.000747
	0.0765	971.65 973.48 985.15 996.26 1022.2	C	2.190321	-1.730186	-0.000807
		1024.1 1056.6 1086.2 1150.8 1156.7	H	3.745825	-3.181955	-0.001165
		1164.3 1181.3 1189.6 1191.9 1209.3	H	1.422571	-2.492380	-0.001352

		1221.1 1227.5 1248 1264.3 1287.4	C	5.292874	1.095852	0.000560
		1306.7 1309.1 1319.7 1343.3 1368.6	C	6.610170	0.770826	0.000713
		1374 1384.4 1395 1415 1419.2 1426.2	C	6.928397	-0.613821	0.000402
		1447.2 1461.2 1463.6 1494 1501.1	C	5.922754	-1.553668	-0.000041
		1517.3 1560.1 1566.9 1584 1612.8	H	7.394676	1.519474	0.001052
		1625.3 1646 1651.5 1658.3 1672.6	H	7.968448	-0.921756	0.000525
		3155.7 3157.1 3158.6 3158.7 3160 3163	H	6.167414	-2.610424	-0.000283
		3163.3 3164.1 3169.7 3176.4 3182	C	-1.200957	1.919885	-0.000356
		3182.3 3183.7 3188.5 3204.6	C	-2.285689	1.018161	-0.000277
			C	-1.995724	-0.397545	0.000028
			C	-0.646835	-0.821169	0.000079
			H	-0.467290	-1.888889	0.000616
			H	-1.405769	2.986033	-0.000529
			C	-3.625495	1.441603	-0.000362
			C	-4.680887	0.532860	-0.000121
			C	-4.391525	-0.885915	0.000239
			C	-3.064621	-1.309609	0.000298
			H	-3.840997	2.505710	-0.000638
			H	-2.848990	-2.373784	0.000545
			C	-6.050167	0.950071	-0.000183
			C	-7.063522	0.036277	0.000114
			C	-6.778186	-1.362614	0.000502
			C	-5.487777	-1.806149	0.000551
			H	-6.266389	2.013319	-0.000499
			H	-8.095887	0.367418	0.000048
			H	-7.598357	-2.071618	0.000770
			H	-5.270365	-2.869159	0.000838
6 ring, singlet	Theory: B3LYP/6-311G(d,p)	29.088 46.055 71.371 84.718 108.24	C	-0.106981	1.392359	-0.224067
		149.62 158.46 191.85 216.06 217.46	C	1.004347	2.286025	-0.353691
	Energy (hartree): -1075.9161092	232.43 278 302.1 314.73 347.65 368.97	C	2.284636	1.844405	-0.282420
		383.33 395.87 428.06 458.93 471.08	C	2.610121	0.447544	-0.088917
	ZPE (hartree): 0.3374310	474.29 478.18 495.63 510.82 524.5	C	1.551339	-0.486035	-0.107927
		537.25 543.5 549.51 563.93 581.26 595.6	C	0.162821	-0.025208	-0.109736
	<S2>: 0	632.13 642.92 661.7 663.3 696.57 732.01	H	0.803449	3.337027	-0.532580
		748.89 752.11 765.22 768.58 774.38	H	3.080908	2.551884	-0.464507
	Rotational constants (GHz):	778.26 807.42 813.51 829.62 836.68	C	3.978978	-0.019344	0.024742
	0.7158	840.3 847.77 850.69 866.11 885.07	C	4.246243	-1.417160	-0.132353
	0.0784	896.59 907.67 910.34 916.39 931.76	C	3.148101	-2.315392	-0.235866

	0.0711	964.74 971.73 975.23 996.22 1007	C	1.860736	-1.874846	-0.176254
		1023.4 1026.3 1033.3 1096.9 1147	H	3.357227	-3.374077	-0.345270
		1154.2 1157.6 1187.8 1189.7 1195.2	H	1.059967	-2.599169	-0.236145
		1201.3 1211.9 1223.8 1229.4 1245.7	C	5.105822	0.812936	0.311891
		1271.2 1288 1305.4 1309.4 1314.4	C	6.393570	0.313981	0.269739
		1322.7 1361.6 1369.3 1377.7 1384.2	C	6.631987	-1.041506	0.002398
		1397.5 1417 1426.3 1438.7 1456.1	C	5.572886	-1.902605	-0.164312
		1465.9 1475 1497.8 1509.9 1547.7	H	7.206528	0.995245	0.488955
		1560.4 1583.2 1586.5 1612.9 1635.7	H	7.651272	-1.409179	-0.026064
		1647.3 1654.1 1658.8 1672.2 3156.1	H	5.736797	-2.964223	-0.310288
		3157.6 3159.3 3160.5 3164.5 3166.4	C	-1.412331	1.858475	-0.232599
		3167 3169.4 3177 3183.4 3186.7 3188.9	C	-2.516154	0.988742	-0.120656
		3197 3208.8 3211.5 3811.5	C	-2.256813	-0.427435	0.008246
			C	-0.919252	-0.884510	0.006944
			H	-0.765038	-1.949987	0.119662
			H	-1.590768	2.925331	-0.325267
			O	4.995334	2.134597	0.665384
			H	4.132281	2.287726	1.064190
			C	-3.846094	1.443402	-0.125159
			C	-4.920240	0.565332	-0.007279
			C	-4.661762	-0.853514	0.125061
			C	-3.345408	-1.308053	0.130253
			H	-4.038134	2.507510	-0.222775
			H	-3.153289	-2.372133	0.228854
			C	-6.279656	1.014195	-0.011356
			C	-7.312024	0.130001	0.106397
			C	-7.057183	-1.268891	0.236818
			C	-5.777528	-1.742144	0.245676
			H	-6.472553	2.077247	-0.110752
			H	-8.336538	0.484567	0.101803
			H	-7.892314	-1.954025	0.329046
			H	-5.583459	-2.805048	0.344622
6 ring, triplet	Theory: B3LYP/6-311G(d,p)	28.917 46.129 69.461 85.554 105.86	C	-0.076018	1.394667	-0.200795
		145.54 155.1 191.47 214.51 215.07	C	1.005150	2.280911	-0.333332
	Energy (hartree): -1075.8684015	233.27 277.02 296.41 313.54 328.94	C	2.314449	1.841338	-0.273902
		367.84 376.57 391.9 411.5 438.22 456.42	C	2.632998	0.474384	-0.089965
	ZPE (hartree): 0.3343900	461.41 472.67 491.3 509.34 527.21	C	1.546607	-0.465126	-0.084794
		536.55 542.64 548.49 554.59 577.85	C	0.189994	-0.001961	-0.082505

	Relative energy, scaled, w/ZPE (kcal/mol): -6.749e+005	592.82 626.67 629.68 658.81 668.71	H	0.804148	3.335191	-0.491769
		693.35 711.98 727.33 746.02 746.98	H	3.098748	2.562216	-0.455609
		760.15 766.41 775.58 787.35 803.19	C	4.003415	-0.015736	0.014831
	<S2>: 2.03	809.1 813.61 827.9 835 835.76 842.77	C	4.250450	-1.413283	-0.143780
		849.39 866.87 878.99 895.82 906.47	C	3.134896	-2.305992	-0.233700
	Rotational constants (GHz):	926.66 935.85 966.61 975.38 976.89	C	1.855558	-1.861765	-0.153636
	0.7203	979.33 1026.7 1035.5 1054.4 1095.2	H	3.337320	-3.366262	-0.340618
	0.0778	1126.3 1136.8 1153.3 1180.7 1187.2	H	1.051276	-2.583028	-0.197877
	0.0706	1191.8 1196.2 1204.9 1225.1 1228.9	C	5.136353	0.800878	0.296443
		1238.3 1253.1 1255.4 1276.8 1282.9	C	6.422924	0.284287	0.256686
		1291.6 1311.7 1318.9 1334.6 1335.2	C	6.641109	-1.069370	-0.008063
		1370 1377.9 1412.7 1433.7 1448.5	C	5.564593	-1.916825	-0.176491
		1459.3 1464.8 1474.9 1478.2 1482.3	H	7.243940	0.957999	0.468911
		1509.9 1521.5 1533.4 1564.1 1580.3	H	7.654157	-1.453674	-0.038211
		1591.1 1596.6 1601.3 1639 1651.5 3158	H	5.714473	-2.980563	-0.322161
		3158.8 3160.7 3162.6 3165.3 3166.3	C	-1.425246	1.861174	-0.217952
		3167.2 3169.5 3177 3183.5 3190.5	C	-2.520859	0.999305	-0.113436
		3191.1 3197.6 3210 3212.1 3789.3	C	-2.260007	-0.426169	0.017992
			C	-0.930180	-0.877228	0.027383
			H	-0.772469	-1.941192	0.144572
			H	-1.599002	2.927783	-0.318899
			O	5.044545	2.123129	0.642510
			H	4.170298	2.294825	1.010617
			C	-3.851104	1.447138	-0.126348
			C	-4.960507	0.554778	-0.012233
			C	-4.703794	-0.849228	0.121194
			C	-3.347638	-1.301864	0.132648
			H	-4.047201	2.510121	-0.224972
			H	-3.158609	-2.366177	0.232073
			C	-6.290209	1.002862	-0.025326
			C	-7.352628	0.106217	0.088963
			C	-7.102742	-1.258880	0.218805
			C	-5.789384	-1.729770	0.234688
			H	-6.486399	2.065206	-0.126407
			H	-8.372281	0.473681	0.076660
			H	-7.927242	-1.956825	0.307629
			H	-5.596596	-2.792783	0.335721

7 ring, radical	Theory: B3LYP/6-311G(d,p)	23.314 42.113 54.877 72.379 102.5	C	1.359578	1.569884	0.000036
		114.46 142.2 162.34 184.05 191.55 208.7	C	2.489126	2.459795	0.000007
	Energy (hartree): -1153.6608594	233.03 265.87 282.43 318.83 337.46	C	3.756967	1.988843	0.000000
		361.1 390.72 391.43 427.25 449.8 467.19	C	4.033423	0.575547	-0.000003
	ZPE (hartree): 0.3659920	472.79 473.37 478.64 501.36 508.01	C	2.976923	-0.350437	0.000017
		517.88 521.33 529.75 542.16 563.74	C	1.595097	0.134702	0.000047
	<S2>: 0.759	592.64 596.59 627.37 633.96 646.57	H	2.299189	3.527894	0.000008
		680.52 697.79 712.49 733.17 740.15	H	4.599588	2.670781	0.000007
	Rotational constants (GHz):	748.02 749.99 758.31 759.74 773.67	C	5.392876	0.111478	-0.000020
	0.7210	780.6 797.03 817.66 820.24 827.22	C	5.679473	-1.292890	-0.000003
	0.0535	832.98 844.32 846.66 868.94 875.63	C	4.580026	-2.194916	0.000015
	0.0498	879.71 885.16 888.27 898.63 914.55	C	3.291053	-1.741601	0.000023
		919.46 922.44 929.66 958.64 973.07	H	4.780985	-3.261184	0.000023
		973.5 985.11 996.03 1018.9 1020.6	H	2.490318	-2.469142	0.000041
		1055.7 1084.8 1142.8 1150.8 1163.9	C	6.514343	0.944654	-0.000059
		1181.2 1187.3 1191.6 1202.7 1209.8	C	7.815854	0.562273	-0.000078
		1221.6 1228.1 1245.6 1254.3 1274.7	C	8.073421	-0.835305	-0.000048
		1289.2 1299.1 1309.8 1320.6 1332.6	C	7.027823	-1.730226	-0.000013
		1345 1366.1 1373.8 1387 1397 1410.2	H	8.632395	1.275868	-0.000117
		1417.2 1423.1 1428.8 1446.6 1460.7	H	9.099072	-1.188215	-0.000056
		1463.9 1487.2 1496 1515.4 1544.2	H	7.225726	-2.796706	0.000006
		1561.9 1564.7 1578.3 1599.7 1622.4	C	0.067755	2.060768	0.000040
		1634.3 1644.3 1651.5 1662.3 1673.3	C	-1.062440	1.209349	0.000020
		3155.5 3157.1 3157.8 3158.9 3159.2	C	-0.835758	-0.223300	0.000038
		3160.3 3161.8 3163.5 3163.8 3164.7	C	0.498201	-0.705788	0.000080
		3170 3176.7 3182.1 3182.6 3184.5	H	0.629469	-1.780519	0.000186
		3188.6 3204.7	H	-0.088129	3.135130	0.000028
			C	-2.372540	1.694170	0.000008
			C	-3.479845	0.832977	0.000010
			C	-3.253858	-0.603115	0.000022
			C	-1.935812	-1.084189	0.000043
			H	-2.539160	2.766893	0.000011
			H	-1.768386	-2.156890	0.000070
			C	-4.807933	1.311336	0.000001
			C	-5.897610	0.452190	-0.000012
			C	-5.671769	-0.982394	-0.000013
			C	-4.370976	-1.465732	0.000010
			H	-4.976814	2.383823	0.000006

			H	-4.203208	-2.538406	0.000018
			C	-7.249853	0.929846	-0.000029
			C	-8.301275	0.063278	-0.000052
			C	-8.078754	-1.350180	-0.000056
			C	-6.812019	-1.852052	-0.000036
			H	-7.417898	2.001752	-0.000023
			H	-9.318073	0.439456	-0.000067
			H	-8.930870	-2.020479	-0.000072
			H	-6.643178	-2.923838	-0.000037
7 ring, singlet	Theory: B3LYP/6-311G(d,p)	22.877 38.378 54.138 69.234 91.379	C	1.107099	1.472982	-0.219220
		112.9 124.61 168.03 178.65 184.36	C	2.255165	2.324695	-0.321189
	Energy (hartree): -1229.5830538	202.81 225.75 251.19 268.41 292.13	C	3.515692	1.833240	-0.241932
		322.16 323.89 360.03 363.35 389.23	C	3.786338	0.419808	-0.071405
	ZPE (hartree): 0.3835730	403.43 423.3 458.66 466.15 469.16	C	2.694311	-0.472234	-0.119827
		472.91 478.19 490.14 517.96 519.59	C	1.322214	0.040531	-0.123226
	<S2>: 0	523.06 535.94 543.99 555.24 560.58	H	2.097039	3.385400	-0.485181
		571.56 625.29 630.15 638.5 648.41	H	4.340508	2.512651	-0.402349
	Rotational constants (GHz):	658.45 692.48 719.45 734.04 740.93	C	5.134980	-0.099944	0.043381
	0.6302	749.24 758.58 758.92 768.14 773.43	C	5.352035	-1.503118	-0.143780
	0.0500	780.83 804.65 811.39 824.46 827.63	C	4.222696	-2.356695	-0.277256
	0.0465	838.75 842.91 843.83 850.4 869.65	C	2.951837	-1.869115	-0.217860
		875.54 888.5 896.06 899.19 914.11	H	4.392869	-3.419588	-0.410719
		914.86 922.39 929.1 964.44 972.72	H	2.124909	-2.560839	-0.303155
		975.33 995.86 1006 1018.7 1025.2	C	6.289366	0.683639	0.358542
		1032.3 1096 1140.9 1148.2 1154.7	C	7.558011	0.138909	0.314188
		1186.4 1188.1 1193.7 1201.5 1204.5	C	7.748798	-1.218261	0.016873
		1211.6 1222.4 1232.5 1249 1253.4	C	6.660609	-2.035861	-0.177410
		1278.5 1289.7 1299.2 1307.8 1315.1	H	8.393608	0.784342	0.555560
		1322.3 1335.1 1361.6 1369.1 1376.2	H	8.754170	-1.622333	-0.012707
		1387.8 1400.3 1411.7 1422.6 1428.9	H	6.787037	-3.099143	-0.346736
		1439.2 1456.2 1464.9 1474.9 1489.3	C	-0.175464	1.988710	-0.235136
		1504.2 1542.4 1547.8 1562.9 1578.2	C	-1.318430	1.160469	-0.146788
		1584.9 1598.8 1632.6 1633.5 1645.9	C	-1.113616	-0.271104	-0.030228
		1656.7 1660.3 1673.2 3155 3156.6	C	0.211312	-0.777111	-0.025265
		3157.5 3158.7 3160 3161.6 3164.3	H	0.324358	-1.848983	0.075817
		3165.9 3166.5 3169.2 3176.8 3183.2	H	-0.311978	3.062808	-0.314188
		3185.8 3188.8 3196.8 3208.5 3211.5	C	-2.620934	1.666159	-0.162485
		3813.3	C	-3.740782	0.827274	-0.067029

			C	-3.536872	-0.607095	0.055381
			C	-2.227016	-1.109112	0.070686
			H	-2.771030	2.737700	-0.250621
			H	-2.076163	-2.180547	0.159795
			C	-5.061324	1.326260	-0.085346
			C	-6.163629	0.489004	0.009674
			C	-5.959855	-0.943706	0.133298
			C	-4.667017	-1.447225	0.152623
			H	-5.213933	2.397267	-0.176893
			H	-4.515609	-2.518423	0.244007
			O	6.223653	1.999893	0.742367
			H	5.363872	2.174584	1.139269
			C	-7.508250	0.987570	-0.009682
			C	-8.572525	0.142287	0.085339
			C	-8.371735	-1.269205	0.207460
			C	-7.113163	-1.790558	0.230523
			H	-7.660048	2.057904	-0.102010
			H	-9.583262	0.534078	0.069450
			H	-9.233871	-1.922343	0.281603
			H	-6.960806	-2.860835	0.322709
7 ring, triplet	Theory: B3LYP/6-311G(d,p)	22.608 38.77 53.676 69.893 90.315	C	1.137262	1.469932	-0.192976
		110.58 126.25 167.67 177.43 180.99	C	2.260398	2.320456	-0.298911
	Energy (hartree): -1229.5513478	204.21 219.59 252.97 267.9 294.71	C	3.540666	1.830754	-0.233042
		320.48 323.09 344.61 360.98 382.5	C	3.806810	0.439064	-0.069587
	ZPE (hartree): 0.3810550	404.09 423.34 429.06 441.01 461.34	C	2.694852	-0.454459	-0.093176
		466.31 472.42 489.01 514.08 519.13	C	1.349044	0.061804	-0.096208
	<S2>: 2.03	524.76 538.34 551.29 554.36 557.97	H	2.100012	3.383225	-0.446749
		574.68 619.16 630.58 631.27 642.31	H	4.356980	2.519964	-0.394964
	Rotational constants (GHz):	657.99 694.1 704.67 720.26 736.39	C	5.156821	-0.098093	0.033344
	0.6342	738.33 751.81 755.47 758.23 767.05	C	5.356368	-1.501313	-0.149327
	0.0497	783.41 794.52 803.91 806.11 813.98	C	4.212901	-2.350426	-0.259839
	0.0462	827.43 832.42 840.49 842.58 847.93	C	2.949266	-1.859334	-0.181604
		860.3 870.83 878.47 884.12 887.39	H	4.376615	-3.415504	-0.384038
		895.96 920.34 922.67 949.47 966.41	H	2.118674	-2.548790	-0.243627
		975.53 984.15 990.47 1029.2 1033.2	C	6.318221	0.673995	0.333506
		1051 1095.5 1135.6 1140.1 1148.7	C	7.584237	0.114820	0.285210
		1179.3 1186.5 1191.8 1195.3 1200.9	C	7.757095	-1.242333	-0.005196
		1203.7 1212.1 1225.9 1243.2 1259.9	C	6.654759	-2.048935	-0.189488

		1265.2 1272.3 1283 1290.9 1303 1314.5	H	8.427720	0.754703	0.513499
		1318.2 1322.9 1350.9 1357.9 1372.1	H	8.756915	-1.659467	-0.040695
		1380.2 1382.7 1417.6 1442.3 1451.4	H	6.768301	-3.114403	-0.354213
		1460.7 1465.9 1468.1 1484.2 1491.9	C	-0.184244	1.986532	-0.214670
		1508.1 1512.9 1528 1537.1 1561.7	C	-1.303595	1.167222	-0.133970
		1581.9 1588.8 1593.2 1613 1622.8	C	-1.099223	-0.265184	-0.020563
		1642.4 1654.6 3155.4 3156.4 3157.5	C	0.201265	-0.768522	-0.008816
		3159.1 3160.9 3162.4 3164.6 3165.5	H	0.316574	-1.840006	0.090581
		3166.2 3169 3176.6 3183.1 3188.3	H	-0.317125	3.060767	-0.297852
		3190.2 3197 3211.1 3211.5 3800.1	C	-2.628635	1.669490	-0.154309
			C	-3.761920	0.830285	-0.064976
			C	-3.557480	-0.608414	0.056427
			C	-2.233898	-1.106166	0.075012
			H	-2.778006	2.741063	-0.241125
			H	-2.082622	-2.177509	0.162643
			C	-5.063357	1.324997	-0.087989
			C	-6.202380	0.476393	0.003114
			C	-6.001180	-0.937116	0.124423
			C	-4.669524	-1.440152	0.147593
			H	-5.219435	2.395569	-0.178539
			H	-4.521285	-2.511844	0.238350
			O	6.270539	1.992645	0.706196
			H	5.408405	2.182889	1.092144
			C	-7.519889	0.977131	-0.021754
			C	-8.607968	0.124790	0.069243
			C	-8.410838	-1.259575	0.188546
			C	-7.127243	-1.779888	0.215524
			H	-7.672557	2.047456	-0.113720
			H	-9.614275	0.527215	0.048635
			H	-9.265410	-1.922666	0.259599
			H	-6.975331	-2.850352	0.307281
8 ring, radical	Theory: B3LYP/6-311G(d,p)	17.502 34.991 42.675 57.996 84.98	C	2.597219	1.600480	0.000181
		86.314 128.71 131.15 150.18 170.93	C	3.755003	2.454139	0.000063
	Energy (hartree): -1307.3269978	173.6 199.06 220.34 239.27 256.53	C	5.006912	1.943454	-0.000086
		291.47 298.66 332.18 336.23 371.92	C	5.239202	0.521329	-0.000042
	ZPE (hartree): 0.4119810	392.35 402.9 425.81 449.49 458.97	C	4.154780	-0.371285	0.000130
		465.22 469.61 474.3 476.5 499.04 501.21	C	2.787747	0.156451	0.000141
	<S2>: 0.768	506.12 516.22 517.7 538.97 554.52	H	3.598785	3.527694	0.000096

		585.71 591.87 594.3 631.73 638.12	H	5.870723	2.598338	-0.000193
	Rotational constants (GHz):	647.59 655.41 695.35 703.02 715.41	C	6.583316	0.015815	-0.000094
	0.6324	726.15 745.64 748.11 748.8 749.73	C	6.826793	-1.396836	0.000098
	0.0361	762.17 762.64 772.86 786.78 796.4	C	5.700283	-2.264331	0.000349
	0.0341	816.33 819.45 824.67 826.84 835.09	C	4.425756	-1.771151	0.000365
		843.51 846.84 859.75 868.99 879.81	H	5.868053	-3.336318	0.000560
		884.27 886.93 888.16 900.48 906.46	H	3.602889	-2.473573	0.000607
		916.1 918.85 926.26 931.9 958.18 973.57	C	7.730018	0.814225	-0.000338
		973.8 985.18 995.84 1016.2 1019.9	C	9.019053	0.391958	-0.000420
		1055.4 1084.8 1129.4 1150.1 1163.1	C	9.233689	-1.012975	-0.000217
		1180.7 1184.6 1191.3 1196.7 1199.4	C	8.161167	-1.875350	0.000038
		1209.5 1217.9 1230.1 1238.5 1256.5	H	9.857175	1.080096	-0.000644
		1267.3 1282.5 1290.2 1298.7 1302.1	H	10.248073	-1.397038	-0.000257
		1320.1 1327.2 1339.1 1347.1 1358.3	H	8.326262	-2.947397	0.000198
		1374.9 1388.5 1397.3 1401.2 1415.5	C	1.323389	2.131836	0.000235
		1418.2 1426 1429.6 1444.8 1460.2	C	0.164088	1.316692	0.000120
		1463.9 1483.1 1492 1513.9 1532 1542.7	C	0.345764	-0.125301	-0.000004
		1558.1 1562.1 1576.6 1586.7 1616.8	C	1.666771	-0.648653	0.000059
		1620.5 1634.3 1646.8 1656.1 1660.1	H	1.764233	-1.727015	-0.000046
		1673 3155.2 3156.7 3156.9 3157.9	H	1.201498	3.210569	0.000371
		3158.9 3159.4 3159.9 3161.2 3162.6	C	-1.125594	1.843021	0.000129
		3163.4 3163.8 3164.8 3170 3176.6	C	-2.265693	1.017258	0.000022
		3181.6 3182.8 3184 3188.5 3204.7	C	-2.084795	-0.429433	-0.000096
			C	-0.776503	-0.950366	-0.000122
			H	-1.258080	2.920465	0.000213
			H	-0.642657	-2.027754	-0.000220
			C	-3.568794	1.538302	0.000037
			C	-4.696806	0.713105	-0.000034
			C	-3.219587	-1.254832	-0.000152
			H	-3.703376	2.615502	0.000093
			C	-6.012885	1.232330	-0.000012
			C	-7.126487	0.408643	-0.000033
			C	-6.945982	-1.034751	-0.000078
			C	-5.663925	-1.559255	-0.000124
			H	-6.147961	2.309592	0.000017
			C	-8.464547	0.928380	0.000000
			C	-9.541866	0.095820	0.000013
			C	-9.364128	-1.325564	-0.000015

			C	-8.115075	-1.867568	-0.000063
			C	-4.516066	-0.732366	-0.000111
			H	-3.085532	-2.332118	-0.000233
			H	-5.530198	-2.636689	-0.000171
			H	-8.598736	2.005050	0.000012
			H	-10.546456	0.503454	0.000040
			H	-10.237464	-1.967977	0.000007
			H	-7.980546	-2.944197	-0.000090
8 ring, singlet	Theory: B3LYP/6-311G(d,p)	17.934 33.324 43.057 56.697 79.367	C	-2.321926	-1.508165	-0.208392
		85.947 106.86 136.42 149.02 159.46	C	-3.493995	-2.329613	-0.291439
	Energy (hartree): -1383.2492078	175.31 194.51 220.49 228.79 245.9	C	-4.739754	-1.803426	-0.209869
		271.75 285.97 303.41 333.31 337.14	C	-4.971526	-0.380048	-0.057404
	ZPE (hartree): 0.4296570	354.97 372.41 393.06 417.31 422.32	C	-3.857118	0.481765	-0.126667
		457.58 459.36 464.51 468.57 473.47	C	-2.498090	-0.067094	-0.129570
	<S2>: 0	476.08 487.86 497.92 506.33 523.01	H	-3.365678	-3.396236	-0.442541
		536.7 540.52 546.49 555.24 566.21	H	-5.583713	-2.462390	-0.355557
	Rotational constants (GHz):	594.86 618.47 629.82 639.91 648.38	C	-6.304888	0.176229	0.057822
	0.5642	656.22 682.02 703.78 707.66 735.09	C	-6.486982	1.581456	-0.151135
	0.0338	747.35 748.06 750.03 761.76 762.42	C	-5.336932	2.402666	-0.306042
	0.0320	768.15 772.28 785.6 806.84 810.31	C	-4.078588	1.882775	-0.246348
		818.76 821.37 835.81 841.02 842.14	H	-5.480010	3.467253	-0.456658
		843.14 847.2 859.97 870.46 884.9 887.3	H	-3.234480	2.551028	-0.348954
		896.14 901.28 906.12 915.18 915.27	C	-7.476866	-0.572241	0.393554
		925.77 931.55 964.32 973.27 975.43	C	-8.731291	0.003964	0.347876
		995.62 1004.5 1016.2 1024.8 1032.1	C	-8.889161	1.360675	0.029047
		1095.6 1127.6 1150 1151.2 1185.3	C	-7.781898	2.146872	-0.185531
		1187.3 1193.1 1199.4 1200.5 1204.5	H	-9.581583	-0.615504	0.605441
		1211.4 1220.1 1232.2 1239.2 1262.2	H	-9.884070	1.789820	-0.001146
		1267.3 1284.2 1290.5 1298.9 1301.8	H	-7.882410	3.210064	-0.371934
		1313 1322 1327.2 1343.4 1356.6 1365.6	C	-1.055849	-2.058467	-0.225264
		1378.8 1390.8 1403.4 1407.5 1417.7	C	0.112361	-1.260526	-0.153778
		1426.4 1430.3 1438.6 1456 1464.1	C	-0.053335	0.180202	-0.051914
		1474.5 1484.5 1500 1530.6 1546.3	C	-1.367157	0.720969	-0.046347
		1551.7 1558.5 1576.8 1583.9 1586.2	H	-1.451122	1.796587	0.043047
		1616 1628.6 1637.4 1652.2 1656 1659.9	H	-0.948844	-3.136769	-0.291299
		1673.2 3154.7 3156.3 3156.4 3157.6	C	1.396055	-1.801774	-0.171924
		3158.6 3159.5 3160.8 3162.4 3164.2	C	2.544865	-0.992618	-0.092702
		3165.7 3166.1 3169.1 3176.6 3183.1	C	2.380203	0.452054	0.016508

		3185.2 3188.7 3196.4 3208.1 3210.2	C	1.078389	0.988077	0.033652
		3814.3	H	1.516298	-2.877893	-0.248987
			H	0.956767	2.064054	0.111676
			C	3.842121	-1.528147	-0.115163
			C	4.978861	-0.719302	-0.036292
			C	3.524216	1.260809	0.098093
			H	3.964754	-2.603656	-0.196939
			C	6.289146	-1.252832	-0.061719
			C	7.411538	-0.445272	0.016338
			C	7.247243	0.995815	0.129726
			C	5.971434	1.534220	0.155941
			H	6.412365	-2.328270	-0.145168
			O	-7.441714	-1.882946	0.799556
			H	-6.583126	-2.073034	1.191911
			C	8.743755	-0.979438	-0.010424
			C	9.830073	-0.162581	0.068043
			C	9.668291	1.256398	0.180153
			C	8.425589	1.811782	0.209747
			C	4.814358	0.723963	0.075527
			H	3.402141	2.336418	0.179505
			H	5.849660	2.609829	0.239326
			H	8.866154	-2.054188	-0.094843
			H	10.829946	-0.581071	0.046610
			H	10.548675	1.886116	0.241313
			H	8.303137	2.886530	0.294120
8 ring, triplet	Theory: B3LYP/6-311G(d,p)	17.608 33.58 42.837 57.26 79.052 85.156	C	-2.348696	-1.503170	-0.186598
		108.33 136.37 146.15 160.63 176.05	C	-3.501389	-2.325978	-0.273948
	Energy (hartree): -1383.2293208	193.27 220.42 229.88 238.2 273.48	C	-4.761254	-1.801350	-0.204113
		285.42 308.38 333.94 336.78 352.57	C	-4.989982	-0.394342	-0.056254
	ZPE (hartree): 0.4274600	360.64 387.49 419.22 423.97 429.34	C	-3.860863	0.467500	-0.103436
		440.17 454.86 459.58 462.57 477.98	C	-2.522362	-0.084792	-0.107389
	Relative energy, scaled, w/ZPE (kcal/mol): -8.677e+005	487.31 493.84 505.59 525.39 539.5	H	-3.370331	-3.393941	-0.412910
		546.91 551.44 557.66 567.36 591.73	H	-5.599051	-2.467670	-0.351527
		619.46 629.75 632.3 636.56 657.36	C	-6.324555	0.175156	0.048330
	<S2>: 2.03	684.17 696.1 707.64 718.81 730.96	C	-6.492166	1.580622	-0.153905
		743.42 751.12 753.43 762.9 765.6 767.57	C	-5.330773	2.398424	-0.286186
	Rotational constants (GHz): 0.5674	786.69 802.95 808.77 810.96 814.16	C	-4.078440	1.875453	-0.211278
		823.71 832.31 838.44 841.48 843.54	H	-5.468107	3.465243	-0.426310

	0.0336	847.74 853.94 862.9 880.26 887.68	H	-3.230860	2.542047	-0.291590
	0.0318	891.02 895.3 895.69 897.53 920.27	C	-7.502879	-0.564806	0.368079
		928.07 957.58 965.94 975.52 988.56	C	-8.754477	0.023054	0.318145
		994.98 1030.3 1031.5 1044.4 1095.6	C	-8.897419	1.380496	0.007625
		1130 1140.1 1149.5 1176.1 1185 1189.3	C	-7.778870	2.158025	-0.194805
		1193.8 1198.4 1202 1204 1208.7 1220.1	H	-9.611565	-0.592389	0.562442
		1237.1 1257.8 1270 1276.4 1285.4	H	-9.887635	1.819941	-0.028163
		1289.2 1294.4 1297.6 1313 1317.8	H	-7.868410	3.223256	-0.375133
		1328.2 1338 1361 1366.5 1381.2 1383.8	C	-1.051074	-2.054275	-0.207392
		1392.4 1398.6 1421.8 1435.8 1452.5	C	0.090061	-1.262166	-0.141229
		1454.9 1465.5 1466.5 1481.4 1482.2	C	-0.074435	0.171550	-0.044170
		1501.3 1509 1519.9 1533.1 1538.7	C	-1.360557	0.712249	-0.034286
		1555.7 1587 1589.7 1595.8 1605.5	H	-1.445529	1.787859	0.052024
		1624.3 1638.5 1644 1655.8 3154.3	H	-0.946008	-3.132655	-0.276358
		3155.6 3155.9 3156.9 3158.5 3159.2	C	1.405139	-1.801783	-0.161496
		3160.9 3162.4 3164.2 3165.3 3165.8	C	2.546813	-0.998478	-0.087713
		3168.8 3176.3 3182.9 3186.7 3189.4	C	2.381649	0.452991	0.019339
		3196.6 3210.2 3210.4 3805.7	C	1.087734	0.984684	0.037870
			H	1.523203	-2.878243	-0.236996
			H	0.964270	2.060575	0.114169
			C	3.844760	-1.529397	-0.112011
			C	5.007108	-0.716823	-0.036793
			C	3.526877	1.257586	0.097197
			H	3.968765	-2.604877	-0.191844
			C	6.291577	-1.248885	-0.064655
			C	7.446652	-0.433286	0.010869
			C	7.284571	0.988441	0.121309
			C	5.975019	1.526883	0.149066
			H	6.416929	-2.324251	-0.146794
			O	-7.483354	-1.878550	0.762154
			H	-6.625884	-2.081131	1.151662
			C	8.756203	-0.970416	-0.018528
			C	9.860833	-0.149416	0.057211
			C	9.701511	1.247965	0.166258
			C	8.440021	1.802811	0.197477
			C	4.843031	0.723268	0.073073
			H	3.406292	2.333458	0.177266
			H	5.855291	2.602903	0.231151

			H	8.878544	-2.045327	-0.101918
			H	10.856987	-0.576332	0.033467
			H	10.576307	1.885455	0.225407
			H	8.317413	2.877703	0.280748

Appendix D Matlab Codes used in Analysis

D.1 MultiWell for Matlab

The program is comprised of two classes, MultiwellCase and MultiwellSet. The MultiwellSet will contain multiple MultiwellCase objects, one for each Multiwell run.

```
classdef MultiwellCase < handle
    %MULTIWELLCASE Encapsulates all of the input and output data for a
    %single multiwell job.
    %   Contains all of the data for a single multiwell job including all
    %   of the input information and the results.  Includes methods for
    %   visualizing and analyzing the results

    properties
        Title,Egrain1,Imax1,Isize,Emax2,Idum,Punits,Eunits,Rotatunits,...
            Temp,Tvib,Np,PP,NWells,NProds,IMol,MolName,HMol,MolMom,...
            Molsym,Molele,Molopt,SigM,EpsM,AmuM,Amu,Mol,Sig,Eps,Itype,...
            DC,LJQM,NForward,MolWell,Ito,TS,RR,J,Qel,L,AA,EE,KeyWords,...
            ImFreq,CharFreq,AveReact,BiRateCon,IVREnergy,Civr,Ntrials,...
            Tspec,Tread,KeyTemp,Molinit,IR,Einit,DensLoc,OutFileLoc,...
            OutSave,hPanel,VibEnergy,hSlider,panelH,fracCutOff,hCutOff,...
            hTableCutOff,hRadioButton,hRadio,radioVal,fracFit,fracPlot,...
            hFracPlot,DensDataIndex
    end
    properties
        hData,hText,hFormFigure,hFormPanel,hButton,OldTun,OldIvr,hSet,...
            PopFrac,PopFracError,OutTime,NumRates,ChanIndex,Kinf;
        hResultsFigure,hResPlotPanel,hAxes,GraphToggle,hResDataPanel
        PressureNumber,hTable,hTable1,k1stOrder,k1stOrderR2,MaxError,Status
        StatusChange,runTime,fitToLine=1,largeNtrials=0,hLargeTrials;
        fitStart,fitCut,fitLine,fitP,hfitL,hListBox,hDispPanel,hDispValue;
    end


    methods
        function obj=MultiwellCase(x)
            %Constructor includes default values so that the data form can
```

```
%open.  If there is an input variable the Case will populate
%with some test values
if nargin==0
   o=obj;
   o.Title='Add';o.Egrain1=0;o.Imax1=0;o.Isize=0;...
      o.Emax2=0;o.Idum=1360436544;o.Punits='ADD';...
      o.Eunits='ADD';o.Rotatunits='ADD';o.Temp=0;o.Tvib=0;...
      o.Np=1;o.PP=0;o.NWells=1;o.NProds=1;
   o.IMol=1:2;o.MolName={'update','update'};...
      o.HMol=[0 0];o.MolMom=[0 0];o.Molsym=[0 0];o.Molele=[0 ];...
      o.Molopt=[0 0];o.SigM=0;o.EpsM=0;o.AmuM=0;...
      o.Amu=0;o.Mol=1;o.Sig=0;o.Eps=0;...
      o.Itype=0;o.DC=zeros(1,8);...
      o.LJQM={'LJ'};o.NForward=1;...
      o.MolWell=[1];o.Ito=[2];
   o.TS={'Update'};
   o.RR=[0];o.J=0;o.Qel=0;
   o.L=0;o.AA=0;
   o.EE=[0];
   rev={'upda'};
   notun={'upd'};
   o.ImFreq(4)=1212;o.ImFreq(6)=546.7;
   fast={'upd'};
   cent={'upd'};
   sum1={'upd'};
   o.KeyWords=[rev' notun' fast' cent' sum1'];
   o.Ntrials=0;o.Tspec='update';o.Tread=0;o.KeyTemp='Update';
   o.Molinit=9;o.IR=9;o.Einit=0;o.DensLoc='Unknown';
   o.OutFileLoc='Will Not Save Output Files'; o.OutSave=0;
   o.GraphToggle=0;o.PressureNumber=1;o.Status='Not Ran';
   o.StatusChange=' ';o.runTime=' ';
   o.fracCutOff=0.001;
   o.radioVal=0;
   o.fracPlot=1;
   obj=o;



end
if nargin==1
   o=obj;
   o.Title='Test';o.Egrain1=10;o.Imax1=250;o.Isize=1000;...
      o.Emax2=500000;o.Idum=1360436544;o.Punits='AtM';...
      o.Eunits='KCAL';o.Rotatunits='amua';o.Temp=2500;o.Tvib=2500;...
      o.Np=4;o.PP=[1 10 .1 100];o.NWells=6;o.NProds=1;
   o.IMol=1:7;o.MolName={'A','B','C','D','E','F','G'};...
      o.HMol=[0,63.93,75.97,44.87,31.31,...
      43.85,17];o.MolMom=[1305.3651,724.6828,1807.7228,1194.9234,...
      1051.6413,1392.5259];o.Molsym=ones(1,6);o.Molele=2*ones(1,6);...
```

```
         o.Molopt=[1 2*ones(1,5)];o.SigM=3.47;o.EpsM=114;o.AmuM=40;...
         o.Amu=193;o.Mol=1:6;o.Sig=7.01*ones(1,6);o.Eps=786.3*ones(1,6);...
         o.Itype=ones(1,6);o.DC=[260*ones(6,1) zeros(6,7)];...
         o.LJQM={'LJ','LJ','LJ','LJ','LJ','LJ'};o.NForward=9;...
         o.MolWell=[1 1 1 2 3 4 4 5 6];o.Ito=[2 3 4 5 6 5 6 7 7];
      o.TS={'ABTS','ACTS','ADTS','BETS','CFTS','DETS','DFTS','EGTS','FGTS'};
      o.RR=[1212.482 1533.09 1237.735 1129.445 1593.490 1150.376 ...
         1292.775 1094.469 1413.4];o.J=ones(1,9);o.Qel=2*ones(1,9);
      o.L=2*ones(1,9);o.AA=1e16*ones(1,9);
      o.EE=[65.82 83.29 48.55 4.59 7.13 6.99 12.7 2.35 1.47];
      rev={'rev','rev','rev','rev','rev','rev','rev','rev','rev'};
      notun={'TUN','NOTUN','NOTUN','TUN','NOTUN','notun','NOTUN',...
         'NOTUN','noTUN'};
      o.ImFreq(4)=1212;o.ImFreq(6)=546.7;
      fast={'FAST','Fast','FAST','slow','FAST','FAST','fast','FAST','FAST'};
      cent={'centx','centx','centx','centx','centx','centx','centx',...
         'centx','centx'};
      sum1={'sum','sum','sum','sum','sum','sum','sum','sum','sum'};
      o.KeyWords=[rev' notun' fast' cent' sum1'];
      o.CharFreq(4)=1221.1;o.AveReact(4)=1e13;
      o.ImFreq(4)=123;o.ImFreq(9)=123134;
      o.BiRateCon(4)=54;o.IVREnergy(4)=2344; o.Civr(4,1:3)=[3.1 4.1 5.1];
      o.Ntrials=1e5;o.Tspec='TIME';o.Tread=3e-10;o.KeyTemp='THERMAL';
      o.Molinit=1;o.IR=7;o.Einit=0;o.DensLoc='Unknown';
      o.OutFileLoc='C:\Users\David Edwards\Desktop\Matlab Input reading'; o.OutSave=0;
      o.GraphToggle=0;o.PressureNumber=1;o.Status='Not Ran';
      o.StatusChange=' ';o.runTime=' ';
      obj=o;
   end
end

function [FlagIvr,FlagTun]=checktun(obj,check)
   %Check for Tunneling or IVR keyword and return results
   FlagIvr=0;
   FlagTun=0;
   for i=1:5
      if isequal(upper(check{i}),'TUN')
         FlagTun=1;
      end
      if isequal(upper(check{i}),'SLOW')
         FlagIvr=1;
      end
   end
end

function updateN(obj,h,d)
   %Save and then update the data form, used to update the form
   %when NWells,NProds, or NForward is changed.
   obj.saveDataForm;
```

```
    close(obj.hFormFigure);
    obj.seeDataForm(2);
end

function saveCloseForm(obj)
    %Save and close Data form
    %obj=obj.saveDataForm();
    close(obj.hFormFigure);
    obj.hSet.getMainScreen


end

function hCopy(new,old,oldName)
    %Used with the copy function in MultiwellSet.  This takes the
    %values from the old Case and adds it to this new case.
    p=fieldnames(new);
    for i=1:59
        new.(p{i})=old.(p{i});
    end
    new.(p{90})=old.(p{90});
    new.Title=oldName;
end

function getDensData(obj)
    %Get location of the DensData folder
    saveDir=uigetdir;
    if ~(saveDir==0)
        obj.DensLoc=saveDir;
        set(obj.hData(obj.DensDataIndex),'String',saveDir);
    end
end

function getOutLoc(obj)
    %Get location of folder where multiwell output files will be
    %saved
    saveDir=uigetdir;
    if ~(saveDir==0)
        obj.OutSave=1;
        obj.OutFileLoc=saveDir;
        set(obj.hData(obj.DensDataIndex+1),'String',saveDir);
    end
end

function cancelOutLoc(obj)
    %Cancel save multiwell output files
    obj.OutFileLoc='Will Not Save Output Files';
    obj.OutSave=0;
    set(obj.hData(obj.DensDataIndex+1),'String',obj.OutFileLoc);
```

```
end

function fitUpdate(o)
   %Called when fit is updated on the results page
   tempStart=round(str2num(get(o.hfitL(1),'String')));
   tempCut=round(str2num(get(o.hfitL(2),'String')));
   stop=0;
   if tempStart>=tempCut
      stop=1;
   end
   if tempStart<0
     stop=1;
   end
   if tempCut>101
      stop=1;
   end

   if stop==0
     o.fitStart(o.PressureNumber)=tempStart;
     o.fitCut(o.PressureNumber)=tempCut;
     o.calcFit;
     h=findobj(o.hResultsFigure);
     delete(h(2:end));
     o.getResultsForm

   end

end

function changePanel(o,h,d)
   val=get(h,'Value');
   set(o.hDispPanel(o.hDispValue),'Visible','off');
   set(o.hDispPanel(val),'Visible','on');
   o.hDispValue=val;
   if (val==3 || val==4 || val==5)
      figLoc=get(o.hFormFigure,'Position');
      set(o.hSlider,'SliderStep',[.1 figLoc(4)/(1-o.panelH(val))]);
      set(o.hSlider,'Visible','on');
   else
      set(o.hSlider,'Visible','off');
   end
end

function moveSlider(o,h,d)
  figLoc=get(o.hFormFigure,'Position');
  pos=get(o.hDispPanel(o.hDispValue),'Position');
  gap=1-o.panelH(o.hDispValue)-figLoc(4);
  val=get(o.hSlider,'Value');
  set(o.hDispPanel(o.hDispValue),'Position',[pos(1),(1-val)*gap,pos(3),pos(4)]);
```

```
end

function updateCutOff(o)
   o.fracCutOff=str2double(get(o.hCutOff,'String'));
   [frac,names] = o.getSpeciesFraction;
   if length(names)<o.fracPlot
     o.fracPlot=1;
   end
   if o.radioVal==1
       names{o.fracPlot}=[names{o.fracPlot} '***'];
   end
   names=[names, 'tot'];
   frac=[frac, sum(frac)];

   ScSize=get(0,'MonitorPositions');
   figHt=round(ScSize(1,4)*.8);
   figWd=round(ScSize(1,3)*.7);

   dataFrac=[names' num2cell(frac')];
   if ishandle(o.hTableCutOff)
      delete(o.hTableCutOff);
   end
   o.hTableCutOff=uitable('Parent',o.hResDataPanel,...
      'Data',dataFrac,...
      'ColumnName','Name',...
      'Visible','off',...
      'ColumnWidth',{50,60});
   extent=get(o.hTableCutOff,'Extent');
   set(o.hTableCutOff,'Position',[175 figHt-extent(4)-130 extent(3:4)],...
      'Visible','on');
end

function moveFit(o,dir)
   data=get(o.hTableCutOff,'Data');
   sz=size(data);
   N=sz(1)-1;
   o.fracPlot=mod(o.fracPlot+dir,N);
   if o.fracPlot==0
      o.fracPlot=N;
   end
   if ishandle(o.hFracPlot)
      set(o.hFracPlot,'Visible','off');
   end
   hold on
  %Change if quadratic or linear
   %o.hFracPlot=plot(o.hAxes,o.OutTime,exp(polyval(o.fracFit(o.fracPlot,:),...
   %    o.OutTime)));
   o.hFracPlot=plot(o.hAxes,o.OutTime,polyval(o.fracFit(o.fracPlot,:),...
      o.OutTime));
```

```
            o.updateCutOff;
        end

        writeInput(obj)
        obj=saveDataForm(obj)
        getResults(obj,FileName);
        getResultsForm(obj);
        fullScreenPlot(obj);
        fullScreenData(obj);
        readInDat(obj,fileName);
        list=seeDataForm(obj,status);
        calcFit(obj);
        EnergyGraph(obj);
        [h,d]=getSpeciesFraction(o);
    end

    methods(Static)
        %Used to find the r2 values for the fits used.
        function r2=regress(P,x,y,change)
            if nargin==3
                SStot=sum((y-mean(y)).^2);
                SSerr=sum((y-polyval(P,x)).^2);
                r2=1-SSerr/SStot;
            else
                SStot=sum((y-mean(y)).^2);
                SSerr=sum((y-(P(1)-P(2)*log(x)-P(3)*x)).^2);
                r2=1-SSerr/SStot;
            end

        end
    end

end




function calcFit(o)
%CALCFIT Calculate value for fit
st=o.fitStart(1);
en=o.fitCut(1);
ind=st:en;
for i=1:o.NProds+1

    if i==1
        o.fitP(:,i)=polyfit(o.OutTime(ind,1),log(o.PopFrac(ind,o.Molinit,1)),1);
        o.k1stOrder(i)=-o.fitP(1,i);
        o.k1stOrderR2(i)=o.regress(o.fitP(:,i),o.OutTime(ind,1),log(o.PopFrac(ind,o.Molinit,1)));
        o.MaxError(i)=100*max(max(o.PopFracError(ind,o.Molinit,1)./o.PopFrac(ind,o.Molinit,1)));
```

```
    else
        loc=o.NWells+i-1;
        fun=@(x,xdata) x/o.k1stOrder(1)*(1-exp(-o.k1stOrder(1).*xdata));
        opt=optimset('MaxFunEvals',200,'TolFun',1e-18);
        fail=false;
        try
            [out,res]=lsqcurvefit(fun,1e3,o.OutTime(ind,1),o.PopFrac(ind,loc,1),10,1e13,opt);
        catch
            fail=true;
            o.k1stOrder(i)=0;
            o.k1stOrderR2(i)=0;
            o.MaxError(i)=100;
        end
        if fail==false
            %       o.fitP(:,i)=polyfit(o.OutTime(ind,1),log(1-o.PopFrac(ind,loc,1)),1);
            o.k1stOrder(i)=out;
            o.k1stOrderR2(i)=res;
            o.MaxError(i)=100*max(max(o.PopFracError(ind,loc,1)./o.PopFrac(ind,loc,1)));
        end
    end

end


end




function EnergyGraph(o)
%ENERGYGRAPH Plot the energy and species fractions together in the results
%window.

h=figure;
ind=1:85;
startFit=5;
xtext=1e-8;
ytext=32000;
clear y2tickVal y1tickVal
Case=o.CaseList{4};
PopFrac=Case.PopFrac(ind,1);
Energy=Case.VibEnergy(ind,1);
time=Case.OutTime(ind);
name=Case.MolName{1};
name='1';
tickNum=round(abs(log10(min(PopFrac))))+1;
sizeE=floor(log10(max(Energy)))-2;
EnergyStep=round(max(Energy)/(tickNum-1)/10^(sizeE))*10^sizeE;
for i=1:tickNum
```

```
    y1tickVal(i)=10^-(tickNum-i);
    y2tickVal(i)=(i-1)*EnergyStep;

end
figure(3)
[AX,h1,h2]=plotyy(time,PopFrac,time,Energy,'semilogy','plot');
set(AX(1),'YLim',[min(PopFrac)*.1 1],'Box','off','XLim',[time(1) time(end)])
set(AX(1),'YTick',y1tickVal,'FontSize',11,'FontWeight','bold')
set(AX(2),'YTick',y2tickVal,'FontSize',11,'FontWeight','bold');
set(AX(2),'YTickLabel',sprintf('%d|',y2tickVal));
set(AX(2),'XLim',[time(1) time(end)],'YLim',[0 max(Energy)]);
set(AX(2),'XAxisLocation','top','XTickLabel',[]);
set(AX(1),'XTickLabel',sprintf('%.2g|',get(AX(1),'XTick')))
set(get(AX(1),'Ylabel'),'String',['Species ' name ' Fraction'],'FontSize',22);
set(get(AX(2),'Ylabel'),'String','Vibrational Energy','FontSize',22);
title(['Decay of Species ' name ' with time, T=' num2str(Case.Temp) ' K'],'FontSize',23);
xlabel('Time (sec)')
set(h1,'LineWidth',2,'Marker','o','LineStyle','none')
set(h2,'LineWidth',1)
fitdata=PopFrac(startFit:end);
fittime=time(startFit:end);
P=polyfit(fittime,log(fitdata),1);
plottime=time(1):(time(end)-time(1))/1000:time(end);
fitresults=exp(P(2))*exp(plottime*P(1));
hold on
h3=semilogy(AX(1),plottime,fitresults,'r','LineWidth',2);
hLegend=legend([h1 h2 h3],[' ' name ' Fraction, 1 atm'],' Vibrational Energy'...
    ,' Fit to Linear part');
set(hLegend,'Box','off')
textuse=['y=' sprintf('%.3G',exp(P(2))) '*e^{' sprintf('%.3G',P(1)) '*t}'];
h1text=text(xtext,ytext,textuse,'FontSize',13);
set(h1text,'Parent',AX(2),'Color',[1 0 0]);
hold off
ktext=['k_\infty =' sprintf('%.3G',Case.Kinf(1))];
h2text=text(xtext/2,ytext*1.9,ktext);
set(h2text,'Parent',AX(2),'FontSize',14);
text3=['k(Thermal)=' sprintf('%.3G',-P(1)) ' s^-^1'];
text4=['k(chem act=' sprintf('%.3G',exp(P(2))) '*k_\infty= '...
    sprintf('%.3G',exp(P(2))*Case.Kinf(1))];
h3text=text(xtext/4,ytext/4,text3,'FontSize',14);
h4text=text(xtext/4,ytext/8,text4,'FontSize',14);
set(h3text,'Parent',AX(2));
set(h4text,'Parent',AX(2));
end
```

```
function fullScreenData(o)
%FULLSCREENDATA displays a full screen of the population fractions from the
%button on getResultsForm
%%%%%%%%%%%%%%%%%%%%Setup figure
ScSize=get(0,'MonitorPositions');
figHt=round(ScSize(1,4)*.7);
figWd=round(ScSize(1,3)*.7);
hFull=figure('Units','pixels',...
    'CloseRequestFcn',@(h,d) eval('delete(hFull);o.getResultsForm'),...
    'Visible','off');
%%%%%%%%%%%%%%%%%%%%Setup uitable
hTable=uitable('Parent',hFull,...
    'Units','pixels',...
    'Data',[o.OutTime(:,o.PressureNumber) o.PopFrac(:,:,o.PressureNumber)],...
    'ColumnName',['Time(sec)' o.MolName]);
extent=get(hTable,'Extent');
extent(3)=extent(3)+40;
if extent(4)>ScSize(1,4)*.85
    extent(4)=ScSize(1,4)*.85;
end

if extent(3)>ScSize(1,3)*.95
    extent(3)=ScSize(1,3)*.95;
end

set(hTable,'Position',extent);
extent(2)=40;
set(hFull,'Position',extent,...
    'Visible','on');
%%%%%%%%%%%%%%%%%%%%Do it again, for some reason the extent changes... If
%%%%%%%%%%%%%%%%%%%%you don't do it again, the table is not the right size,
%%%%%%%%%%%%%%%%%%%%I'm not sure why.
extent=get(hTable,'Extent');
extent(3)=extent(3)+40;
if extent(4)>ScSize(1,4)*.85
    extent(4)=ScSize(1,4)*.85;
end

if extent(3)>ScSize(1,3)*.95
    extent(3)=ScSize(1,3)*.95;
end

set(hTable,'Position',extent);
extent(2)=40;
set(hFull,'Position',extent,...
    'Visible','on');

end
```

```
function fullScreenPlot(o)
%GETFULLSCREENPLOT will display a full screen version of the plot in
%getResultsForm

hFull=figure('Units','normalized',...
    'Position',[0 .05 .95 .85],...
    'CloseRequestFcn',@(h,d) eval('delete(hFull);o.getResultsForm'));
set(o.hAxes,'Parent',hFull,...
   'Units','normalized',...
   'Position',[.05 .05 .9 .9]);
legend(o.hAxes,'Location','Best')
 end
```

```
function writeInput(obj)
%WRITEINPUT This function takes the Cases muliwell data values and creates
%the properely formatted multiwell.dat file and puts it in the same
%folder as the mexMulti function.  The line numbers are the muliwell.dat
%line numbers

%%%%%%%%%%%%%%%%%%%%%%%Find File Location and open file
o=obj;
if o.largeNtrials==0
    fileLocation=fileparts(which('mexMulti'));
elseif o.largeNtrials==1
    fileLocation=fileparts(which('mexMultiLargeTrials'));
end
Fid=fopen(fullfile(fileLocation,'multiwell.dat'),'wt');
%%%%%%%%%%%%%%%%%%%%%%%Write out lines
fprintf(Fid,'%s\n',o.Title);   %Line 1
fprintf(Fid,'%i\t',[o.Egrain1 o.Imax1 o.Isize o.Emax2 o.Idum]);fprintf(Fid,'\n'); %Line 2
fprintf(Fid,'%s\t', ['''' upper(o.Punits) '''' ], ['''',upper(o.Eunits), '''']...%Line 3
    ,['''',upper(o.Rotatunits), '''']);fprintf(Fid,'\n');
fprintf(Fid,'%g\t',o.Temp,o.Tvib);fprintf(Fid,'\n');    %Line 4
fprintf(Fid,'%i\n',o.Np);                              %Line 5
fprintf(Fid,'%g\t',o.PP(1:o.Np));fprintf(Fid,'\n');             %Line 6
fprintf(Fid,'%i\t',o.NWells,o.NProds);fprintf(Fid,'\n');%Line 7
for i=1:o.NWells                                       %Line 8
    fprintf(Fid,'%i\t',o.IMol(i));fprintf(Fid,'%s\t',['''' o.MolName{i} '''']);
    fprintf(Fid,'%.4f\t',o.HMol(i),o.MolMom(i));
    fprintf(Fid,'%g\t',o.Molsym(i),o.Molele(i),o.Molopt(i));
    fprintf(Fid,'\n');
```

```
end
for i=(1+o.NWells):(o.NProds+o.NWells)                  %Line 9
   fprintf(Fid,'%i\t',o.IMol(i));fprintf(Fid,'%s\t',['''' o.MolName{i} '''']);
   fprintf(Fid,'%.4f\n',o.HMol(i));
end
fprintf(Fid,'%.3f\t',o.SigM,o.EpsM,o.AmuM,o.Amu);fprintf(Fid,'\n');   %Line 10
for i=1:o.NWells                                        %Line 11
   fprintf(Fid,'%i\t',o.Mol(i));
   fprintf(Fid,'%.3f\t',[o.Sig(i) o.Eps(i)]);
   fprintf(Fid,'%i\t',o.Itype(i));fprintf(Fid,'%.3f\t',o.DC(i,:));
   fprintf(Fid,'\n');
   fprintf(Fid,'%s\n',['''' o.LJQM{i} '''']); %Line 12
end
fprintf(Fid,'%i\n',o.NForward);                         %Line 13
for i=1:o.NForward                                      %Line 14
   IVRFlag=0;
   TunFlag=0;
   fprintf(Fid,'%i\t',o.MolWell(i),o.Ito(i));
   fprintf(Fid,'%s\t',['''' o.TS{i} '''']);
   fprintf(Fid,'%.4f\t',o.RR(i));
   fprintf(Fid,'%i\t',o.J(i),o.Qel(i),o.L(i));
   fprintf(Fid,'%.4g\t',o.AA(i));
   fprintf(Fid,'%.4f\t',o.EE(i));
   for j=1:5
      fprintf(Fid,'%s\t',['''' upper(o.KeyWords{i,j}) '''']);
      if isequal(upper(o.KeyWords{i,j}),'SLOW')
         IVRFlag=1;
      end
      if isequal(upper(o.KeyWords{i,j}),'TUN')
         TunFlag=1 ;
      end
   end
   fprintf(Fid,'\n');
   if IVRFlag==1                                        %Line 14b
     fprintf(Fid,'%s\t',['''' 'SLOW' '''']);
     fprintf(Fid,'%.4f\t',o.CharFreq(i),o.AveReact(i),o.BiRateCon(i),...
        o.IVREnergy(i),o.Civr(i,:));fprintf(Fid,'\n');
   end
   if TunFlag==1                                        %Line 14a
      fprintf(Fid,'%s\t',['''' 'TUN' '''']);
      fprintf(Fid,'%.4f\t',o.ImFreq(i));fprintf(Fid,'\n');
   end
end
fprintf(Fid,'%i\t',o.Ntrials);fprintf(Fid,'%s\t',['''' o.Tspec '''']); %Line 15
fprintf(Fid,'%g\t',o.Tread);fprintf(Fid,'%s\t',['''' o.KeyTemp '''']);
fprintf(Fid,'%g\t',o.Molinit,o.IR);fprintf(Fid,'%.4f\t',o.Einit);
fprintf(Fid,'\n');                                      %End with carriage return
fclose(Fid);
end
```

```
function getResults(o,FileName)
%GETRESULTS After a multiwell run is comleted, this function will pull out
%the data from the output files and store it in the Case.  If FileName is
%not specified it will just look at where mexMulti is and grab from there.

%%%%%%%%%%%%%%%%%%%%%Find where the mexMulti function is and open .out file.
if nargin==1
   if o.largeNtrials==0
      fileLoc=fileparts(which('mexMulti'));
   elseif o.largeNtrials==1
      fileLoc=fileparts(which('mexMultiLargeTrials'));
   end
   fIdOut=fopen(fullfile(fileLoc,'multiwell.out'));
else
   fIdOut=fopen(FileName);
end
%%%%%%%%%%%%%%%%%%%%%Extract population frac results and unimolecular rate
%%%%%%%%%%%%%%%%%%%%%constants from multiwell.out
i=0;
p=1;
FracFlag=0;
RateFlag=0;
while feof(fIdOut)==0
   tline=fgetl(fIdOut) ;

   %Detect if it is the population fractions and flag it
   if ~isempty(strfind(tline,'Time  Collisns(Mol=1)'))
      FracFlag=1;
      continue
   end

   %Look for rate constants
   if ~isempty(strfind(tline,'k(E) RATE CONSTANTS'))
      RateFlag=1;
      o.NumRates=str2double(strtok(tline));
      continue
   end

   if FracFlag==1 && ~isempty(str2num(tline))
      i=i+1;
      temp=str2num(tline);
      o.OutTime(i,p)=temp(1);
      for j=1:(o.NWells+o.NProds)
         o.PopFrac(i,j,p)=temp(3+3*(j-1));
         o.PopFracError(i,j,p)=temp(4+3*(j-1));
         o.VibEnergy(i,j,p)=temp(5+3*(j-1));
```

```
        end

        %Stop getting fractions and index pressure number
        if i==101
            FracFlag=0;
            i=0;
            p=p+1;
        end
    end
    if RateFlag==1
        i=i+1;
        if i==2
            remain=tline;
            for j=1:o.NumRates
                [token,remain]=strtok(remain,'... ');
                o.ChanIndex(j,1)=str2double(token);
                [token,remain]=strtok(remain,'... ');
                o.ChanIndex(j,2)=str2double(token);
            end
        end
        if i==15
            for j=1:o.NumRates
                [~,remain]=strtok(tline);
                temp=textscan(remain,'%n');
                o.Kinf=temp{1};
            end
        end
        if i==24
            i=0;
            RateFlag=0;
        end
    end


end
fclose(fIdOut);
%%%%%%%%%%%%%%%%%%%%Calculate assumed 1st order reaction rate for entire system
%%%%%%%%%%%%%%%%%%%%Based on 1-product.

%%%%%%Find Change in scales to use the best for fitting.

o.fitStart(1:o.Np)=1;
o.fitCut(1:o.Np)=101;
o.calcFit;

%%%%%%%%%%%%%%%%%%%%Save and backup the multiwell output files
if o.OutSave==1 && nargin==1
    %Change file names if bad tokens used
    badTokens={':' '\' '/' '*' '<' '>' '?' '|' '"'};
```

```
    toRemove=regexp(o.Title,badTokens);
    useTitle=o.Title;
    useTitle(horzcat(toRemove{:,:}))=' ';
    movefile(fullfile(fileLoc,'multiwell.array'),...
        fullfile(o.OutFileLoc,[useTitle '.array']));
    movefile(fullfile(fileLoc,'multiwell.dat'),...
        fullfile(o.OutFileLoc,[useTitle '.dat']));
    movefile(fullfile(fileLoc,'multiwell.dist'),...
        fullfile(o.OutFileLoc,[useTitle '.dist']));
    movefile(fullfile(fileLoc,'multiwell.flux'),...
        fullfile(o.OutFileLoc,[useTitle '.flux']));
    movefile(fullfile(fileLoc,'multiwell.out'),...
        fullfile(o.OutFileLoc,[useTitle '.out']));
    movefile(fullfile(fileLoc,'multiwell.rate'),...
        fullfile(o.OutFileLoc,[useTitle '.rate']));
    movefile(fullfile(fileLoc,'multiwell.sum'),...
        fullfile(o.OutFileLoc,[useTitle '.sum']));
end
end



function getResultsForm(o)
%GETRESULTSFORM Pulls up the result form for the Case.  Includes graphs and
%data and buttons for other graphs.

%%%%%%%%%%%%%%%%%%%%Plot variations
pVar={'b' 'g' 'r' 'c' 'm' 'y' 'k' 'b:' 'g:' 'r:' 'c:' 'm:' 'y:' 'k:'...
    'b-.' 'g-.' 'r-.' 'c-.' 'm-.' 'y-.' 'k-.''b--' 'g--' 'r--' 'c--'...
    'm--' 'y--' 'k--' 'b.' 'g.' 'r.' 'c.' 'm.' 'y.' 'k.' 'bo' 'go' 'ro'...
    'co' 'mo' 'yo' 'ko'};
pColor={'b' 'r' 'c' 'm' 'y' 'k' 'g'};
pSymbol={'-' ':' '-.' '--' '.' 'o'};
%%%%%%%%%%%%%%%%%%%%Setup figure
ScSize=get(0,'MonitorPositions');
figHt=round(ScSize(1,4)*.8);
figWd=round(ScSize(1,3)*.7);
if isempty(o.hResultsFigure) || ~ishandle(o.hResultsFigure)
    o.hResultsFigure=figure('MenuBar','none',...
        'NumberTitle','off',...
        'Units','normalized',...
        'Position',[.10 .15 .8 .8],...
        'Name','Matlab Multiwell Results Screen');
end
FigColor=get(o.hResultsFigure,'Color');
%%%%%%%%%%%%%%Setup Two Panels, one for data one for figure
o.hResPlotPanel=uipanel('Parent',o.hResultsFigure,...
    'Units','normalized',...
    'Position',[0 0 .7 1],...
```

```
    'BackgroundColor',FigColor);
o.hResDataPanel=uipanel('Parent',o.hResultsFigure,...
    'Units','normalized',...
    'Position',[.7 0 .3 1],...
    'BackgroundColor',FigColor);
%%%%%%%%%%%%%%%%%%%Graph population fractions and a 1st order fit to the
%%%%%%%%%%%%%%%%%%%data
o.hAxes=axes('Parent',o.hResPlotPanel,...
    'Position',[.10 .3 .8 .65]);
%%%Used for regular plot
if o.GraphToggle==0
    for i=1:(o.NWells+o.NProds)
        if i==2
            hold on
        end
        %Plot the energy and fraction on same plot
        if i==1
            [AX,h1,h2]=plotyy(o.hAxes,o.OutTime(:,o.PressureNumber),...
                o.PopFrac(:,i,o.PressureNumber),o.OutTime(:,o.PressureNumber),...
                o.VibEnergy(:,i,o.PressureNumber),'plot','plot');
        else
            h1(i)=plot(AX(1),o.OutTime(:,o.PressureNumber),...
                o.PopFrac(:,i,o.PressureNumber));
        end
        %Determine what symbol and what color should be used for the line
        ColInd=mod(i,7);
        SymInd=(i-ColInd)/7+1;
        if ColInd==0
            ColInd=7;
        end
        set(h1(i),'Color',pColor{ColInd})
        if SymInd>4
            set(h1(i),'Marker',pSymbol{SymInd});
        else
            set(h1(i),'LineStyle',pSymbol{SymInd});
        end

    end
    %Setup graph to make it look nicer.
    set(h2,'LineWidth',2)
    ytickPop=0:.1:1;
    maxEnergy=max(o.VibEnergy(:,1,o.PressureNumber));
    EnergySize=round(log10(maxEnergy));
    EnergySpace=ceil(maxEnergy/10^EnergySize)*10^(EnergySize-1);
    EnergySteps=ceil(maxEnergy/EnergySpace);
    ytickEnergy=0:EnergySpace:EnergySteps*EnergySpace;
    set(AX(1),'Box','off','XLim',[0 o.OutTime(end,o.PressureNumber)],...
        'YLim',[0 1]);
    set(AX(2),'XAxisLocation','top','XTickLabel',[],'FontWeight','bold');
```

```
    set(AX(1),'YTick',ytickPop,'YTickLabel',sprintf('%g|',ytickPop));
    set(AX(2),'YTick',ytickEnergy,'YTickLabel',sprintf('%d|',ytickEnergy));
    set(AX(2),'YLim',[0 maxEnergy],'XLim',[0 o.OutTime(end,o.PressureNumber)]);
    set(get(AX(2),'Ylabel'),'String','Vibrational Energy','FontWeight','bold');
    hold off
    ylabeltext='Population Fraction';


%%%%%Graph the Population Fraction on a Log Scale
elseif o.GraphToggle==1
    for i=1:(o.NWells+o.NProds)
        if i==2
            hold on
        end
        %Plot the energy and fraction on same plot
        if i==1
            [AX,h1,h2]=plotyy(o.hAxes,o.OutTime(:,o.PressureNumber),...
                o.PopFrac(:,i,o.PressureNumber),o.OutTime(:,o.PressureNumber),...
                o.VibEnergy(:,i,o.PressureNumber),'semilogy','plot');
        else
            h1(i)=semilogy(AX(1),o.OutTime(:,o.PressureNumber),...
                o.PopFrac(:,i,o.PressureNumber));
        end
        %Determine what symbol and what color should be used for the line
        ColInd=mod(i,7);
        SymInd=(i-ColInd)/7+1;
        if ColInd==0
            ColInd=7;
        end
        set(h1(i),'Color',pColor{ColInd})
        if SymInd>4
            set(h1(i),'Marker',pSymbol{SymInd});
        else
            set(h1(i),'LineStyle',pSymbol{SymInd});
        end

    end

    %Make Graph look nicer
    set(h2,'LineWidth',2)
    PopMin=floor(log10(1/cast(o.Ntrials,'double')));
    %Plot lines to show were fit starts and stops

    semilogy(o.hAxes,o.OutTime(o.fitStart(o.PressureNumber),o.PressureNumber)*ones(1,2),...
        [10^(PopMin) 1],'r','LineWidth',.5);
    semilogy(o.hAxes,o.OutTime(o.fitCut(o.PressureNumber),o.PressureNumber)*ones(1,2),...
        [10^(PopMin) 1],'r','LineWidth',.5);
    PopSteps=-PopMin+1;
    for i=1:PopSteps
```

```
        ytickPop(i)=10^(1-i);
    end
    ytickPop=fliplr(ytickPop);
    maxEnergy=max(o.VibEnergy(:,1,o.PressureNumber));
    EnergySize=round(log10(maxEnergy));
    EnergySpace=ceil(maxEnergy/10^EnergySize)*10^(EnergySize-1);
    EnergySteps=ceil(maxEnergy/EnergySpace);
    ytickEnergy=0:EnergySpace:EnergySteps*EnergySpace;
    set(AX(1),'Box','off','YLim',[10^PopMin 1])
    set(AX(2),'XAxisLocation','top','XTickLabel',[],'FontWeight','bold');
    set(AX(1),'YTick',ytickPop,'XLim',[0 o.OutTime(end,o.PressureNumber)]);
    set(AX(2),'YTick',ytickEnergy,'YTickLabel',sprintf('%d|',ytickEnergy));
    set(AX(2),'YLim',[0 maxEnergy],'XLim',[0 o.OutTime(end,o.PressureNumber)]);
    set(get(AX(2),'Ylabel'),'String','Vibrational Energy','FontWeight','bold');
    set(AX(1),'YTickLabelMode','auto');
    ylabeltext='Population Fraction (log scale)';
    hold off
end
%Add title's and labels to graph
set(AX(1),'YColor','k');
hYlabel=get(o.hAxes,'YLabel');
set(hYlabel,'String',ylabeltext)
hXlabel=get(o.hAxes,'XLabel');
set(hXlabel,'String','Time (sec)')
hTitle=get(o.hAxes,'Title');
%If there are less pressures, make sure that the pressurenumber isn't too
%big.
if o.PressureNumber>length(o.PP)
    o.PressureNumber=1;
end
%Add title to graph
set(hTitle,'String',['Population Fraction versus Time.  Pressure ='...
    num2str(o.PP(o.PressureNumber)) ' ' upper(o.Punits)]);
%legend(h1,o.MolName,'Location','NorthEast');


%%%%%Toggles between fitting to the decay or the growth.
if o.fitToLine==1
    fit=exp(polyval(o.fitP(:,1),o.OutTime(:,1)));
else
    %fit=1-exp(polyval(o.fitP(:,o.fitToLine),o.OutTime(:,1)));
    k=o.k1stOrder(o.fitToLine);
    kA=o.k1stOrder(1);
    fit=k/kA*(1-exp(-kA*o.OutTime(:,1)));
end
if ~isnan(o.fitP(1,o.PressureNumber))
    if o.GraphToggle==0
        hold on
        hfit=plot(o.hAxes,o.OutTime(:,o.PressureNumber),fit,'k+');
```

```
        hold on
    else
        hold on
        %Values of fit are transformed back to linear system and then the
        %semilogy function transforms it back to log system.
        hfit=semilogy(o.hAxes,o.OutTime(:,1),fit,'k+');
        hold off
    end
    molName=o.MolName;
    if o.fitToLine==1
        loc=o.Molinit;
    else
        loc=o.NWells+o.fitToLine-1;
    end
    molName{loc}=[molName{loc} '**'];
    legend([h1 hfit h2],[molName '1st Order Fit' 'Energy (cm-1)'],...
        'Location','NorthEast');

end
%%%%%%%%%%%%%%%%%%%Create k Table
kColumn(1)=o.MolName(o.Molinit);
for i=1:o.NProds
    kColumn(i+1)=o.MolName(o.NWells+i);
end

ind=1:o.NProds+1;
tData=[o.k1stOrder(ind)' o.k1stOrderR2(ind)' o.MaxError(ind)'];
    %o.fitStart(ind)' o.fitCut(ind)'];
tData=num2cell(tData)';
colWid=num2cell(65*ones(1,o.NProds+1));
o.hTable1(1)=uitable('Parent',o.hResPlotPanel,...
    'Data',tData,...
    'RowName',{'k' 'r^2' 'max error (%)' },...
    'ColumnName',kColumn,...
    'ColumnWidth',colWid,...
    'Visible','off');
extent=get(o.hTable1(1),'Extent');
set(o.hTable1(1),'Position',[5 figHt*.35*.20 extent(3:4)],...
    'Visible','on');

%%%%%%%%%%%%%%%%%%%Add Table for the unimolecular rate constants provided
%%%%%%%%%%%%%%%%%%%%by multiwell
for i=1:o.NumRates
    RowName{i}=[o.MolName{o.ChanIndex(i,1)} '  to  ' o.MolName{o.ChanIndex(i,2)}];
end
data=[RowName' num2cell(o.Kinf)];
o.hTable1(2)=uitable('Parent',o.hResDataPanel,...
    'Data',data,...
    'ColumnName','k(inf)',...
```

```
    'Visible','off',...
    'ColumnWidth',{55,'auto'});
extent=get(o.hTable1(2),'Extent');
set(o.hTable1(2),'Position',[5 figHt-extent(4)-30 extent(3:4)],...
    'Visible','on');
uicontrol('Parent',o.hResDataPanel,...
    'Position',[5 figHt-30 figWd*.3-10 20],...
    'String',['Case Title=' o.Title],...
    'FontSize',10,...
    'BackgroundColor',FigColor,...,...
    'Style','text');

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% Table of species fractions fractions
o.hCutOff=uicontrol('Parent',o.hResDataPanel,...
    'Units','normalized',...
    'Style','edit',...
    'Position',[.75 .865 .25 .03],...
    'String',num2str(o.fracCutOff));
o.hRadioButton=uibuttongroup('Parent',o.hResDataPanel,...
    'Units','pixels',...
    'Position',[175 .925*figHt 150 25],...
    'SelectionChangeFcn',@(h,d) eval('o.radioVal=mod(o.radioVal+1,2);o.updateCutOff;'));
o.hRadio(1)=uicontrol('Parent',o.hRadioButton,...
    'Style','radiobutton',...
    'String','Str',...
    'Position',[5 1 45 20]);
o.hRadio(2)=uicontrol('Parent',o.hRadioButton,...
    'Style','radiobutton',...
    'String','Curv',...
    'Position',[55 1 45 20]);


o.updateCutOff;


if o.radioVal==0
    set(o.hRadio(1),'Value',1);
    set(o.hRadio(2),'Value',0);
    if ishandle(o.hFracPlot)
        set(o.hFracPlot,'Visible','off');
    end
else
    set(o.hRadio(1),'Value',0);
    set(o.hRadio(2),'Value',1);
    hold on
    %o.hFracPlot=plot(o.hAxes,o.OutTime,exp(polyval(o.fracFit(o.fracPlot,:),o.OutTime)));
    o.hFracPlot=plot(o.hAxes,o.OutTime,polyval(o.fracFit(o.fracPlot,:),o.OutTime));
    set(o.hFracPlot,'Visible','on');
end
```

```
uicontrol('Parent',o.hResDataPanel,...
    'Units','normalized',...
    'Position',[.75 .90 .25 .03],...
    'String','Vi Pop. Frac.',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) o.fullScreenData);

uicontrol('Parent',o.hResDataPanel,...
    'Units','normalized',...
    'Position',[.51 .90 .1 .03],...
    'String','UP',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) o.moveFit(1));

uicontrol('Parent',o.hResDataPanel,...
    'Units','normalized',...
    'Position',[.64 .90 .1 .03],...
    'String','DN',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) o.moveFit(-1));

uicontrol('Parent',o.hResDataPanel,...
    'Units','normalized',...
    'Position',[.75 .83 .25 .03],...
    'String','Upd. Cut Off',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) o.updateCutOff);

%%%%%%%%%%%%%%%%%%Buttons
uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[5 5 100 20],...
    'String','Log/Linear Plot',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) eval('o.GraphToggle=mod(o.GraphToggle+1,2);o.getResultsForm'));

uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[270 5 150 20],...
    'String','Next Pressure Plot',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) eval('o.PressureNumber=mod(o.PressureNumber,o.Np)+1;o.getResultsForm'));

uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[110 5 150 20],...
    'String','Previous Pressure Plot',...
    'BackgroundColor',FigColor,...
```

```
    'CallBack',@(h,d) eval('o.PressureNumber=mod(o.PressureNumber-2,o.Np)+1;o.getResultsForm'));

uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[430 30 150 20],...
    'String','Update Fit Start and Cut',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) o.fitUpdate);

uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[590 30 100 20],...
    'Style','text',...
    'BackgroundColor',FigColor,...
    'String','Fit Start:');

o.hfitL(1)=uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[690 30 30 20],...
    'Style','edit',...
    'String',num2str(o.fitStart(o.PressureNumber)));

uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[590 5 100 20],...
    'Style','text',...
    'BackgroundColor',FigColor,...
    'String','Fit Cut:');

o.hfitL(2)=uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[690 5 30 20],...
    'Style','edit',...
    'String',num2str(o.fitCut(o.PressureNumber)));

uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[270 30 150 20],...
    'String','Change Fit Line',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) eval('o.fitToLine=mod(o.fitToLine,o.NProds+1)+1;o.getResultsForm'));

uicontrol('Parent',o.hResultsFigure,...
    'Units','pixels',...
    'Position',[430 5 150 20],...
    'String','Full Screen Plot',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) o.fullScreenPlot);
```

```
uicontrol('Parent',o.hResDataPanel,...
    'Units','normalized',...
    'Position',[.65 .01 .3 .03],...
    'String','Close Figure',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) delete(findobj(o.hResultsFigure)));
end


function [ frac,names ] = getSpeciesFraction( o )
%GETSPECIESFRACTION Summary of this function goes here
%   Detailed explanation goes here

if o.radioVal==0
    o.radioVal
    frac=o.PopFrac();
    frac=frac(end,:);
    index=frac > o.fracCutOff;
    names=o.MolName;
    names=names(index);
    frac=frac(index);

    if sum(index)==0
        o.fracPlot=0;
    end
    if isempty(o.fracPlot)
        o.fracPlot=1;
    end
    if ishandle(o.hFracPlot)
        set(o.hFracPlot,'Visible','off');
        clear o.hFracPlot;
    end
elseif o.radioVal==1
    o.radioVal
    st=o.fitStart;
    ct=o.fitCut;
    time=o.OutTime(st:ct);
    frac=o.PopFrac(st:ct,:);
    sz=size(frac);
    %changed to 1
    %N=1;
    N=2;
    xint=zeros(1,sz(2));
    o.fracFit=zeros(sz(2),N+1);
    for i=1:sz(2)
       val=frac(:,i);
       %Added ln(val)
```

```
        %P=polyfit(time,log(val),N);
        P=polyfit(time,val,N);
        o.fracFit(i,:)=P;
        %Added exp of the results.
        %xint(i)=exp(polyval(P,0));
        xint(i)=polyval(P,0);
    end
    index=xint > o.fracCutOff;
    names=o.MolName;
    names=names(index);
    frac=xint(index);
    o.fracFit=o.fracFit(index,:);

    if sum(index)==0
        o.fracPlot=0;
    end
    if isempty(o.fracPlot)
        o.fracPlot=1;
    end
    if ishandle(o.hFracPlot)
        set(o.hFracPlot,'Visible','on');
    end

end


end


function readInDat(o,fileName)
%READINDAT Reads in a muliwell.dat file and saves all values in a new Case.
%Line numbers are from muliwell.dat file
%%%%%%%%%%%%%%%%%%%Open file
fid=fopen(fileName);
temp=fgetl(fid);
tindex=strfind(temp,'!');
if ~isempty(tindex)
    temp=temp(1:tindex);
end
%%%%%%%%%%%%%%%%%%%Line 1
o.Title=strtrim(temp);
%%%%%%%%%%%%%%%%%%%%Line 2
temp1=fgetl(fid);
temp=textscan(temp1,'%d');
temp=temp{1};
o.Egrain1=temp(1);
o.Imax1=temp(2);
o.Isize=temp(3);
o.Emax2=temp(4);
```

```
o.Idum=temp(5);
%%%%%%%%%%%%%%%%%%%%Line 3
temp=textscan(fgetl(fid),'%s','delimiter',''' \t','MultipleDelimsAsOne',1);
temp1=temp{1};
o.Punits=temp1{1};
o.Eunits=temp1{2};
o.Rotatunits=temp1{3};
%%%%%%%%%%%%%%%%%%%%Line 4
temp1=fgetl(fid);
temp=sscanf(temp1,'%g',2);
o.Temp=temp(1);
o.Tvib=temp(2);
%%%%%%%%%%%%%%%%%%%%Line 5
temp1=fgetl(fid);
temp=sscanf(temp1,'%d',1);
o.Np=temp(1);
%%%%%%%%%%%%%%%%%%%%Line 6
temp1=fgetl(fid);
temp=sscanf(temp1,'%g',o.Np);
for i=1:o.Np
   o.PP(i)=temp(i);
end
%%%%%%%%%%%%%%%%%%%%Line 7
temp1=fgetl(fid);
temp=sscanf(temp1,'%d',2);
o.NWells=temp(1);
o.NProds=temp(2);
%%%%%%%%%%%%%%%%%%%%Line 8
for i=1:o.NWells
   temp1=fgetl(fid);
   temp=textscan(temp1,'%d %s %f %f %f %f %f','delimiter',''' \t','MultipleDelimsAsOne',1);
   o.IMol(i)=temp{1};
   o.MolName{i}=temp{2}{1};
   o.HMol(i)=temp{3};
   o.MolMom(i)=temp{4};
   o.Molsym(i)=temp{5};
   o.Molele(i)=temp{6};
   o.Molopt(i)=temp{7};
end
%%%%%%%%%%%%%%%%%%%%Line 9
for i=(1+o.NWells):(o.NProds+o.NWells)
   temp1=fgetl(fid);
   temp=textscan(temp1,'%d %s %f','delimiter',''' \t','MultipleDelimsAsOne',1);
   o.IMol(i)=temp{1};
   o.MolName{i}=temp{2}{1};
   o.HMol(i)=temp{3};
end
%%%%%%%%%%%%%%%%%%%%Line 10
temp1=fgetl(fid);
```

```
temp=sscanf(temp1,'%g',4);
o.SigM=temp(1);
o.EpsM=temp(2);
o.AmuM=temp(3);
o.Amu=temp(4);
%%%%%%%%%%%%%%%%%%%%Line 11
for i=1:o.NWells
    temp1=fgetl(fid);
    temp=textscan(temp1,'%d %f %f %d %f %f %f %f %f %f %f %f');
    o.Mol(i)=temp{1};
    o.Sig(i)=temp{2};
    o.Eps(i)=temp{3};
    o.Itype(i)=temp{4};
    o.DC(i,1)=temp{5};
    o.DC(i,2)=temp{6};
    o.DC(i,3)=temp{7};
    o.DC(i,4)=temp{8};
    o.DC(i,5)=temp{9};
    o.DC(i,6)=temp{10};
    o.DC(i,7)=temp{11};
    o.DC(i,8)=temp{12};
%%%%%%%%%%%%%%%%%%%%Line 12
    temp1=fgetl(fid);
    temp=textscan(temp1,'%s','delimiter',''' \t','MultipleDelimsAsOne',1);
    o.LJQM{i}=temp{1}{1};
end
%%%%%%%%%%%%%%%%%%%%Line 13
temp1=fgetl(fid);
temp=sscanf(temp1,'%d',1);
o.NForward=temp(1);
%%%%%%%%%%%%%%%%%%%%Line 14
for i=1:o.NForward
    temp1=fgetl(fid);
    temp=textscan(temp1,'%d %d %s %f %f %f %f %f %f %s %s %s %s %s',14,...
        'delimiter',''' \t','MultipleDelimsAsOne',1);
    o.MolWell(i)=temp{1};
    o.Ito(i)=temp{2};
    o.TS{i}=temp{3}{1};
    o.RR(i)=temp{4};
    o.J(i)=temp{5};
    o.Qel(i)=temp{6};
    o.L(i)=temp{7};
    o.AA(i)=temp{8};
    o.EE(i)=temp{9};
    o.KeyWords{i,1}=temp{10}{1};
    o.KeyWords{i,2}=temp{11}{1};
    o.KeyWords{i,3}=temp{12}{1};
    o.KeyWords{i,4}=temp{13}{1};
    o.KeyWords{i,5}=temp{14}{1};
```

```
    [ivrFlag,tunFlag]=o.checktun(o.KeyWords(i,:));
    if ivrFlag==1
        temp1=fgetl(fid);
        temp=textscan(temp1,'%s %f %f %f %f %f %f %f %f');
        o.CharFreq(i)=temp{2};
        o.AveReact(i)=temp{3};
        o.BiRateCon(i)=temp{4};
        o.IVREnergy(i)=temp{5};
        o.Civr(i,1)=temp{6};
        o.Civr(i,2)=temp{7};
        o.Civr(i,3)=temp{8};
    end
    if tunFlag==1
        temp1=fgetl(fid);
        temp=textscan(temp1,'%s %f');
        o.ImFreq(i)=temp{2};
    end
end
%%%%%%%%%%%%%%%%%%%Line 15
temp1=fgetl(fid);
temp=textscan(temp1,'%d64 %s %f %s %d %d %f',...
    'delimiter',''' \t','MultipleDelimsAsOne',1);
o.Ntrials=temp{1};
o.Tspec=temp{2}{1};
o.Tread=temp{3};
o.KeyTemp=temp{4}{1};
o.Molinit=temp{5};
o.IR=temp{6};
o.Einit=temp{7};

fclose(fid);

end



function [o] = saveDataForm(o)
%SAVEDATAFORM Saves all the values in the Data form GUI.  The line numbers
%are the muliwell.dat line numbers

%%%%%%%%%%%%%%%%%%%Line 1
o.Title=get(o.hData(1),'String');
%%%%%%%%%%%%%%%%%%%Line 2
o.Egrain1=str2double(get(o.hData(2),'String'));
o.Imax1=str2double(get(o.hData(3),'String'));
o.Isize=str2double(get(o.hData(4),'String'));
o.Emax2=str2double(get(o.hData(5),'String'));
o.Idum=str2double(get(o.hData(6),'String'));
%%%%%%%%%%%%%%%%%%%Line 3
```

```
o.Punits=upper(get(o.hData(7),'String'));
o.Eunits=upper(get(o.hData(8),'String'));
o.Rotatunits=upper(get(o.hData(9),'String'));
%%%%%%%%%%%%%%%%%%Line 4
o.Temp=str2double(get(o.hData(10),'String'));
o.Tvib=str2double(get(o.hData(11),'String'));
%%%%%%%%%%%%%%%%%%Line 5
o.Np=str2double(get(o.hData(12),'String'));
%o.largeNtrials=get(o.hLargeTrials,'Value');
%%%%%%%%%%%%%%%%%%Line 6
o.PP=str2num(get(o.hData(13),'String'));
%%%%%%%%%%%%%%%%%%Check that the correct number of pressures was given
if length(o.PP)~=o.Np
   error(['number of input pressures doesn''t equal number of'...
      'specified pressure'])
end
%%%%%%%%%%%%%%%%%%Save the previous NWells and NProds for reading in.
oldNWells=o.NWells;
oldNProds=o.NProds;
%%%%%%%%%%%%%%%%%%Line 7
o.NWells=str2double(get(o.hData(14),'String'));
o.NProds=str2double(get(o.hData(15),'String'));
%%%%%%%%%%%%%%%%%%Line 8
for i=1:oldNWells
   o.IMol(i)=str2double(get(o.hData(16+7*(i-1)),'String'));
   o.MolName{i}=get(o.hData(17+7*(i-1)),'String');
   o.HMol(i)=str2double(get(o.hData(18+7*(i-1)),'String'));
   o.MolMom(i)=str2double(get(o.hData(19+7*(i-1)),'String'));
   o.Molsym(i)=str2double(get(o.hData(20+7*(i-1)),'String'));
   o.Molele(i)=str2double(get(o.hData(21+7*(i-1)),'String'));
   o.Molopt(i)=str2double(get(o.hData(22+7*(i-1)),'String'));
end
Index=23+7*(oldNWells-1);
%%%%%%%%%%%%%%%%%%Line 9
for i=(oldNWells+1):(oldNProds+oldNWells)
   o.IMol(i)=str2double(get(o.hData(Index+3*(i-oldNWells-1)),'String'));
   o.MolName{i}=get(o.hData(Index+1+3*(i-oldNWells-1)),'String');
   o.HMol(i)=str2double(get(o.hData(Index+2+3*(i-oldNWells-1)),'String'));
end
%%%%%%%%%%%%%%%%%%Line 10
Index=23+(oldNWells-1)*7+3*(oldNProds);
o.SigM=str2double(get(o.hData(Index),'String'));
o.EpsM=str2double(get(o.hData(Index+1),'String'));
o.AmuM=str2double(get(o.hData(Index+2),'String'));
o.Amu=str2double(get(o.hData(Index+3),'String'));
%%%%%%%%%%%%%%%%%%Line 11 & 12

for i=1:oldNWells
   o.Mol(i)=str2double(get(o.hData(Index+4+6*(i-1)),'String'));
```

```
    o.Sig(i)=str2double(get(o.hData(Index+5+6*(i-1)),'String'));
    o.Eps(i)=str2double(get(o.hData(Index+6+6*(i-1)),'String'));
    o.Itype(i)=str2double(get(o.hData(Index+7+6*(i-1)),'String'));
    o.DC(i,1:8)=str2num(get(o.hData(Index+8+6*(i-1)),'String'));
    o.LJQM{i}=get(o.hData(Index+9+6*(i-1)),'String');
end
%%%%%%%%%%%%%%%%%%%%Expand the arrays that depend on NWells if the size is
%%%%%%%%%%%%%%%%%%%%changing.
if o.NWells>oldNWells
    new=o.NWells;
    old=oldNWells;
    dif=new-old;
    o.IMol=[o.IMol (o.IMol(end)+1):(o.IMol(end)+dif)];
    o.MolName=[o.MolName(1:old) cellstr(num2str(zeros(dif,1)))' o.MolName(old+1:end)];
    o.HMol=[o.HMol(1:old) zeros(1,dif) o.HMol(old+1:end)];
    o.MolMom=[o.MolMom(1:old) zeros(1,dif)];
    o.Molsym=[o.Molsym(1:old) zeros(1,dif)];
    o.Molele=[o.Molele(1:old) zeros(1,dif)];
    o.Molopt=[o.Molopt(1:old) zeros(1,dif)];
    o.Mol=[o.Mol (o.Mol(end)+1):(o.Mol(end)+dif)];
    o.Sig=[o.Sig(1:old) zeros(1,dif)];
    o.Eps=[o.Eps(1:old) zeros(1,dif)];
    o.Itype=[o.Itype(1:old) zeros(1,dif)];
    if old==0
        o.DC=zeros(dif,8);
    else
        o.DC=vertcat(o.DC(1:old,:),zeros(dif,8));
    end
    o.LJQM=[o.LJQM(1:old) cellstr(num2str(zeros(dif,1)))'];

end
%%%%%%%%%%%%%%%%%%%%Make sure if NWells gets smaller it doesn't steal
%%%%%%%%%%%%%%%%%%%%NProds stuff
if o.NWells<oldNWells
    new=o.NWells;
    old=oldNWells;
    o.MolName=[o.MolName(1:new) o.MolName(old+1:end)];
    o.HMol=[o.HMol(1:new) o.HMol(old+1:end)];

end
%%%%%%%%%%%%%%%%%%%%Expand arrays that depend on NProds if the new is
%%%%%%%%%%%%%%%%%%%%bigger then old
if o.NProds>oldNProds
    dif=o.NProds-oldNProds;
    old=oldNProds;
    o.IMol=[o.IMol (o.IMol(end)+1):(o.IMol(end)+dif) ];
    o.MolName=[o.MolName(1:(o.NWells+old)) cellstr(num2str(zeros(dif,1)))'];
    o.HMol=[o.HMol(1:(o.NWells+old)) zeros(1,dif)];
```

```
end


Index=Index+10+6*(oldNWells-1);
%%%%%%%%%%%%%%%%%%Line 13
oldNForward=o.NForward;
o.NForward=str2double(get(o.hData(Index),'String'));
%%%%%%%%%%%%%%%%%%Line 14
for i=1:oldNForward
  o.MolWell(i)=str2double(get(o.hData(Index+1+14*(i-1)),'String'));
  o.Ito(i)=str2double(get(o.hData(Index+2+14*(i-1)),'String'));
  o.TS{i}=get(o.hData(Index+3+14*(i-1)),'String');
  o.RR(i)=str2double(get(o.hData(Index+4+14*(i-1)),'String'));
  o.J(i)=str2double(get(o.hData(Index+5+14*(i-1)),'String'));
  o.Qel(i)=str2double(get(o.hData(Index+6+14*(i-1)),'String'));
  o.L(i)=str2double(get(o.hData(Index+7+14*(i-1)),'String'));
  o.AA(i)=str2double(get(o.hData(Index+8+14*(i-1)),'String'));
  o.EE(i)=str2double(get(o.hData(Index+9+14*(i-1)),'String'));
  for j=1:5
    o.KeyWords{i,j}=get(o.hData(Index+9+j+14*(i-1)),'String');
  end

  if o.OldIvr(i)==1
    OIndex=Index+16+14*(i-1);
    o.CharFreq(i)=str2double(get(o.hData(OIndex),'String'));
    o.AveReact(i)=str2double(get(o.hData(OIndex+1),'String'));
    o.BiRateCon(i)=str2double(get(o.hData(OIndex+2),'String'));
    o.IVREnergy(i)=str2double(get(o.hData(OIndex+3),'String'));
    o.Civr(i,1:3)=str2num(get(o.hData(OIndex+4),'String'));
    Index=Index+6;
  end

  if o.OldTun(i)==1
    OIndex=Index+16+14*(i-1);
    o.ImFreq(i)=str2double(get(o.hData(OIndex),'String'));
    Index=Index+2;
  end
end

%%%%%%%%%%%%%%%%%%Update matrix values if Nforward gets bigger
if o.NForward>oldNForward
  dif=o.NForward-oldNForward;
  old=oldNForward;
  o.MolWell=[o.MolWell(1:old) zeros(1,dif)];
  o.Ito=[o.Ito(1:old) zeros(1,dif)];
  o.TS=[o.TS(1:old) cellstr(num2str(zeros(dif,1)))'];
  o.RR=[o.RR(1:old) zeros(1,dif)];
  o.J=[o.J(1:old) zeros(1,dif)];
  o.Qel=[o.Qel(1:old) zeros(1,dif)];
```

```
    o.L=[o.L(1:old) zeros(1,dif)];
    o.AA=[o.AA(1:old) zeros(1,dif)];
    o.EE=[o.EE(1:old) zeros(1,dif)];
    for j=1:dif
        o.KeyWords=vertcat(o.KeyWords(1:(old+j-1),:),cellstr(num2str(zeros(5,1)))');
    end

end
%%%%%%%%%%%%%%%%%%Update supplemental for proper length

if length(o.CharFreq)<o.NForward
    dif=o.NForward-length(o.CharFreq);
    o.CharFreq=[o.CharFreq zeros(1,dif)];
    o.AveReact=[o.AveReact zeros(1,dif)];
    o.BiRateCon=[o.BiRateCon zeros(1,dif)];
    o.IVREnergy=[o.IVREnergy zeros(1,dif)];
    o.Civr=vertcat(o.Civr,zeros(dif,3));
end
if length(o.ImFreq)<o.NForward
    o.ImFreq=[o.ImFreq zeros(1,o.NForward-length(o.ImFreq))];
end
Index=Index+1+14*(oldNForward);
%%%%%%%%%%%%%%%%%%Line 15
o.Ntrials=str2double(get(o.hData(Index),'String'));
o.Tspec=get(o.hData(Index+1),'String');
o.Tread=str2double(get(o.hData(Index+2),'String'));
o.KeyTemp=get(o.hData(Index+3),'String');
o.Molinit=str2double(get(o.hData(Index+4),'String'));
o.IR=str2double(get(o.hData(Index+5),'String'));
o.Einit=str2double(get(o.hData(Index+6),'String'));
o.DensLoc=get(o.hData(Index+7),'String');
o.OutFileLoc=get(o.hData(Index+8),'String');
Index+8;
end



function o=seeDataForm(o,status)
%SEEDATAFORM Replace getDataForm.
%17-May-2012.  I believe that it is done, but a bit more testing should be
%completed to ensure that it is correct.  I have not swapped out the old
%form for this form in the MutliwellSet program.

%Jan-2013.  I am using.  It takes 7 seconds to load.  I"m going to try and
%modify the code for faster loading.  No luck.  Much faster if a smaller
%case is used, but the OH+Phenanthrene example exceeds 27 channels and 25
%intermeidates (or something like that).
if isempty(o.hFormFigure)
o.hFormFigure=figure('MenuBar','none',...
```

```
    'NumberTitle','off',...
    'Units','normalized',...
    'Position',[.05,.15,.9,.7],...
    'Color',[1 1 1],...
    'Name','Multiwell Input Data Form');
end
%%%%%%%%%%%%%%%%%%%Redraw the figure if it needs to
if ~ishandle(o.hFormFigure)
o.hFormFigure=figure('MenuBar','none',...
    'NumberTitle','off',...
    'Units','normalized',...
    'Position',[.05,.15,.9,.7],...
    'Color',[1 1 1],...
    'Name','Multiwell Input Data Form');
end
%%%%%%%%%%%%%%%%%%%Add List Box for selecting what section
list={'Run Properties','Computational Information','Well and Products','Colliders','Reaction Channels'};
FigColor=[1 1 1];
o.hListBox=uicontrol('Parent',o.hFormFigure,...
    'Style','listbox',...
    'Units','normalized',...
    'String',list,...
    'FontSize',14,...
    'BackgroundColor',FigColor,...
    'Position',[0 .1 .25 .9],...
    'Callback',@(h,d) o.changePanel(h,d));
o.hDispPanel(1)=uipanel('Parent',o.hFormFigure,...
    'Units','normalized',...
    'Position',[.25 0 .75 1],...
    'BackgroundColor',FigColor,...
    'Visible','on');
o.hDispValue=1;
o.hDispPanel(2)=uipanel('Parent',o.hFormFigure,...
    'Units','normalized',...
    'Position',[.25 0 .75 1],...
    'BackgroundColor',FigColor,...
    'Visible','off');
o.hDispPanel(3)=uipanel('Parent',o.hFormFigure,...
    'Units','normalized',...
    'Position',[.25 0 .75 1],...
    'BackgroundColor',FigColor,...
    'Visible','off');
o.hDispPanel(4)=uipanel('Parent',o.hFormFigure,...
    'Units','normalized',...
    'Position',[.25 0 .75 1],...
    'BackgroundColor',FigColor,...
    'Visible','off');
o.hDispPanel(5)=uipanel('Parent',o.hFormFigure,...
    'Units','normalized',...
```

```
    'Position',[.25 0 .75 1],...
    'BackgroundColor',FigColor,...
    'Visible','off');
o.hSlider=uicontrol('Parent',o.hFormFigure,...
    'Style','slider',...
    'Units','normalized',...
    'Position',[.985 0 .015 1],...
    'Visible','off',...
    'Value',1,...
    'CallBack',@(h,d) o.moveSlider(h,d));
%Setup organization
xstarttext=.03;
xstartinput=.58;
xlengthtext=.55;
xlengthinput=.4;
ystart=.955;
yheight=.03;
gap=.01;
biggap=4;
fontsize=11;

%%%%%%%%%%%%%%%%%%Line 1
o.hText(1)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','text',...
    'Units','normalized',...
    'String','Title:',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ystart,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(1)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','edit',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'String',o.Title,...
    'Position',[xstartinput,ystart,xlengthinput,yheight],...
    'HorizontalAlignment','left');
ycurrent1=ystart-biggap*gap-yheight;

%%%%%%%%%%%%%%%%%%Line 2
o.hText(2)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Energy grain size of first segment in arrays (Egrain1-cm^-1):',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent1,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
```

```
o.hData(2)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Egrain1),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent1,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent1-gap-yheight;

o.hText(3)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Number of elements of first segment of array (imax1): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(3)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Imax1),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-gap-yheight;

o.hText(4)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Total number of elements in array (Isize): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(4)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Isize),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-gap-yheight;

o.hText(5)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
```

```
    'String','Maximum energy of 2nd segment of double arrays (Emax2-cm^-1): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(5)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Emax2),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-gap-yheight;

o.hText(6)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Random # Seed (Integer): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);

o.hData(6)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Idum),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-biggap*gap-yheight;

%%%%%%%%%%%%%%%%%%%%%%Line 3

o.hText(7)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','text',...
    'String','Pressure Units(BAR, ATM or MCC): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent1,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(7)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','edit',...
    'String',o.Punits,...
    'Units','normalized',...
```

```
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent1,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent1=ycurrent1-gap-yheight;

o.hText(8)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','text',...
    'String','Energy Units(CM-1, KCAL, or KJOU): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent1,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(8)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','edit',...
    'String',o.Eunits,...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent1,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent1=ycurrent1-gap-yheight;

o.hText(9)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','text',...
    'String','Rot. Info (AMUA, GMCM, CM-1, MHZ, or GHZ): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent1,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(9)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','edit',...
    'String',o.Rotatunits,...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent1,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent1=ycurrent1-biggap*gap-yheight;

% %%%%%%%%%%%%%%%%%%%%%%Line 4
o.hText(10)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','text',...
    'String','Translational Temp (K): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent1,xlengthtext,yheight],...
```

```
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(10)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','edit',...
    'String',num2str(o.Temp),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent1,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent1=ycurrent1-gap-yheight;

o.hText(11)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','text',...
    'String','Vibrational Temp (K): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent1,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(11)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','edit',...
    'String',num2str(o.Tvib),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent1,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent1=ycurrent1-biggap*gap-yheight;

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%Line 5
o.hText(12)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','text',...
    'String','Number of Pressures: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent1,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(12)=uicontrol('Parent',o.hDispPanel(1),...
    'Style','edit',...
    'String',num2str(o.Np),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent1,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent1=ycurrent1-gap-yheight;
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%Line 6
o.hText(13)=uicontrol('Parent',o.hDispPanel(1),...
   'Style','text',...
   'String','List each pressure sepereated by a space: ',...
   'Units','normalized',...
   'FontSize',fontsize,...
   'Position',[xstarttext,ycurrent1,xlengthtext,yheight],...
   'HorizontalAlignment','left',...
   'BackgroundColor',FigColor);
o.hData(13)=uicontrol('Parent',o.hDispPanel(1),...
   'Style','edit',...
   'String',num2str(o.PP),...
   'Units','normalized',...
   'FontSize',fontsize,...
   'Position',[xstartinput,ycurrent1,xlengthinput,yheight],...
   'HorizontalAlignment','left');


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%Line 7
o.hText(14)=uicontrol('Parent',o.hDispPanel(3),...
   'Style','text',...
   'String','Number of Wells: ',...
   'Units','normalized',...
   'FontSize',fontsize,...
   'Position',[xstarttext,ystart,xlengthtext,yheight],...
   'HorizontalAlignment','left',...
   'BackgroundColor',FigColor);
o.hData(14)=uicontrol('Parent',o.hDispPanel(3),...
   'Style','edit',...
   'String',num2str(o.NWells),...
   'Units','normalized',...
   'Position',[xstartinput,ystart,xlengthinput,yheight],...
   'FontSize',fontsize,...
   'HorizontalAlignment','left');

ycurrent2=ystart-gap-yheight;

o.hText(15)=uicontrol('Parent',o.hDispPanel(3),...
   'Style','text',...
   'String','Number of Products: ',...
   'Units','normalized',...
   'FontSize',fontsize,...
   'Position',[xstarttext,ycurrent2,xlengthtext,yheight],...
   'HorizontalAlignment','left',...
   'BackgroundColor',FigColor);
o.hData(15)=uicontrol('Parent',o.hDispPanel(3),...
   'Style','edit',...
   'String',num2str(o.NProds),...
   'Units','normalized',...
```

```
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent2,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent2=ycurrent2-biggap*gap-yheight;

if status==2
o.hButton(1)=uicontrol('Parent',o.hDispPanel(3),...
    'Style','pushbutton',...
    'CallBack',@(h,d) o.updateN(h,d),...
    'String','Update Form',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput+xlengthinput/4,ycurrent2,xlengthinput/2,yheight],...
    'HorizontalAlignment','center');
    ycurrent2=ycurrent2-biggap*gap-yheight;
end

%%%%%%%%%%%%%%%%%%%%%%%%%%Line 8 Header

xgap=.01;
xcurrent=xstarttext;
xspace=.12;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Index #',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Well Name',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Enth. Formation',...
```

```
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Moment of Int.',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Ext. Sym. #',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Elect. Part. Func.',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','# Opt. Isom.',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%Line 8
for i=1:o.NWells
    ycurrent2=ycurrent2-gap-yheight;
    xcurrent=xstarttext;

    o.hData(16+(i-1)*7)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',num2str(o.IMol(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(17+(i-1)*7)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',o.MolName{i},...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(18+(i-1)*7)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',num2str(o.HMol(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(19+(i-1)*7)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',num2str(o.MolMom(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(20+(i-1)*7)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',num2str(o.Molsym(i)),...
```

```
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(21+(i-1)*7)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',num2str(o.Molele(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(22+(i-1)*7)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',num2str(o.Molopt(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');
end


%%%%%%%%%%%%%%%%%%%%%%%%%Line 9 Header
ycurrent2=ycurrent2-biggap*gap-yheight;
xgap=.01;
xcurrent=xstarttext;
xspace=.12;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Index #',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Prod Name',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
```

```
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(3),...
    'Style','text',...
    'String','Enth. Formation',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent2,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);


%%%%%%%%%%%%%%%%%%%%%%%%%Line 9
hDataIndex=22+(o.NWells-1)*7;
for i=(o.NWells+1):(o.NWells+o.NProds)

    ycurrent2=ycurrent2-gap-yheight;
    xcurrent=xstarttext;
    o.hData(hDataIndex+1+(i-o.NWells-1)*3)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',num2str(o.IMol(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hDataIndex+2+(i-o.NWells-1)*3)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',o.MolName{i},...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hDataIndex+3+(i-o.NWells-1)*3)=uicontrol('Parent',o.hDispPanel(3),...
        'Style','edit',...
        'String',num2str(o.HMol(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent2,xspace,yheight],...
        'HorizontalAlignment','left');
```

```
end
o.panelH(3)=ycurrent2;

hDataIndex=hDataIndex+3*(o.NProds);
LineIndex=8+o.NWells+o.NProds;
%%%%%%%%%%%%%%%%%%%%%%%%%%%Line 10
ycurrent3=ystart;
o.hText(hDataIndex+1)=uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','LJ Sigma for Collider: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent3,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+1)=uicontrol('Parent',o.hDispPanel(4),...
    'Style','edit',...
    'String',num2str(o.SigM),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent3,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent3=ycurrent3-gap-yheight;

o.hText(hDataIndex+2)=uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','LJ e/k (Kelvins), for Collider: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent3,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+2)=uicontrol('Parent',o.hDispPanel(4),...
    'Style','edit',...
    'String',num2str(o.EpsM),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent3,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent3=ycurrent3-gap-yheight;

o.hText(hDataIndex+3)=uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','Mass (g/mole) of Collider: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent3,xlengthtext,yheight],...
```

```
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+3)=uicontrol('Parent',o.hDispPanel(4),...
    'Style','edit',...
    'String',num2str(o.AmuM),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent3,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent3=ycurrent3-gap-yheight;

o.hText(hDataIndex+4)=uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','Mass (g/mole) of Reactant: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent3,xlengthtext,yheight],...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+4)=uicontrol('Parent',o.hDispPanel(4),...
    'Style','edit',...
    'String',num2str(o.Amu),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent3,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent3=ycurrent3-biggap*gap-yheight;

%%%%%%%%%%%%%%%%%%%%%%%%%%%Line 11
hDataIndex=hDataIndex+5;
%Header to Columns
xgap=.01;
xcurrent=xstarttext-.01;
xspace=.09;

uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','Index #',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent3,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(4),...
```

```
    'Style','text',...
    'String','LJ Sigma',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent3,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','LJ e/K',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent3,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','Model Type',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent3,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','8 coefficients for energy transfer model (seperated by spaces)',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent3,xspace*4.6,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace*4.6;

uicontrol('Parent',o.hDispPanel(4),...
    'Style','text',...
    'String','Coll. Type (LJ QM)',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent3,xspace*1.5,yheight],...
```

```
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);


for i=1:o.NWells
    xcurrent=xstarttext-.01;
    ycurrent3=ycurrent3-gap-yheight;
    o.hData(hDataIndex+(i-1)*6)=uicontrol('Parent',o.hDispPanel(4),...
        'Style','edit',...
        'String',num2str(o.Mol(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent3,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hDataIndex+1+(i-1)*6)=uicontrol('Parent',o.hDispPanel(4),...
        'Style','edit',...
        'String',num2str(o.Sig(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent3,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hDataIndex+2+(i-1)*6)=uicontrol('Parent',o.hDispPanel(4),...
        'Style','edit',...
        'String',num2str(o.Eps(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent3,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hDataIndex+3+(i-1)*6)=uicontrol('Parent',o.hDispPanel(4),...
        'Style','edit',...
        'String',num2str(o.ltype(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent3,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hDataIndex+4+(i-1)*6)=uicontrol('Parent',o.hDispPanel(4),...
        'Style','edit',...
```

```
        'String',num2str(o.DC(i,:)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent3,xspace*4.6,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace*4.6;

    o.hData(hDataIndex+5+(i-1)*6)=uicontrol('Parent',o.hDispPanel(4),...
        'Style','edit',...
        'String',o.LJQM{i},...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent3,xspace*1.5,yheight],...
        'HorizontalAlignment','left');
end
o.panelH(4)=ycurrent3;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%Line 13
hDataIndex=hDataIndex+6*o.NWells;
LineIndex=LineIndex+o.NWells+2;
ycurrent4=ystart;
o.hText(hDataIndex)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Number of Forward Reactions:  ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent4,xlengthtext,yheight],...
    'HorizontalAlignment','left',....
    'BackgroundColor',FigColor);
o.hData(hDataIndex)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.NForward),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent4,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent4=ycurrent4-biggap*gap-yheight;

if status==2
o.hButton(1)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','pushbutton',...
    'CallBack',@(h,d) o.updateN(h,d),...
    'String','Update Form',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput+xlengthinput/4,ycurrent4,xlengthinput/2,yheight],...
    'HorizontalAlignment','center');
    ycurrent4=ycurrent4-biggap*gap-yheight;
```

```
end

%%%%%%%%%%%%%%%%%%%%%%%%%Line 14

%Header to Columns
xgap=.005;
xcurrent=0;
xspace=.065;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Well',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Exit',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','TS Name',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Mom. Int.',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
```

```
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Ex Sym #',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Qel',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','#Opt Iso',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','AA',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
```

```
    'Style','text',...
    'String','Ets-Ewell',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Key1',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Key2',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Key3',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Key4',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
```

```
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

xcurrent=xcurrent+xgap+xspace;

uicontrol('Parent',o.hDispPanel(5),...
    'Style','text',...
    'String','Key5',...
    'Units','normalized',...
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','center',...
    'BackgroundColor',FigColor);

hDataIndex=hDataIndex+1;
LineIndex=LineIndex+1;
ivrTot=0;
tunTot=0;
o.OldTun=zeros(1,o.NForward);
o.OldIvr=o.OldTun;

for i=1:o.NForward
    xcurrent=xgap;
    ycurrent4=ycurrent4-gap-yheight;
    o.hData(hDataIndex+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
        'Style','edit',...
        'String',num2str(o.MolWell(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent4,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hDataIndex+1+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
        'Style','edit',...
        'String',num2str(o.Ito(i)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent4,xspace,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hDataIndex+2+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
        'Style','edit',...
        'String',o.TS{i},...
        'Units','normalized',...
        'FontSize',fontsize,...
```

```
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap+xspace;

o.hData(hDataIndex+3+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.RR(i)),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap+xspace;

o.hData(hDataIndex+4+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.J(i)),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap+xspace;

o.hData(hDataIndex+5+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.Qel(i)),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap+xspace;

o.hData(hDataIndex+6+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.L(i)),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap+xspace;

o.hData(hDataIndex+7+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.AA(i),'%g'),...
    'Units','normalized',...
```

```
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap+xspace;

o.hData(hDataIndex+8+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.EE(i)),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap+xspace;

for j=1:5
    o.hData(hDataIndex+8+j+(i-1)*14)=uicontrol('Parent',o.hDispPanel(5),...
        'Style','edit',...
        'String',o.KeyWords{i,j},...
        'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace,yheight],...
    'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap+xspace;
end
[ivrFlag,tunFlag]=o.checktun(o.KeyWords(i,:));
ivrTot=ivrTot+ivrFlag;
tunTot=tunTot+tunFlag;
%%%%%%%Slow supplementary Line
if ivrFlag==1
    xcurrent=2*xgap;
    ycurrent4=ycurrent4-2*gap-yheight;
    hData=hDataIndex+i*14;
    LIndex=LineIndex+i+1;
    o.OldIvr(i)=1;

    %Put up description for inputs
    uicontrol('Parent',o.hDispPanel(5),...
        'Style','text',...
        'String','Key: ',...
        'Units','normalized',...
        'FontSize',fontsize-2,...
        'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
        'BackgroundColor',FigColor,...
        'HorizontalAlignment','center');

    xcurrent=xcurrent+xgap*2+xspace*2;
```

```
uicontrol('Parent',o.hDispPanel(5),...
   'Style','text',...
   'String','Char. Freq (cm-1):',...
   'Units','normalized',...
   'FontSize',fontsize-2,...
   'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
   'BackgroundColor',FigColor,...
   'HorizontalAlignment','center');

xcurrent=xcurrent+xgap*2+xspace*2;

uicontrol('Parent',o.hDispPanel(5),...
   'Style','text',...
   'String','Ave. Freq (cm-1): ',...
   'Units','normalized',...
   'FontSize',fontsize-2,...
   'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
   'BackgroundColor',FigColor,...
   'HorizontalAlignment','center');

xcurrent=xcurrent+xgap*2+xspace*2;

uicontrol('Parent',o.hDispPanel(5),...
   'Style','text',...
   'String','Bimol k: ',...
   'Units','normalized',...
   'FontSize',fontsize-2,...
   'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
   'BackgroundColor',FigColor,...
   'HorizontalAlignment','center');

xcurrent=xcurrent+xgap*2+xspace*2;

uicontrol('Parent',o.hDispPanel(5),...
   'Style','text',...
   'String','IVR Threshold: ',...
   'Units','normalized',...
   'FontSize',fontsize-2,...
   'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
   'BackgroundColor',FigColor,...
   'HorizontalAlignment','center');

xcurrent=xcurrent+xgap*2+xspace*2;

uicontrol('Parent',o.hDispPanel(5),...
   'Style','text',...
   'String','3 coef (use spaces): ',...
   'Units','normalized',...
```

```
    'FontSize',fontsize-2,...
    'Position',[xcurrent,ycurrent4,xspace*3,yheight],...
    'BackgroundColor',FigColor,...
    'HorizontalAlignment','center');


%Put in inputs
xcurrent=2*xgap;
ycurrent4=ycurrent4-gap-yheight;

o.hData(hData)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String','SLOW',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap*2+xspace*2;

o.hData(hData+1)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.CharFreq(i)),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap*2+xspace*2;

o.hData(hData+2)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.AveReact(i),'%g'),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap*2+xspace*2;

o.hData(hData+3)=uicontrol('Parent',o.hDispPanel(5),...
    'Style','edit',...
    'String',num2str(o.BiRateCon(i),'%g'),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
    'HorizontalAlignment','left');

xcurrent=xcurrent+xgap*2+xspace*2;
```

```
    o.hData(hData+4)=uicontrol('Parent',o.hDispPanel(5),...
        'Style','edit',...
        'String',num2str(o.IVREnergy(i),'%g'),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent4,xspace*2,yheight],...
        'HorizontalAlignment','left');

    xcurrent=xcurrent+xgap*2+xspace*2;

    o.hData(hData+5)=uicontrol('Parent',o.hDispPanel(5),...
        'Style','edit',...
        'String',num2str(o.Civr(i,:)),...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent4,xspace*3,yheight],...
        'HorizontalAlignment','left');


    LineIndex=LineIndex+1;
    hDataIndex=hDataIndex+6;
    ycurrent4=ycurrent4-gap;
end

if tunFlag==1
    hIndex=hDataIndex+i*14;
    LIndex=LineIndex+i+1;
    xcurrent=xgap;
    ycurrent4=ycurrent4-2*gap-yheight;
    o.OldTun(i)=1;
    uicontrol('Parent',o.hDispPanel(5),...
        'Style','text',...
        'String','Key: ',...
        'Units','normalized',...
        'FontSize',fontsize-2,...
        'Position',[xcurrent,ycurrent4,xspace,yheight],...
        'BackgroundColor',FigColor,...
        'HorizontalAlignment','right');

    xcurrent=xcurrent+xgap+xspace;

    o.hData(hIndex)=uicontrol('Parent',o.hDispPanel(5),...
        'Style','edit',...
        'String','TUN',...
        'Units','normalized',...
        'FontSize',fontsize,...
        'Position',[xcurrent,ycurrent4,xspace,yheight],...
        'HorizontalAlignment','left');
```

```
        xcurrent=xcurrent+xgap+xspace;

        uicontrol('Parent',o.hDispPanel(5),...
            'Style','text',...
            'String','Imaginary Freq (cm-1): ',...
            'Units','normalized',...
            'FontSize',fontsize-2,...
            'Position',[xcurrent,ycurrent4,xspace*3,yheight],...
            'BackgroundColor',FigColor,...
            'HorizontalAlignment','right');

        xcurrent=xcurrent+xgap+xspace*3;

        o.hData(hIndex+1)=uicontrol('Parent',o.hDispPanel(5),...
            'Style','edit',...
            'String',num2str(o.ImFreq(i)),...
            'Units','normalized',...
            'FontSize',fontsize,...
            'Position',[xcurrent,ycurrent4,xspace,yheight],...
            'HorizontalAlignment','left');

        LineIndex=LineIndex+1;
        hDataIndex=hDataIndex+2;
        ycurrent4=ycurrent4-gap;


    end

end
hDataIndex=hDataIndex+14*o.NForward;
o.panelH(5)=ycurrent4;
%%%%%%%%%%%%%%%%%Line 15
%ycurrent5=ycurrent5-biggap*gap-yheight;
uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','# of Trials: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Ntrials,'%g'),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
```

```
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-biggap*gap-yheight;

uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','TIME/COLL: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+1)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',o.Tspec,...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-gap-yheight;

uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Max Time or # of Collisions: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+2)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Tread,'%g'),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-biggap*gap-yheight;

uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Initial Energy Distribution: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
```

```
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+3)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',o.KeyTemp,...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-gap-yheight;

uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Initial Well #: ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+4)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Molinit),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-gap-yheight;

uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Initial Product Set (for chemical activiation): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+5)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.IR),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-gap-yheight;
```

```
uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Initial energy (relative to initial well): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);
o.hData(hDataIndex+6)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',num2str(o.Einit),...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

ycurrent5=ycurrent5-biggap*gap-yheight;
%%%%%%%%%%%%%%%%%%Find DensData folder and output location
uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'String','Location of DensData Folder : ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);

    o.DensDataIndex=hDataIndex+7;
o.hData(hDataIndex+7)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',o.DensLoc,...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');



if status==2
    ycurrent5=ycurrent5-gap-yheight;
o.hButton(5)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','pushbutton',...
    'String','Get DensData Loc.',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthtext/4,yheight],...
```

```
    'CallBack',@(h,d) o.getDensData,...
    'HorizontalAlignment','center');
end

ycurrent5=ycurrent5-biggap*gap-yheight;

uicontrol('Parent',o.hDispPanel(2),...
    'Style','text',...
    'TooltipString',['Push button to specify where to save the Multiwell'...
    'output files.  The title of this case will be used with'...
    ' the standard Multiwell file extensions.  If you do not specify'...
    'a location the files will not be saved'],...
    'String','Output file save Loc(see mouse tip): ',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstarttext,ycurrent5,xlengthtext,yheight],...
    'FontWeight','light',...
    'HorizontalAlignment','left',...
    'BackgroundColor',FigColor);

o.hData(hDataIndex+8)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','edit',...
    'String',o.OutFileLoc,...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthinput,yheight],...
    'HorizontalAlignment','left');

if status==2
     ycurrent5=ycurrent5-gap-yheight;
o.hButton(3)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','pushbutton',...
    'String','Set Out. File Loc.',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput,ycurrent5,xlengthtext/4,yheight],...
    'CallBack',@(h,d) o.getOutLoc,...
    'HorizontalAlignment','center');
o.hButton(6)=uicontrol('Parent',o.hDispPanel(2),...
    'Style','pushbutton',...
    'String','Do Not Save',...
    'Units','normalized',...
    'FontSize',fontsize,...
    'Position',[xstartinput+xlengthtext/2,ycurrent5,xlengthtext/4,yheight],...
    'CallBack',@(h,d) o.cancelOutLoc,...
    'HorizontalAlignment','center');

o.hButton(4)=uicontrol('Parent',o.hFormFigure,...
    'Style','pushbutton',...
```

```
    'String','Save',...
    'Units','normalized',...
    'Position',[.03,.03,.06,.04],...
    'CallBack',@(h,d) o.saveDataForm(),...
    'HorizontalAlignment','center');
end

o.hButton(4)=uicontrol('Parent',o.hFormFigure,...
    'Style','pushbutton',...
    'String','Close',...
    'Units','normalized',...
    'Position',[.13,.03,.06,.04],...
    'CallBack',@(h,d) o.saveCloseForm(),...
    'HorizontalAlignment','center');
```

MultiwellSet class

```
classdef MultiwellSet < handle
    %MULTIWELLSET Manage multiple multiwell cases and outputs.
    %It contians the GUI's to view and manage many cases, changing input
    %parameters for multiwell.  It also contians methods to view the
    %results of the runs and to compare multiple runs.


    properties
        CaseList,hMainFigure,hMainPanel,hListBox,hStatusListBox,hMainButton,Name
        hCompareResultsFigure,hFull,hArr,hTime,GraphToggle=1;GraphToggle2=1;
        hData,arrA,arrE,r2,narrA,narrE,arrN,nr2,PressNum=1;hCrossScreen
        hButtonGroup=NaN(1,3);,CrossDensLoc=' ';CrossOutFileLoc=' ';hTable
        hRadio,hCrossPanel,hMenu,SaveLocation=[];
    end

    methods
        getMainScreen(obj)
        getCompareResults(obj)
        getCompareGraphs(obj,countP)
        getArrhenius(obj)
        getTimeSeries(obj)
        getCrossScreen(obj)
        getkinfCompareScreen(obj)
        saveCrossScreen(obj,toClose,Index)


        function obj=MultiwellSet()
            %Define name of MulitwellSet
            obj.Name='Define Name';
```

```
end

function newCase(o)
   %Create a new empty Case and add to end of Case List
   o.CaseList{end+1}=MatlabMultiwell.MultiwellCase();
   o.CaseList{end}.hSet=o;
   o.CaseList{end}.seeDataForm(2);
   o.getMainScreen;
end

function modCase(o)
   %Allows a Case to be opened and viewed.  Manages the status of
   %the case if it is after it has been run.
   Index=get(o.hListBox,'Value');
   Case=o.CaseList{Index(1)};
   Case.seeDataForm(2);
   if strcmp('Ran',Case.Status)
      Case.StatusChange='   Input: Changed';
      o.getMainScreen;
   end

end

function viewCase(o,state)
   %Just view Case without allowing changes to be made
   Index=get(o.hListBox,'Value');
   if state==1
      if length(Index)==1
         o.CaseList{Index(1)}.seeDataForm(1);
      else
         o.getCrossScreen
      end
   elseif state==2
      temp=length(get(o.hListBox,'String'));
      temp1=length(get(o.hStatusListBox,'String'));
      set(o.hListBox,'Value',1:temp);
      set(o.hStatusListBox,'Value',1:temp1);
      o.getCrossScreen

   end
end

function delCase(o)
   %Remove Case from the Case list
   Index=get(o.hListBox,'Value');
   for i=0:length(Index)-1
      o.CaseList=[o.CaseList(1:(Index(length(Index)-i)-1))...
         o.CaseList((Index(length(Index)-i)+1):end)];
   end
```

```
    o.getMainScreen;
end

function copyCase(o)
    %Allows the copying of a case.  This will copy all of the
    %multiwell input variables, it does not copy any of the
    %results.
    Index=get(o.hListBox,'Value');
    for i=1:length(Index)
        new=MatlabMultiwell.MultiwellCase();
        o.CaseList=[o.CaseList(1:(Index(i)+i-1)) {new} o.CaseList((Index(i)+i):end)];
        new.hCopy(o.CaseList{Index(i)+i-1},[o.CaseList{Index(i)+i-1}.Title ' Copy']);
        o.CaseList{Index(i)+i}.hSet=o;
        if length(Index)<2
            o.CaseList{Index(i)+i}.seeDataForm(2);
        end
    end

    o.getMainScreen;
end

function setup(o)
    %Creates a series of cases best on a master copy that varies
    %only the temperature and pressure.  Usefully in setting up a
    %large amount of runs.
    Index=get(o.hListBox,'Value');
    Master=o.CaseList{Index(1)};
    answer=inputdlg({'list pressures:','List Temperature:'},...
        'Setup values',2,{'0.01 0.1 1 10',...
        '1500 1600 1700 1800 1900 2000 2100 2200 2300 2400 2500'});
    press=str2num(answer{1});
    temps=str2num(answer{2});
    lenCases=length(o.CaseList);
    put=lenCases+1;
    for i=1:length(temps)
        for j=1:length(press)
            new=MatlabMultiwell.MultiwellCase();
            o.CaseList{put}=new;
            title=['T=' num2str(temps(i)) ' P=' num2str(press(j))];
            new.hCopy(Master,title)
            new.PP=press(j);
            new.Temp=temps(i);
            new.Tvib=temps(i);
            new.hSet=o;
            put=put+1;


        end
    end
```

```
    o.getMainScreen;
end

function saveSet(o,closeFig)
    %Saves the entire set at a specified location
    if isempty(o.SaveLocation)
        saveDir=uigetdir;
        o.SaveLocation=saveDir;
    else
        saveDir=o.SaveLocation;
    end
    if ~(saveDir==0)
        o.Name=get(o.hData(1),'String');
        saveName=[o.Name '.mat'];
        saveFile=fullfile(saveDir,saveName);
        save(saveFile,'o')
        if closeFig==1
            close(o.hMainFigure)
        end
    end
end

function saveAsSet(o)
    %Saves the entire set at a specified location
    saveDir=uigetdir;
    o.SaveLocation=saveDir;
    if ~(saveDir==0)
        o.Name=get(o.hData(1),'String');
        saveName=[o.Name '.mat'];
        saveFile=fullfile(saveDir,saveName);
        save(saveFile,'o')
    end
end

function loadSet(o)
    %Load an entire set from a specified location
    [loadName loadDir]=uigetfile;
    if ~(loadName==0)
        newSt=load(fullfile(loadDir,loadName));
        new=newSt.o;
        new.hMainFigure=o.hMainFigure;
        delete(o.hMenu);
        o=new;
        o.getMainScreen;
    end
end

function runCaseSetup(o,state)
```

```
    if state==1
        o.runCase;
    elseif state==2
        temp=length(get(o.hListBox,'String'));
        temp1=length(get(o.hStatusListBox,'String'));
        set(o.hListBox,'Value',1:temp);
        set(o.hStatusListBox,'Value',1:temp1);
        o.runCase;
    end

end

function runCase(o)
    %Runs the case by locating the mexMulti function and moving the
    %necessary files and folders to that location.
    %If you don’t have mexMulti you can replace the function call to mexMulti with
    %a system call to the multiwell executable.  If you do this you’ll need to change how
    %the program finds the executable location.  It will work.
    o.saveSet(false);
    oldDir=pwd;
    Index=get(o.hListBox,'Value');
    Len=length(Index);
    for i=1:Len
       o.CaseList{Index(i)}.Status='In Queue';
       o.CaseList{Index(i)}.StatusChange=' ';
       o.CaseList{Index(i)}.runTime=' ';
    end
    for i=1:Len
        runner=o.CaseList{Index(i)};
        if runner.largeNtrials==0
            mexLocation=fileparts(which('mexMulti'));
        elseif runner.largeNtrials==1
            mexLocation=fileparts(which('mexMultiLargeTrials'));
        end
        cd(mexLocation);
        if ~(exist(fullfile(mexLocation,'DensData'),'dir')==0)
            rmdir(fullfile(mexLocation,'DensData'),'s');
        end
        copyfile(runner.DensLoc,fullfile(mexLocation,'DensData'));
        runner.writeInput;
        runner.Status='Running';
        runner.StatusChange=' ';
        runner.runTime=' ';
        o.getMainScreen;
        pause(1);
        tic;
        if runner.largeNtrials==0
            mexMulti;
        elseif runner.largeNtrials==1
```

```
            mexMultiLargeTrials;
        end
        tocOut=toc;
        if tocOut<60
            runner.runTime=['  ' num2str(tocOut,'%.2f') ' sec'];
        elseif tocOut<3600
            runner.runTime=['   ' num2str(tocOut/60,'%.2f') ' min'];
        else
            runner.runTime=['   ' num2str(tocOut/3600,'%.2f') ' hrs'];
        end
        runner.getResults;
        runner.Status='Ran';
        runner.StatusChange='   Input: Unchanged';
        o.getMainScreen;
        o.saveSet(false);
    end
    cd(oldDir);
end

function readDat(o)
    %Read in muliwell .dat file and creates new Case to hold the
    %data.
    [loadName loadDir]=uigetfile('*.dat');
    if ~(loadName==0)
        [~,~,ext]=fileparts(loadName);
        if strcmp(ext,'.dat')
            new=MatlabMultiwell.MultiwellCase();
            o.CaseList{end+1}=new;
            new.readInDat(fullfile(loadDir,loadName));
            new.hSet=o;
            o.getMainScreen;
        end
    end
end

function seeResultsForm(o,state)
    %Show Case Result form
    Index=get(o.hListBox,'Value');
    if state==1
        if length(Index)==1
            o.CaseList{Index(1)}.getResultsForm();
        else
            o.getCompareResults;
        end
    elseif state==2
        temp=length(get(o.hListBox,'String'));
        temp1=length(get(o.hStatusListBox,'String'));
        set(o.hListBox,'Value',1:temp);
        set(o.hStatusListBox,'Value',1:temp1);
```

```
        o.getCompareResults;
    end
end

function getDensData(o,Index)
    %Get location of the DensData folder
    saveDir=uigetdir;
    if ~(saveDir==0)
        o.saveCrossScreen(0,Index);
        o.CrossDensLoc=saveDir;
        o.getCrossScreen;
    end
end

function getOutLoc(o,Index)
    %Get location of folder where multiwell output files will be
    %saved
    saveDir=uigetdir;
    if ~(saveDir==0)
        o.saveCrossScreen(0,Index);
        o.CrossOutFileLoc=saveDir;
        o.getCrossScreen;
    end
end

function moveCaseUp(o)
    Index=get(o.hListBox,'Value');
    if Index(1)~=1 && length(Index(1):Index(end))==length(Index)...
            && ~isempty(o.CaseList)
        temp=o.CaseList{Index(1)-1};
        for i=1:length(Index)
            o.CaseList{Index(i)-1}=o.CaseList{Index(i)};
        end
        o.CaseList{Index(end)}=temp;
        set(o.hListBox,'Value',Index-1);
        set(o.hStatusListBox,'Value',Index-1);
        o.getMainScreen
    end
end

function moveCaseDown(o)
    Index=get(o.hListBox,'Value');
    if Index(end)~=length(o.CaseList) && ...
            length(Index(1):Index(end))==length(Index) &&...
            ~isempty(o.CaseList)
        set(o.hListBox,'Value',Index+1)
        set(o.hStatusListBox,'Value',Index+1)
        temp=o.CaseList{Index(end)+1};
        for i=length(Index):-1:1
```

```
        o.CaseList{Index(i)+1}=o.CaseList{Index(i)};
      end
      o.CaseList{Index(1)}=temp;

      o.getMainScreen
    end
  end

  function getAllFiles(o)
    %Reads in a completed Multiwell set.  It will read in the input
    %file and the result file.  Note it will not move the multiwell
    %files to a backup location.
    [loadName loadDir]=uigetfile('*.dat');

    if ~(loadName==0)
      [~,newName,ext]=fileparts(loadName);
      if strcmp(ext,'.dat')
        new=MatlabMultiwell.MultiwellCase();
        o.CaseList{end+1}=new;
        new.readInDat(fullfile(loadDir,loadName));
        new.getResults(fullfile(loadDir,[newName '.out']));
        new.Status='Results Imported';
        new.hSet=o;
        o.getMainScreen;
      end
    end
  end

  function updCase(o)
    Index=get(o.hListBox,'Value');
    for i=1:length(Index)
      Ind=Index(i);
      Case=o.CaseList[6];
      Case.fitStart(1:Case.Np)=1;
      Case.fitCut(1:Case.Np)=50;
      Case.calcFit;
      Case.fracCutOff=.001;
      Case.radioVal=0;
      Case.fracPlot=1;
    end

  end




end
```

```
end



function getArrhenius(o)
%GETARRHENIUS Creates a new window and plot showing the Arrhenius values
%for the selected cases.  Only works if the Cases are different
%temperatures and if the pressures and numbers of pressures are the same.

%%%%%%%%%%%%%%%%%%Get Cases to compare
Index=get(o.hListBox,'Value');
Cases=o.CaseList(Index);
%%%%%%%%%%%%%%%%%%Setup up Figure
ScSize=get(0,'MonitorPositions');
figHt=round(ScSize(1,4)*.7);
figWd=round(ScSize(1,3)*.5);
if isempty(o.hArr) || ~ishandle(o.hArr)
    o.hArr=figure('MenuBar','none',...
        'NumberTitle','off',...
        'Units','normalized',...
        'Position',[.2 .2 .5 .7],...
        'Name','Matlab Multiwell Arrhenius Fit Screen');
end
FigColor=get(o.hArr,'Color');
%%%%%%%%%%%%%%%%%%Setup plot panel
hPanel=uipanel('Parent',o.hArr,...
    'Position',[0 .3 1 .7],...
    'BackgroundColor',FigColor);
%%%%%%%%%%%%%%%%%%Get k Values and Temperatures
if o.PressNum>Cases{1}.Np
    o.PressNum=1;
end
for i=1:length(Index)
    casek(i)=log(Cases{i}.k1stOrder(o.PressNum));
    caseT(i)=1/Cases{i}.Temp;
end
%%%%%%%%%%%%%%%%%%Get Arrhenius values
P=polyfit(caseT,casek,1);
o.arrE(o.PressNum)=-P(1);
o.arrA(o.PressNum)=exp(P(2));
o.r2(o.PressNum)=MatlabMultiwell.MultiwellCase.regress(P,caseT,casek);
A=[ones(length(Index),1) -log(caseT)' -caseT'];
x=lscov(A,casek');
o.narrA(o.PressNum)=exp(x(1));
o.arrN(o.PressNum)=x(2);
o.narrE(o.PressNum)=x(3);
o.nr2(o.PressNum)=MatlabMultiwell.MultiwellCase.regress(x,caseT,casek,1);
%%%%%%%%%%%%%%%%%%Setup and Plot fit and data points
```

```
hAxes=axes('Parent',hPanel);
Tinv=min(caseT):(max(caseT)-min(caseT))/100:max(caseT);
Kfit=polyval(P,Tinv);
Knfit=(x(1)-x(2)*log(Tinv)-x(3)*Tinv);
plot(hAxes,1000*Tinv,Kfit)
hold on
plot(hAxes,1000*Tinv,Knfit,'r')
plot(1000*caseT,casek,'go','LineWidth',3)
set(hAxes,'XLim',[1000*min(caseT) 1000*max(caseT)]);
title(['Arrhenius Fit, k versus 1000/T' ', Pressure=' num2str(Cases{1}.PP(o.PressNum)) ' ' Cases{1}.Punits]);
xlabel('1000/Temperature (1/K)');
ylabel('Natural Log of k');
legend('Arrhenius Fit, Form:k=A*e^(^-^E^a^/^(^R^T^)^)',...
   'Arrhenius Fit, Form:k=A*T^n*e^(^-^E^a^/^(^R^T^)^)','Values from Cases')
%%%%%%%%%%%%%%%%%%%Display Data Values
hTable=uitable('Parent',o.hArr,...
   'Data',{o.arrE(o.PressNum),o.arrA(o.PressNum),'  ',...
   o.r2(o.PressNum);o.narrE(o.PressNum),o.narrA(o.PressNum),o.arrN(o.PressNum),o.nr2(o.PressNum)},...
   'ColumnName',{'Ea/R (K)','A (1/sec)','n','r^2 value'},...
   'RowName',{'A with No T Dependence','A with T Dependence'},...
   'Visible','off');
extent=get(hTable,'Extent');
set(hTable,'Position',[10 40 extent(3:4)],...
   'Visible','on')
uicontrol('Parent',o.hArr,...
   'Style','text',...
   'Position', [10 65+extent(4) figWd-10 15],...
   'BackgroundColor',FigColor,...
   'String','The r^2 values are calculated by: 1-SSerr/SSTot',...
   'HorizontalAlignment','left');
%%%%%%%%%%%%%%%%%%%Buttons to move from different pressures.
uicontrol('Parent',o.hArr,...
   'Units','pixels',...
   'Position',[270 5 150 20],...
   'String','Next Pressure Plot',...
   'BackgroundColor',FigColor,...
   'CallBack',@(h,d) eval('o.PressNum=mod(o.PressNum,Cases{1}.Np)+1;o.getArrhenius'));
uicontrol('Parent',o.hArr,...
   'Units','pixels',...
   'Position',[110 5 150 20],...
   'String','Previous Pressure Plot',...
   'BackgroundColor',FigColor,...
   'CallBack',@(h,d) eval('o.PressNum=mod(o.PressNum-2,Cases{1}.Np)+1;o.getArrhenius'));
end


function getCompareGraphs(o,countP)
%GETCOMPAREGRAPHS Creates window to view graphs of all cases and all
%pressures in the cases.
```

```
%Plot variations
pVar={'b' 'g' 'r' 'c' 'm' 'y' 'k' 'b:' 'g:' 'r:' 'c:' 'm:' 'y:' 'k:'...
   'b-.' 'g-.' 'r-.' 'c-.' 'm-.' 'y-.' 'k-.' 'b--' 'g--' 'r--' 'c--' 'm--' 'y--' 'k--'...
   'b.' 'g.' 'r.' 'c.' 'm.' 'y.' 'k.' 'bo' 'go' 'ro' 'co' 'mo' 'yo' 'ko'};
%%%%%%%%%%%%%%%%%%Get Cases to plot
Index=get(o.hListBox,'Value');
Cases=o.CaseList(Index);
%%%%%%%%%%%%%%%%%%Determine the grid layout of graphs.
len=countP;
if sqrt(len)==round(sqrt(len))
   aWd=sqrt(len);
   aHt=sqrt(len);
else
   aHt=ceil(sqrt(len));
   aWd=floor(sqrt(len));
   if aWd*aHt<len;
      aWd=aWd+1;
   end
end
%%%%%%%%%%%%%%%%%%Create figure
if isempty(o.hFull) || ~ishandle(o.hFull)
o.hFull=figure('Units','normalized',...
   'Position',[.01 .05 .95 .85],...
   'MenuBar','none',...
   'NumberTitle','off',...
   'CloseRequestFcn',@(h,d) eval('delete(o.hFull);o.getCompareResults'));
end
%%%%%%%%%%%%%%%%%%Plot on figure using subplots
countP2=1;
for i=1:length(Index)
   Case=Cases{i};
   numPres=Case.Np;
   for j=1:numPres
      h=subplot(aWd,aHt,countP2);
      for k=1:(Case.NWells+Case.NProds)
         if o.GraphToggle==0
            semilogy(h,Case.OutTime(:,j),Case.PopFrac(:,k,j),pVar{k});
         else
            plot(h,Case.OutTime(:,j),Case.PopFrac(:,k,j),pVar{k});
         end
         if k==1
            hold on
         end
      end
      countP2=countP2+1;
      set(h,'XLim',[Case.OutTime(1) Case.OutTime(end)]);
      title(h,[Case.Title ', P=' num2str(Case.PP(j)) ' ' Case.Punits]);
      xlabel(h,'Time (sec)');
```

```
        ylabel(h,'Population Fraction')
        if countP2==2
            hLegend=legend(h,Case.MolName);
            extent=get(hLegend,'Position');
            set(hLegend,'Position',[ .01 .99-extent(4) .06 extent(4)]);
        end
        hold off
    end


end
%%%%%%%%%%%%%%%%%%%Button for toggling log on and off
uicontrol('Parent',o.hFull,...
    'Units','pixels',...
    'Position',[5 5 100 20],...
    'String','Log/Linear Plot',...
    'CallBack',@(h,d) eval('o.GraphToggle=mod(o.GraphToggle+1,2);o.getCompareGraphs(countP)'));


end




function getCompareResults(o)
%GETCOMPARERESULTS Opens the main window for comparing multiple case's
%results to oneanother.

%%%%%%%%%%%%%%%%%%%Get Cases to compare
Index=get(o.hListBox,'Value');
Cases=o.CaseList(Index);
%%%%%%%%%%%%%%%%%%%Setup Figure
ScSize=get(0,'MonitorPositions');
figHt=round(ScSize(1,4)*.6);
figWd=round(ScSize(1,3)*.6);
if isempty(o.hCompareResultsFigure) || ~ishandle(o.hCompareResultsFigure)
    o.hCompareResultsFigure=figure('MenuBar','none',...
        'NumberTitle','off',...
        'Units','normalized',...
        'Position',[.2 .2 .6 .6],...
        'Name','Matlab Multiwell Compare Results Screen');
end
FigColor=get(o.hCompareResultsFigure,'Color');
%%%%%%%%%%%%%%%%%%%Setup Panels
hPanel=uipanel('Parent',o.hCompareResultsFigure,...
    'Units','normalized',...
    'Position',[0 0 1 1],...
    'BackgroundColor',FigColor);
%%%%%%%%%%%%%%%%%%%Create uitable compring 1st order k values, Temperature
```

```
%%%%%%%%%%%%%%%%%%%%,time and other things.
countC=1;
countP=1;
while countC<=length(Index)
   numPres=Cases{countC}.Np;
   for j=1:numPres
   caseTitle{countP}=[Cases{countC}.Title ', P=' num2str(Cases{countC}.PP(j))...
         ' ' Cases{countC}.Punits];
   caseT{countP}=Cases{countC}.Temp;
   casek{countP}=Cases{countC}.k1stOrder(j);
   caser2{countP}=Cases{countC}.k1stOrderR2(j);
   caseErr{countP}=Cases{countC}.MaxError(j);
   caseTime{countP}=Cases{countC}.OutTime(end,j);
   countP=countP+1;
   end
   countC=countC+1;
end
hTable=uitable('Parent',hPanel,...
   'Data',[caseTitle' caseT' casek' caser2' caseErr' caseTime'],...
   'ColumnName',{'Case Title','T of Case','k of Case','r^2 fit value','% Frac error',...
   'Time (sec)'},...
   'Visible','off',...
   'ColumnWidth',{300 'auto'});
extent=get(hTable,'Extent');
set(hTable,'Position',[5 figHt-extent(4)-5 extent(3:4)],...
   'Visible','on');
%%%%%%%%%%%%%%%%%%%Add buttons for additional windows
uicontrol('Parent',hPanel,...
   'String','View All Graphs',...
   'Position',[(figWd-extent(3))/2+extent(3)-50 figHt*.90 100 25],...
   'Callback',@(h,d) o.getCompareGraphs(countP-1));

uicontrol('Parent',hPanel,...
   'String','Arrhenius Fit',...
   'Position',[(figWd-extent(3))/2+extent(3)-50 figHt*.90-30 100 25],...
   'Callback',@(h,d) o.getArrhenius);

uicontrol('Parent',hPanel,...
   'String','Time Series Plot',...
   'Position',[(figWd-extent(3))/2+extent(3)-50 figHt*.90-60 100 25],...
   'Callback',@(h,d) o.getTimeSeries);

uicontrol('Parent',hPanel,...
   'String','Compare k(inf)',...
   'Position',[(figWd-extent(3))/2+extent(3)-50 figHt*.90-90 100 25],...
   'Callback',@(h,d) o.getkinfCompareScreen);
end
```

```
function getCrossScreen(o)
%GETCROSSSCREEN Used to change the variables of Cases across multiple
%Cases from one screen.  Some variables will only change all of the
%selected cases to match this values, while other variables for each of the
%selected cases can be changed.

%Pressures, number of pressures, DensData location, and Output file save
%location are changes that will be the same for all of the cases.

%Temperature, Time, # of trials, and random number seed can be
%updated for each case selected.

%%%%%%%%%%%%%%%%%%%Get Cases to compare
Index=get(o.hListBox,'Value');
Cases=o.CaseList(Index);
%%%%%%%%%%%%%%%%%%%Setup Figure
ScSize=get(0,'MonitorPositions');
figHt=round(ScSize(1,4)*.8);
figWd=round(ScSize(1,3)*.4);
if isempty(o.hCrossScreen) || ~ishandle(o.hCrossScreen)
  o.hCrossScreen=figure('MenuBar','none',...
    'NumberTitle','off',...
    'Units','normalized',...
    'Position',[.3 .1 .4 .8],...
    'Name','Matlab Multiwell Input Cross Compare');
end
FigColor=get(o.hCrossScreen,'Color');
%%%%%%%%%%%%%%%%%%%Setup Panels
o.hCrossPanel=uipanel('Parent',o.hCrossScreen,...
  'Units','normalized',...
  'Position',[0 0 1 1],...
  'BackgroundColor',FigColor);
%%%%%%%%%%%%%%%%%%%Add selection for pressures
if ~ishandle(o.hButtonGroup(1))
  o.hButtonGroup(1)=uibuttongroup('Parent',o.hCrossPanel,...
    'Position',[0 .83 1 .17],...
    'BackgroundColor',FigColor);
  o.hRadio(1)=uicontrol('Parent',o.hButtonGroup(1),...
    'Style','Radio',...
    'String','Do NOT update all of the cases to match these pressures',...
    'Position',[5,figHt*.17-30,350,20],...
    'BackgroundColor',FigColor);
  o.hRadio(2)=uicontrol('Parent',o.hButtonGroup(1),...
    'Style','Radio',...
    'String','Update all of the cases to match these pressures:',...
    'Position',[5,figHt*.17-50,350,20],...
    'BackgroundColor',FigColor);
end
```

```
uicontrol('Parent',o.hButtonGroup(1),...
  'Style','text',...
  'String','Number of Pressures: ',...
  'Position',[5,figHt*.17-70,130,15],...
  'HorizontalAlignment','right',...
  'BackgroundColor',FigColor);
o.hData(2)=uicontrol('Parent',o.hButtonGroup(1),...
  'Style','edit',...
  'String',num2str(Cases{1}.Np),...
  'Position',[145,figHt*.17-70,50,15],...
  'HorizontalAlignment','left');
uicontrol('Parent',o.hButtonGroup(1),...
  'Style','text',...
  'String','List each pressure sepereated by a space: ',...
  'Position',[8,figHt*.17-90,230,15],...
  'HorizontalAlignment','right',...
  'BackgroundColor',FigColor);
o.hData(3)=uicontrol('Parent',o.hButtonGroup(1),...
  'Style','edit',...
  'String',num2str(Cases{1}.PP),...
  'Position',[238,figHt*.17-90,300,15],...
  'HorizontalAlignment','left');
%%%%%%%%%%%%%%%%%%%%Add selection for DensData Location
if ~ishandle(o.hButtonGroup(2))
  o.hButtonGroup(2)=uibuttongroup('Parent',o.hCrossPanel,...
    'Position',[0 .67 1 .15],...
    'BackgroundColor',FigColor);
  o.hRadio(3)=uicontrol('Parent',o.hButtonGroup(2),...
    'Style','Radio',...
    'String','Do NOT update all of the cases to match this File Location',...
    'Position',[5,figHt*.15-30,350,20],...
    'BackgroundColor',FigColor);
  o.hRadio(4)=uicontrol('Parent',o.hButtonGroup(2),...
    'Style','Radio',...
    'String','Update all of the cases to match this DensData File Location:',...
    'Position',[5,figHt*.15-50,350,20],...
    'BackgroundColor',FigColor);
end
uicontrol('Parent',o.hButtonGroup(2),...
  'Style','text',...
  'String','Location of DensData Folder : ',...
  'Position',[15,figHt*.15-70,150,15],...
  'HorizontalAlignment','right',...
  'BackgroundColor',FigColor);
o.hData(4)=uicontrol('Parent',o.hButtonGroup(2),...
  'Style','edit',...
  'String',o.CrossDensLoc,...
  'Position',[165,figHt*.15-70,350,15],...
  'HorizontalAlignment','left');
```

```
uicontrol('Parent',o.hButtonGroup(2),...
    'Style','pushbutton',...
    'String','Get DensData Loc.',...
    'Position',[365,figHt*.15-90,100,15],...
    'CallBack',@(h,d) o.getDensData(Index),...
    'HorizontalAlignment','center');
%%%%%%%%%%%%%%%%%%%Add Location for Saving files
if ~ishandle(o.hButtonGroup(3))
    o.hButtonGroup(3)=uibuttongroup('Parent',o.hCrossPanel,...
        'Position',[0 .49 1 .18],...
        'BackgroundColor',FigColor);
    o.hRadio(5)=uicontrol('Parent',o.hButtonGroup(3),...
        'Style','Radio',...
        'String','Do NOT update or modify any of the cases to match this File Location',...
        'Position',[5,figHt*.18-30,400,20],...
        'BackgroundColor',FigColor);
    o.hRadio(6)=uicontrol('Parent',o.hButtonGroup(3),...
        'Style','Radio',...
        'String','Update all of the cases to not save the output files',...
        'Position',[5,figHt*.18-50,350,20],...
        'BackgroundColor',FigColor);
    o.hRadio(7)=uicontrol('Parent',o.hButtonGroup(3),...
        'Style','Radio',...
        'String','Update all of the cases to save the output files at this File Location:',...
        'Position',[5,figHt*.18-70,350,20],...
        'BackgroundColor',FigColor);
end
uicontrol('Parent',o.hButtonGroup(3),...
    'Style','text',...
    'String','Location of Output File Folder : ',...
    'Position',[15,figHt*.18-90,150,15],...
    'HorizontalAlignment','right',...
    'BackgroundColor',FigColor);
o.hData(5)=uicontrol('Parent',o.hButtonGroup(3),...
    'Style','edit',...
    'String',o.CrossOutFileLoc,...
    'Position',[165,figHt*.18-90,350,15],...
    'HorizontalAlignment','left');
uicontrol('Parent',o.hButtonGroup(3),...
    'Style','pushbutton',...
    'String','Get File Save Loc',...
    'Position',[365,figHt*.18-110,100,15],...
    'CallBack',@(h,d) o.getOutLoc(Index),...
    'HorizontalAlignment','center');
%%%%%%%%%%%%%%%%%%%Insert UI Table for Other variables
%First get all data from the Cases to be looked at.
for i=1:length(Index);
    rowname{i}=i;
    name{i}=Cases{i}.Title;
```

```
    temp(i)=Cases{i}.Temp;
    RandSeed(i)=Cases{i}.Idum;
    timeORcoll{i}=Cases{i}.Tspec;
    tORcValue(i)=Cases{i}.Tread;
    trials(i)=Cases{i}.Ntrials;
    dat(i,1:6)={name{i} temp(i) RandSeed(i) timeORcoll{i} tORcValue(i) trials(i)};
end
o.hTable=uitable('Parent',o.hCrossPanel,...
    'Data',dat,...
    'Visible','off',...
    'RowName',rowname,....
    'ColumnName',{'Name of Case','Temp (K)','RandomSeed','Time/Coll',...
    'Time/Coll Value','# of Trials'});
extent=get(o.hTable,'Extent');
set(o.hTable,'Units','normalized',...
    'Position',[0,.03,1,.47],...
    'Visible','on',...
    'ColumnEditable',[true true true true true true]);

%%%%%%%%%%%%%%%%%%Add Buttons for saving
uicontrol('Parent',o.hCrossPanel,...
    'Style','pushbutton',...
    'String','Save and Close',...
    'Position',[5,5,100,20],...
    'CallBack',@(h,d) o.saveCrossScreen(1,Index),...
    'HorizontalAlignment','center');
uicontrol('Parent',o.hCrossPanel,...
    'Style','pushbutton',...
    'String','Cancel (No Save)',...
    'Position',[110,5,100,20],...
    'CallBack',@(h,d) close(o.hCrossScreen),...
    'HorizontalAlignment','center');
end


function getkinfCompareScreen(o)
%GETKINFCOMPARESCREEN Used to compare the k(inf) from Multiwell across
%different cases

%%%%%%%%%%%%%%%%%%Get Cases to compare
Index=get(o.hListBox,'Value');
Cases=o.CaseList(Index);
%%%%%%%%%%%%%%%%%%Setup Figure
ScSize=get(0,'MonitorPositions');
figHt=round(ScSize(1,4));
figWd=round(ScSize(1,3));
hkinf=figure('Units','pixels',...,...
    'Visible','off',...
    'MenuBar','none',...
```

```
    'NumberTitle','off',...
    'Name','Matlab Multiwell Compare k(inf) Screen');
FigColor=get(o.hCompareResultsFigure,'Color');
%%%%%%%%%%%%%%%%%%%Setup Panels
hPanel=uipanel('Parent',hkinf,...
    'Units','normalized',...
    'Position',[0 0 1 1],...
    'BackgroundColor',FigColor);
for i=1:length(Index)
   dat(:,i)=Cases{i}.Kinf;
   ColumnName{i}=Cases{i}.Title;
end

for i=1:Cases{1}.NumRates
    RowName{i}=[Cases{1}.MolName{Cases{1}.ChanIndex(i,1)}...
        '  to  ' Cases{1}.MolName{Cases{1}.ChanIndex(i,2)}];
end
kTable=uitable('Parent',hPanel,...
    'Data',dat,...
    'RowName',RowName,...
    'ColumnName',ColumnName,...
    'Visible','on');
set(kTable,'Units','normalized',...
    'Position',[0 0 1 1],...
    'Visible','on');
set(hkinf,'Position',[40 100 figWd*.9 figHt*.6],...
    'Visible','on');
end


function getMainScreen(o)
%GETMAINSCREEN The main screen for the MatlabMultiwell program.  Contains a
%list of all Cases and buttons to allow for the addition/modification of
%Cases.  Can run cases, and view results and save set.

%%%%%%%%%%%%%%%%%%%Setup Window, including redrawing if list changes
ScSize=get(0,'MonitorPositions');
figHt=round(ScSize(1,4)*.6);
figWd=round(ScSize(1,3)*.6);
if isempty(o.hMainFigure)
    o.hMainFigure=figure('MenuBar','none',...
        'NumberTitle','off',...
        'Units','normalized',...
        'Position',[.2 .1 .5 .6],...
        'Name','Matlab Multiwell Main Screen');
end
if ~ishandle(o.hMainFigure)
    o.hMainFigure=figure('MenuBar','none',...
        'NumberTitle','off',...
```

```
        'Units','normalized',...
        'Position',[.2 .1 .5 .6],...
        'Name','Matlab Multiwell Main Screen');
end
%%%%%%%%%%%%%%%%%%%%Setup up Menu
if isempty(o.hMenu) || ~ishandle(o.hMenu(1))
    o.hMenu(1)=uimenu('Parent',o.hMainFigure,...
        'Label','File');
    uimenu('Parent',o.hMenu(1),...
        'Label','New',...
        'Accelerator','n',...
        'Callback',@(h,d) o.newCase);
    uimenu('Parent',o.hMenu(1),...
        'Label','Open',...
        'Accelerator','o',...
        'Callback',@(h,d) o.loadSet);
    uimenu('Parent',o.hMenu(1),...
        'Label','Close',...
        'Callback',@(h,d) close(o.hMainFigure));
    uimenu('Parent',o.hMenu(1),...
        'Label','Setup',...
        'Callback',@(h,d) o.setup);
    uimenu('Parent',o.hMenu(1),...
        'Label','&Save ',...
        'Accelerator','s',...
        'Separator','on',...
        'Callback',@(h,d) o.saveSet(0));
    uimenu('Parent',o.hMenu(1),...
        'Label','Save As',...
        'Callback',@(h,d) o.saveAsSet);

    o.hMenu(2)=uimenu('Parent',o.hMainFigure,...
        'Label','View');
    uimenu('Parent',o.hMenu(2),...
        'Label','Input Parameter of Selected Jobs',...
        'Callback',@(h,d) o.viewCase(1));
    uimenu('Parent',o.hMenu(2),...
        'Label','Input Parameters of All of the Jobs',...
        'Callback',@(h,d) o.viewCase(2));
    uimenu('Parent',o.hMenu(2),...
        'Label','Results of Selected Jobs',...
        'Separator','on',...
        'Callback',@(h,d) o.seeResultsForm(1));
    uimenu('Parent',o.hMenu(2),...
        'Label','Results of All Jobs',...
        'Callback',@(h,d) o.seeResultsForm(2));

    o.hMenu(3)=uimenu('Parent',o.hMainFigure,...
        'Label','Import');
```

```
    uimenu('Parent',o.hMenu(3),...
        'Label','Multiwell.dat File',...
        'Callback',@(h,d) o.readDat);
    uimenu('Parent',o.hMenu(3),...
        'Label','All Multiwell Files',...
        'Callback',@(h,d) o.getAllFiles);

    o.hMenu(4)=uimenu('Parent',o.hMainFigure,...
        'Label','Run');
    uimenu('Parent',o.hMenu(4),...
        'Label','Run Selected Jobs',...
        'Callback',@(h,d) o.runCaseSetup(1));
    uimenu('Parent',o.hMenu(4),...
        'Label','Run All Jobs',...
        'Callback',@(h,d) o.runCaseSetup(2));
end
%%%%%%%%%%%%%%%%%%%%Making sure to save name of set if window is updated
if ~isempty(o.hData)
    if ishandle(o.hData(1))
        o.Name=get(o.hData(1),'String');
    end
end
%%%%%%%%%%%%%%%%%%%%Reseting the main panel if calling again
%%%%%%%%%%%%%%%%%%%%ValuePass is keeps the highlights on the list box at
%%%%%%%%%%%%%%%%%%%%the same spots.
if ~isempty(o.hMainPanel) && ishandle(o.hMainPanel)
    ValuePass=get(o.hListBox,'Value');
    ValuePass=ValuePass(~(ValuePass>length(o.CaseList)));
    if isempty(ValuePass)
        ValuePass=length(o.CaseList);
    end
    if ValuePass==0
        ValuePass=1;
    end
    delete(o.hMainPanel);
else
    ValuePass=1;
end
%%%%%%%%%%%%%%%%%%%%Creating main panel
FigColor=get(o.hMainFigure,'Color');
o.hMainPanel=uipanel('Parent',o.hMainFigure,...
    'Units','normalized',...
    'Position',[0 0 1 1],...
    'BackgroundColor',FigColor);
%%%%%%%%%%%%%%%%%%%%Setting up the two text boxes, one for Case name and
%%%%%%%%%%%%%%%%%%%%one for the status of the cases.
if isempty(o.CaseList)
    TextBox={'No Cases'};
    TextBoxStat={' '};
```

```
else
  for i=1:length(o.CaseList)
    TextBox{i}=o.CaseList{i}.Title;
    TextBoxStat{i}=[o.CaseList{i}.Status o.CaseList{i}.StatusChange ...
        o.CaseList{i}.runTime];
  end
end
o.hListBox=uicontrol('Parent',o.hMainPanel,...
   'Style','listbox',...
   'Units','normalized',...
   'Position',[.05 .1 .4 .8],...
   'String',TextBox,...
   'Max',100,...
   'Value',ValuePass,...
   'Callback',@(h,d) set(o.hStatusListBox,'Value',get(o.hListBox,'Value')));
o.hStatusListBox=uicontrol('Parent',o.hMainPanel,...
   'Style','listbox',...
   'Units','normalized',...
   'Position',[.45 .1 .4 .8],...
   'String',TextBoxStat,...
   'Max',100,...
   'Value',ValuePass,...
   'Callback',@(h,d) set(o.hListBox,'Value',get(o.hStatusListBox,'Value')));
%%%%%%%%%%%%%%%%%%Uicontrol items for Set name and text on window
uicontrol('Parent',o.hMainPanel,...
   'Style','text',...
   'Units','normalized',...
   'Position',[.05 .91 .45 .03],...
   'HorizontalAlignment','left',...
   'String','List of Multiwell cases associated with this set',...
   'BackgroundColor',FigColor);
uicontrol('Parent',o.hMainPanel,...
   'Style','text',...
   'Units','normalized',...
   'Position',[.05 .95 .25 .03],...
   'HorizontalAlignment','left',...
   'String','Name of Set (used to save Set): ',...
   'BackgroundColor',FigColor);
o.hData(1)=uicontrol('Parent',o.hMainPanel,...
   'Style','edit',...
   'Units','normalized',...
   'Position',[.3 .95 .3 .03],...
   'HorizontalAlignment','left',...
   'String',o.Name);
%%%%%%%%%%%%%%%%%%Uicontrols for all of the buttons.

o.hMainButton(1)=uicontrol('Parent',o.hMainPanel,...
   'Units','normalized',...
   'Position',[.87 .85 .11 .045],...
```

```
    'String','Modify Case',...
    'Callback',@(h,d) o.modCase);
o.hMainButton(2)=uicontrol('Parent',o.hMainPanel,...
    'Units','normalized',...
    'Position',[.87 .80 .11 .045],...
    'String','Copy Case',...
    'Callback',@(h,d) o.copyCase);

o.hMainButton(3)=uicontrol('Parent',o.hMainPanel,...
    'Units','normalized',...
    'Position',[.87 .75 .11 .045],...
    'String','Delete Case',...
    'Callback',@(h,d) o.delCase);

o.hMainButton(4)=uicontrol('Parent',o.hMainPanel,...
    'Units','normalized',...
    'Position',[.023 .1 .025 .37],...
    'String','D',...
    'Callback',@(h,d) o.moveCaseDown);
o.hMainButton(5)=uicontrol('Parent',o.hMainPanel,...
    'Units','normalized',...
    'Position',[.023 .53 .025 .37],...
    'String','Up',...
    'Callback',@(h,d) o.moveCaseUp);

o.hMainButton(6)=uicontrol('Parent',o.hMainPanel,...
    'Units','normalized',...
    'Position',[.87 .70 .11 .045],...
    'String','Update Case',...
    'Callback',@(h,d) o.updCase);


end


function getTimeSeries(o)
%GETTIMESERIES creates a new figure and plot by combining the selected
%cases into one large set.  Only makes sense if all of the selected cases
%have same number and same Pressures and if the temperatures are the same
%across cases.  And each case should have a different time range.

%%%%%%%%%%%%%%%%%%%Plot variations
pVar={'bo' 'go' 'ro' 'co' 'mo' 'yo' 'ko' 'b.' 'g.' 'r.' 'c.' 'm.' 'y.' 'k.'...
    'bx' 'gx' 'rx' 'cx' 'mx' 'yx' 'kx''bs' 'gs' 'rs' 'cs' 'ms' 'ys' 'ks'...
    'b*' 'g*' 'r*' 'c*' 'm*' 'y*' 'k*' 'b+' 'g+' 'r+' 'c+' 'm+' 'y+' 'k+'};
%%%%%%%%%%%%%%%%%%%Get Cases to compare
Index=get(o.hListBox,'Value');
Cases=o.CaseList(Index);
%%%%%%%%%%%%%%%%%%%Setup up Figure
```

```
ScSize=get(0,'MonitorPositions');
if isempty(o.hTime) || ~ishandle(o.hTime)
   o.hTime=figure('MenuBar','none',...
      'NumberTitle','off',...
      'Units','normalized',...
      'Position',[.01 .1 .98 .85],...
      'Name','Matlab Multiwell Time Series Screen');
end
FigColor=get(o.hTime,'Color');
%%%%%%%%%%%%%%%%%%Setup panel
hPanel=uipanel('Parent',o.hTime,...
   'Units','normalized',...
   'Position',[0 0 1 1],...
   'BackgroundColor',FigColor);
%%%%%%%%%%%%%%%%%%Get Data from all of the cases and combine together
NpCompare=Cases{1}.Np;
for i=2:length(Index)
   if NpCompare~=Cases{i}.Np
      error('Time Series compare files have different # of pressures')
   end
end
allTime=Cases{1}.OutTime(:,o.PressNum);
allFrac=Cases{1}.PopFrac(:,:,o.PressNum);
for i=2:length(Index)
  allTime=[allTime;Cases{i}.OutTime(:,o.PressNum)];
  allFrac=[allFrac;Cases{i}.PopFrac(:,:,o.PressNum)];
end
%%%%%%%%%%%%%%%%%%Plot Data.  Including ways to toggle log on and off
hAxes=axes('Parent',hPanel,...
   'Position',[.1 .12 .89 .80]);
if o.GraphToggle2==0
   for i=1:(Cases{1}.NWells+Cases{1}.NProds)
      if i==2
         hold on
      end
      plot(hAxes,allTime(:),allFrac(:,i),pVar{i});
   end
   hold off
   ylabeltext='Population Fraction';
   xlabeltext='Time (sec)';
elseif o.GraphToggle2==1
   for i=1:(Cases{1}.NWells+Cases{1}.NProds)
      if i==2
         hold on
      end
      loglog(hAxes,allTime(:),allFrac(:,i),pVar{i});
   end
   hold off
   ylabeltext='Population Fraction (log scale)';
```

```
    xlabeltext='Time (sec) (log scale)';
end
hYlabel=get(hAxes,'YLabel');
set(hYlabel,'String',ylabeltext)
hXlabel=get(hAxes,'XLabel');
set(hXlabel,'String',xlabeltext)
hTitle=get(hAxes,'Title');
set(hTitle,'String',['Population Fraction versus Time.  Pressure ='...
    num2str(Cases{1}.PP(o.PressNum)) ' ' upper(Cases{1}.Punits)]);
legend(hAxes,Cases{1}.MolName,'Location','BestOutside')
%%%%%%%%%%%%%%%%%%%Buttons
uicontrol('Parent',hPanel,...
    'Units','pixels',...
    'Position',[5 5 100 20],...
    'String','Log/Linear Plot',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) eval('o.GraphToggle2=mod(o.GraphToggle2+1,2);o.getTimeSeries'));

uicontrol('Parent',hPanel,...
    'Units','pixels',...
    'Position',[270 5 150 20],...
    'String','Next Pressure Plot',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) eval('o.PressNum=mod(o.PressNum,Cases{1}.Np)+1;o.getTimeSeries'));

uicontrol('Parent',hPanel,...
    'Units','pixels',...
    'Position',[110 5 150 20],...
    'String','Previous Pressure Plot',...
    'BackgroundColor',FigColor,...
    'CallBack',@(h,d) eval('o.PressNum=mod(o.PressNum-2,Cases{1}.Np)+1;o.getTimeSeries'));
end


function saveCrossScreen(o,toClose,Index)
%SAVECROSSSCREEN Save the values in the Cross screen window

%%%%%%%%%%%%%%%%%%%Get Cases to compare
Cases=o.CaseList(Index);
%%%%%%%%%%%%%%%%%%%Save Pressures
if o.hRadio(2)==get(o.hButtonGroup(1),'SelectedObject')
    for i=1:length(Index)
        Cases{i}.Np=str2double(get(o.hData(2),'String'));
        Cases{i}.PP=str2num(get(o.hData(3),'String'));
    end
end
%%%%%%%%%%%%%%%%%%%Save Densdata update
if o.hRadio(4)==get(o.hButtonGroup(2),'SelectedObject')
    for i=1:length(Index)
```

```
        Cases{i}.DensLoc=get(o.hData(4),'String');
    end
end
%%%%%%%%%%%%%%%%%%Save Output File Save Location
if o.hRadio(6)==get(o.hButtonGroup(3),'SelectedObject')
    for i=1:length(Index)
        Cases{i}.OutSave=0;
        Cases{i}.OutFileLoc='Will Not Save Output Files';
    end
end
if o.hRadio(7)==get(o.hButtonGroup(3),'SelectedObject')
    for i=1:length(Index)
        Cases{i}.OutSave=1;
        Cases{i}.OutFileLoc=get(o.hData(5),'String');
    end
end
%%%%%%%%%%%%%%%%%%Save Data in Table
data=get(o.hTable,'Data');
for i=1:length(Index)
    Cases{i}.Title=data{i,1};
    Cases{i}.Temp=data{i,2};
    Cases{i}.Tvib=data{i,2};
    Cases{i}.Idum=data{i,3};
    Cases{i}.Tspec=data{i,4};
    Cases{i}.Tread=data{i,5};
    Cases{i}.Ntrials=data{i,6};
end
if toClose==1
    close(o.hCrossScreen);
    o.CrossDensLoc=' ';
    o.CrossOutFileLoc=' ';
    o.getMainScreen;
end
end
```

The following lines can be used to create the mex function for MultiWell. Alternatively, instead of calling the mex function, a system call to the Fortran compiled executable can also be used. You’ll need to make sure you have set up the fortran compiler using the mex –setup command.

```
mex -output mexMulti mexMulti.F book1.f colnorm.f colstep.f datetime.f densarray.f densarrayts.f...
    dents.f denvr.f doubnterp.f doubnterp2.f eckart.f estart.f etherm.f initial.f...
    lenstr.f multiwell.f nterp.f nterp2.f pdown.f qkinf.f qkinftun.f qudint.f...
    ran1.f ratearray.f rivr.f rotunits.f rvr.f stepper.f unittest.f
```

D.2 Extract and Create Hindered Rotor Potentials

```
function [energyunits,InDeg,varname,var,cartOut,carbonCoord]=evalRelaxedScan(name,fileDir,...
    type,status)
%%Reads in the results of a Potential Energy Surface scan from Guassian.
%%It then writes the results to lamm.dat, and finds the reduced moment of
%%inertia.  The program then plots the data and the fit and allows you to
%%very the number of points untill a fit is found you like.  The data
%%points that are required for Multiwell's densum are also printed.
%Input variables:
%   name: the file name of the gaussian log and com file.  Both the
%       name.log and name.com file must be in the same folder as
%       evalRelaxedScan.
%   type: This is used to indicate if there is a relaxed scan parsing of an
%       internal rotor ('IR') or for bond dissociation ('BD')
%   status: f or s.  f if the gaussian file is incomplete, and s if it
%   succedded
%
%Output variables:
%   energyunits: a two columned matrix.  Each row is a step in the
%       rotation. The first column is in units of Kcal/mol and the second
%       column is in cm-1.
%   InDeg: is an array for the the resulting reduced moment of inertia's
%       that are obtained from lamm.
%   varname: is the list of the variable names that gaussian uses to
%       represent the different variables.  Not that important.
%   var: A 2 dimensional matrix.  The rows are the values of the variables
%       that correspond to the varname array.  The columns are each step
%       taken in the scan.
%
%Output Files Generated:
%   lamm.dat: A formatted lamm.dat file required for lamm.exe.  The program
%       overwrites the file each time it is executed.
%   lamm.out: The results of lamm.exe.  The program overwrites the file
%       each time it is executed
%   std.xyz: The standard cartesian coordiates for each rotation in .xyz
%       format.  The title also includes the energy at that time step.
%       Very useful in for viewing the results of the optimization at each
%       time step in Jmol.
%   Zout.xyz: Each step of the scan in A-matrix format.  I don't use it for
%       anything.

import RelaxedScanParsing.MichaelLS
clc
InDeg=0;
%Open the data files
```

```
fid1=fopen(fullfile(fileDir,[name '.inx']));
if fid1 == -1
   fid1=fopen(fullfile(fileDir,[name '.com1']));
end
fid2=fopen(fullfile(fileDir,[name '.log']));

%Read in the .com file and extract the information
[atom,IBond,BondVar,Iangle,AngleVar,idih,DihVar,NumAtoms,stepsize,varnI,...
   varI,varRot,sType,rType,scanVarNum]=RelaxedScanParsing.readRelaxedComFile(fid1);
%Identify the atoms which are the centers of the respecitive seperation
indexB=ismember(BondVar,varnI(varRot));
if sum(indexB)>=2
   error('line 55, too many bond breakings')
end


firstAtom=IBond(indexB);
secAtom=find(indexB)+1;


%Read in the log file and extract the results.
[Nsteps,energy,varname,var]...
   =RelaxedScanParsing.readRelaxedLogFile(fid2,sType,rType,...
   length(atom),status,scanVarNum);
if sType=='S'
   %Used if scan is used in the route section of the gaussian file.
   if ~all(strcmp(varnI(varRot),varname'))
      error('The rotation variable for scan doesn''t match');
   end
   varname=varnI;
   %Collect range of scan variables
   for i=1:Nsteps
      tvar(:,i)=varI;
      tvar(varRot,i)=var(i,1:scanVarNum);
   end
   var=tvar;
end

%Change energy to kcal/mole and wave number
%kcal/mole
energyunits(:,1)=energy*627.51;
energyunits(:,1)=energyunits(:,1)-min(energyunits(:,1));
%wave number cm-1
energyunits(:,2)=energy*219474.6314;
energyunits(:,2)=energyunits(:,2)-min(energyunits(:,2));
%leave in hartree
energyunits(:,3)=energy;
%Write output files
[cartCoord]=RelaxedScanParsing.writeFiles(atom,IBond,BondVar,Iangle,...
```

```
   AngleVar,idih,DihVar,NumAtoms,stepsize,Nsteps,var,varname,...
   energyunits,name,fileDir,varI,rType,scanVarNum);

%Run lamm.exe and read in results
if strcmp(type,'IR')
   InDeg=RelaxedScanParsing.runLamm(fileDir);
end


%Create the standard cartesian coordinate .xyz file
fid4=fopen(fullfile(fileDir,'std.xyz'),'w+');
if strcmp(type,'BD')
   fid5=fopen(fullfile(fileDir,'Bond_Len.txt'),'w+');
   fid6=fopen(fullfile(fileDir,'BondSimple.txt'),'w+');
end
for i =0:(Nsteps)
   fprintf(fid4,'%u\n',NumAtoms);
   if i==0
      fprintf(fid4,'Initial Structure: %s\n',name);
      if strcmp(type,'BD')
         fprintf(fid5,'Name: %s\n',name);
         fprintf(fid6,'Date: %s\n',date);
         fprintf(fid6,'From: %s\n',name);
         for k=1:scanVarNum
            fprintf(fid6,'%-15s',cell2mat(varnI(varRot(k))));
         end
         fprintf(fid6,'%-15s%-15s\n','kcal/mol','Hartree');
      end
      for j=1:NumAtoms
         xcart=cartCoord(Nsteps+1,(j-1)*3+1);
         ycart=cartCoord(Nsteps+1,(j-1)*3+2);
         zcart=cartCoord(Nsteps+1,(j-1)*3+3);
         fprintf(fid4,'%s %f %f %f\n',upper(atom{j}),xcart,...
            ycart,zcart);
         if j==firstAtom
            cartOut(Nsteps+1,1:3)=[xcart,ycart,zcart];
         elseif j==secAtom
            cartOut(Nsteps+1,4:6)=[xcart,ycart,zcart];
         end
      end
   else
      if strcmp(type,'IR')
         fprintf(fid4,'Angle: %u, E: %.1f kcal/mol I: %.1f\n',...
            (i-1)*stepsize,energyunits(i,1),InDeg(i));
      else
         if scanVarNum==1
            fprintf(fid4,'Bond Length: %.2f,  E: %.1f kcal/mol\n',...
               (i-1)*stepsize + var(varRot),energyunits(i,1));
```

```
      fprintf(fid5,'Bond Length: %.6f,  E: %.4f kcal/mol\n',...
         (i-1)*stepsize + var(varRot),energyunits(i,1));
      BL(i)=(i-1)*stepsize + var(varRot);

      fprintf(fid6,'%.6f\t%.4f\t%.8f\n',...
         (i-1)*stepsize + var(varRot),energyunits(i,1),energyunits(i,3));
   else
      prnt1='E: %.1f kcal/mol';
      prnt2='';
      prnt3='';
      for j=1:scanVarNum
         prnt1=strcat(prnt1, varnl(varRot(j)), ': %.2f, ');
         val(j)=var(varRot(j),i);
         BL(i,j)=val(j);
         prnt2=strcat(prnt2, varnl(varRot(j)), ': %.6f, ');
         prnt3=strcat(prnt3, '%-15.6f');
      end
      val1=[val energyunits(i,1)];
      val2=[val energyunits(i,1) energyunits(i,3)];
      prnt1=strcat(prnt1, ' \n');
      prnt2=strcat(prnt2, ' E: %.4f kcal/mol\n');
      prnt3=strcat(prnt3, '%-15.4f%-15.8f\n');
      fprintf(fid4,cell2mat(prnt1),[val1(end) val1(1:end-1)]);
      fprintf(fid5,cell2mat(prnt2),val1);
      fprintf(fid6,prnt3,val2);


   end



end
Ccount=0;
for j=1:NumAtoms
   xcart=cartCoord(i,(j-1)*3+1);
   ycart=cartCoord(i,(j-1)*3+2);
   zcart=cartCoord(i,(j-1)*3+3);
   fprintf(fid4,'%s %f %f %f\n',upper(atom{j}),xcart,...
      ycart,zcart);
   if cell2mat(atom(j))=='c'
      Ccount=Ccount+1;
      ind=Ccount;
      carbonCoord(i,(ind-1)*3+1:3*ind)=[xcart,ycart,zcart];
   end
   if j==firstAtom
      cartOut(i,1:3)=[xcart,ycart,zcart];
   elseif j==secAtom
      cartOut(i,4:6)=[xcart,ycart,zcart];
   end
```

```
        end
    end
end
%Close .log and .com files.
fclose(fid1);
fclose(fid2);
fclose(fid4);
if strcmp(type,'BD')
    fclose(fid5);
    fclose(fid6);
end

%Center on highest point.  This increases the chance that the profiles will
%be centered and make the fit easier and better.


if strcmp(type,'IR')
%Runing the loop that allows you to specify the number of points and see
%how it fits the data.
phiinput='n';
running=1;
nstart=input('Initial number of points in fit?:');
nE=nstart;
nI=nstart;
indE=true(Nsteps,1);
indI=true(Nsteps,1);

    while running==1
        %keyboard
        clc
        figure(1)
        subplot(2,1,1)

        %MichaelLS is a simple Least squares fit that Michael wanted me to use.
        % I had already gotten LSfit to work, so I implemented both of them.
        % They give pretty much the same result, if for some reason they are
        % different it displays the two.  It isn't every significant.

        %Energy plot and fit
        angle=0:stepsize*pi/180:stepsize*pi/180*(Nsteps-1);
        [~,sigmaE,PhiE,x0E,xnE]=LSfit(energyunits(indE,2),angle(indE),nE,phiinput,angle);
        [~,xnE1,angl1,sol1]=MichaelLS(energyunits(indE,2),angle(indE),nE,PhiE);
        if mean(abs(xnE1-[x0E;xnE']))>1e-2
            [xnE1 [x0E;xnE']]
            mean(abs(xnE1-[x0E;xnE']))
            figure(2)
            plot(angl1,sol1);
            inpt=input('MichaelsLS and LSfit do not match in energy continue (1,0):');
            if inpt==0
```

```
        error('done')
    end
end
title('Reduced Inertia and Energy versus diahederal angle')
ylabel('Energy (cm^-^1)');

%The reduced moment of inertia fit and data.
figure(1)
subplot(2,1,2)
[~,sigmaI,PhiI,x0I,xnI]=LSfit(InDeg(indI),angle(indI),nI,phiinput,angle);
[~,xnE1,angl1,sol1]=MichaelLS(InDeg(indI),angle(indI),nI,PhiI);
if mean(abs(xnE1-[x0I;xnI']))>5e-3
    [xnE1 [x0I;xnI']]
    mean(abs(xnE1-[x0I;xnI']))
    figure(2)
    plot(angl1,sol1);
    inpt=input('MichaelsLS and LSfit do not match in inertia');
    if inpt==0
        error('done')
    end
end
ylabel('Reduced moment of inertia, (amu *Ang^2)')
xlabel('Diahederal Angle (radians)');

%Disp the variables and coefficents from the fits.
disp(['Max Energy: ' num2str(max(energyunits(:,1)))]);
disp(['nE=',num2str(nE),' nI=',num2str(nI)]);
disp(['SigmaE=',num2str(sigmaE)]);
disp(['SigmaI=',num2str(sigmaI)]);
disp(['PhiE=',num2str(PhiE)]);
disp(['PhiI=',num2str(PhiI)]);
disp('xn for energy in order, starting with x0:')
fprintf('%f\n',[x0E xnE]);
disp('xn for inertia in order, starting with x0:')
fprintf('%f\n',[x0I xnI]);
disp('Is the fit good enough?');
disp('[0] -yes');
disp('[nE,nI] -no and input fits for energy and inertia')
inp=input('Your choice: ');
inp1=input('Offset:');
inp2=input('Phi:');
inp3=input('Energy Cutoff:');
inp4=input('Inertia Cutoff:');
if inp==0
    running=0;
elseif length(inp)==1;
    nE=inp;
    nI=inp;
elseif isempty(inp)
```

```
else
   nE=inp(1);
   nI=inp(2);
end
if ~isempty(inp1)
   if ~ischar(inp1)
      target=ceil(Nsteps/2)+inp1;
      index=ceil(Nsteps/2);
      if target<=0 || target>Nsteps
         error('error in shifting')
      else
         energyunits=offset(energyunits,index,target);
         indE=offset(indE,index,target);
         InDeg=offset(InDeg,index,target);
         indI=offset(indI,index,target);
      end
   elseif inp1=='m'
      target=ceil(Nsteps/2);
      [~,index]=max(energyunits(:,2));
      energyunits=offset(energyunits,index,target);
      indE=offset(indE,index,target);
      InDeg=offset(InDeg,index,target);
      indI=offset(indI,index,target);
   elseif inp1=='n'
      target=ceil(Nsteps/2);
      [~,index]=min(energyunits(:,2));
      energyunits=offset(energyunits,index,target);
      indE=offset(indE,index,target);
      InDeg=offset(InDeg,index,target);
      indI=offset(indI,index,target);
   end

end
if ~isempty(inp2)
   phiinput=inp2;
end
if ~isempty(inp3)
   indE=energyunits(:,2)<inp3;

end
if ~isempty(inp4)
   if inp4==0
      indI=InDeg>0;
   else
      indI=InDeg<inp4;
   end
end
```

```
    end
else
    plot(BL,energyunits(:,1))
    xlabel('Length (Angstroms)')
    ylabel('Energy (kcal/mol)')
    title(['Name: ' name]);
    var=BL;
    if ~exist('carbonCoord','var')
        carbonCoord=NaN;
    end
end


end

function x=offset(x,ind,target)
    spot=target-ind;
    if round(ind)~=ind || round(target)~=target
       error('error in offsetting')
    end
    if sign(spot)==1
        x=[x((end-spot+1):end,:); x(1:(end-spot),:)];
    elseif sign(spot)==-1
        x=[x((spot*-1+1):end,:); x(1:(spot*-1),:)];
    end
end




function [atom,IBond,BondVar,Iangle,AngleVar,idih,DihVar,NumAtoms,...
    stepsize,varname,var,varRot,sType,rType,scanVarNum]...
    =readRelaxedComFile(fid1)
%%readRelaxedComFile reads in the data from the name.com file and
%%determines how many step sizes they'll be.  Assumes the file is in
%%Z-matrix form with variables at the end.
tline=fgetl(fid1);
ttext=textscan(tline,'%s');
sType='R';
rType='Z';
redo=true;
touch=false;
while redo
    for i=1:length(ttext{1})
        if strcmp(upper(ttext{1}(i)),'SCAN')
            sType='S';
            touch=true;
            redo=false;
```

```
        end
        if ~isempty(strfind(upper(ttext{1}{i}),'MODREDUNDANT'))
            rType='M';
            touch=true;
            redo=false;
        end
        if ~isempty(strfind(upper(ttext{1}{i}),'%MEM'));
            redo=true;
            touch=true;
        end
        if ~isempty(strfind(upper(ttext{1}{i}),'%NPROCSHARED'));
            redo=true;
            touch=true;
        end

        if i==length(ttext{1}) && touch==false
            redo=false;
        end
    end
    if redo==true
        tline=fgetl(fid1)
        ttext=textscan(tline,'%s');
        touch = false;
    end

end
varNum=0;
connDone=0;
varDone=0;
varStart=0;
scanVarNum=0;
while ~feof(fid1)
    %keyboard
    tline=fgetl(fid1);
    %Change to match the multiplicity
    if (strcmp('0 2',tline) || strcmp('0 1',tline) || strcmp('0 3',tline));
        row=1;
        tline=fgetl(fid1);
        while row~=0
            if row==1
                tstr=textscan(tline,'%s');
                atom(row)=tstr{1};
            elseif row==2
                tstr=textscan(tline,'%s %u %s');
                atom(row)=tstr{1};
                IBond(row-1)=tstr{2};
                BondVar(row-1)=tstr{3};
            elseif row==3
                tstr=textscan(tline,'%s %u %s %u %s');
```

```
            atom(row)=tstr{1};
            IBond(row-1)=tstr{2};
            BondVar(row-1)=tstr{3};
            Iangle(row-2)=tstr{4};
            AngleVar(row-2)=tstr{5};
        elseif row>3
            tstr=textscan(tline,'%s %u %s %u %s %u %s');
            atom(row)=tstr{1};
            IBond(row-1)=tstr{2};
            BondVar(row-1)=tstr{3};
            Iangle(row-2)=tstr{4};
            AngleVar(row-2)=tstr{5};
            idih(row-3)=tstr{6};
            DihVar(row-3)=tstr{7};

        end
        tline=fgetl(fid1);
        if isempty(tline) || strcmp('Variables:',tline)
            val{1}=[];
        else
            val=textscan(tline,'%s');
        end

        if isempty(val{1})
            %Get the number of atoms from the number of rows.
            NumAtoms=row;
            row=0;
            connDone=1;
            tline={};
        else
            row=row+1;
        end
    end


end
%Search for the scan variable and determine the step size
if ~isempty(tline) && ischar(tline) && connDone==1 && varDone==0
    tnum=textscan(tline,'%s');
    if ~isempty(tnum{1})
        varStart=1;
        varNum=varNum+1;
        varname(varNum)=tnum{1}(1);
        var(varNum)=str2double(tnum{1}{2});

        if length(tnum{1})==5 && tnum{1}{3}=='S'
            scanVarNum=scanVarNum+1;
            stepsize(scanVarNum)=str2num(tnum{1}{5});
            varRot(scanVarNum)=varNum;
```

```
            end

            if length(tnum{1}) == 4 && sType=='S'
                scanVarNum=scanVarNum+1;
                varRot(scanVarNum)=varNum;
                stepsize(scanVarNum)=str2num(tnum{1}{4});
            end

            if length(tnum{1})==1
                varStart=0;
                varDone=1;
            end

        elseif varStart==1 && isempty(tnum{1})
            varStart=0;
            varDone=1;
        end
    end
    if varStart==1 && isempty(tline)
        varStart=0;
        varDone=1;
    end

    if ~isempty(tline) && ischar(tline) && connDone==1 && varDone==1 && rType=='M'
        tnum=textscan(tline,'%s');
        if length(tnum{1})==7 && tnum{1}{5}=='S'
            stepsize=str2double(tnum{1}{7});
            varRot=str2double(tnum{1}{1});
        end
    end
end




function [Nsteps,energy,varname,var]=readRelaxedLogFile(fid2,sType,rType,...
    nAtoms,type,scanVarNum)
%%readRelaxedLogFile, Reads in the energy and optimized location of each
%%step of the relaxed scan.
Nsteps=0;
%Get the data from the .log file, read each line
if sType=='R' && rType=='Z' && type=='s'
    while ~feof(fid2)
        tline=fgetl(fid2);
        match=strfind(tline,'Summary of Optimized Potential Surface Scan');
        %If at the right location in file continue
        if ~isempty(match)
            %Count the number of block down,  This is not the number of variable
            %rows, but rather how many blocks are in the file.
```

```
block=1;
tline=fgetl(fid2);
%Step into the loop for each set of variables.
while block~=0
  %tsteps is the index number of each column.
  tsteps=str2num(tline);
  %Add to the total number of steps in the file
  Nsteps=Nsteps+length(tsteps);
  tline=fgetl(fid2);
  strloc=strfind(tline,'EIGENVALUES --');
  values=tline(20:end);
  %Get the values of energy from the first line
  C=textscan(values,'%.6f');
  values=C{1};
  for i=1:length(tsteps)
    energy(tsteps(i))=values(i);
  end
  %Rows is the row index in the block
  rows=1;
  tline=fgetl(fid2);
  %Get all of the variables from one block
  %Initialize the information from the fist line
  varinfo=textscan(tline,'%s');
  varinfo=varinfo{1};
  while rows>0
    varname(rows,block)=varinfo(1);

    for i=1:length(tsteps)
      %If in the file the variables are negative, they may
      %have no space between them and the the string parse of
      %textscan will only return one string.  This checks for
      %that and if it is the case it parse that string as a
      %float which will work

      if length(varinfo)==2 && length(tsteps)~=1
        if i==1
          tvar=textscan(varinfo{2},'%.5f');
        end
        var(rows,tsteps(i))=tvar{1}(i);

      elseif length(varinfo)==3 && length(tsteps)~=2

        if i==1
          tvar=textscan(varinfo{2},'%.5f');
          tvar=tvar{1};
          tvar1=textscan(varinfo{3},'%.5f');
          tvar1=tvar1{1};
        end
        if i<=length(tvar)
```

```
            var(rows,tsteps(i))=tvar(i);
        else
            var(rows,tsteps(i))=tvar1(i-length(tvar));
        end
    elseif length(varinfo)==4 && length(tsteps)~=3
        if i==1
            tvar=textscan(varinfo{2},'%.5f');
            tvar=tvar{1};
            tvar1=textscan(varinfo{3},'%.5f');
            tvar1=tvar1{1};
            tvar2=textscan(varinfo{4},'%.5f');
            tvar2=tvar2{1};
        end
        if i<=length(tvar)
            var(rows,tsteps(i))=tvar(i);
        elseif i<=(length(tvar)+length(tvar1))
            var(rows,tsteps(i))=tvar1(i-length(tvar));
        else
            var(rows,tsteps(i))=tvar2(i-length(tvar)-length(tvar1));
        end


        elseif length(varinfo)==5 && length(tsteps)~=4
        if i==1
            tvar=textscan(varinfo{2},'%.5f');
            tvar=tvar{1};
            tvar1=textscan(varinfo{3},'%.5f');
            tvar1=tvar1{1};
            tvar2=textscan(varinfo{4},'%.5f');
            tvar2=tvar2{1};
            tvar3=textscan(varinfo{5},'%.5f');
            tvar3=tvar3{1};
        end
        if i<=length(tvar)
            var(rows,tsteps(i))=tvar(i);
        elseif i<=(length(tvar)+length(tvar1))
            var(rows,tsteps(i))=tvar1(i-length(tvar));
        elseif i<=(length(tvar)+length(tvar1)+length(tvar2))
            var(rows,tsteps(i))=tvar2(i-length(tvar)-length(tvar1));
        else
            var(rows,tsteps(i))=tvar3(i-length(tvar)-length(tvar1)-length(tvar2));
        end
    else
        var(rows,tsteps(i))=str2double(varinfo(1+i));
    end

end
tline=fgetl(fid2);
varinfo=textscan(tline,'%s');
```

```
            varinfo=varinfo{1};
            if length(varinfo)~= length(tsteps)+1
               if length(varinfo)~=1
                  truelength=1;
                  for i=2:length(varinfo)
                     tvar=textscan(varinfo{i},'%.5f');
                     truelength=truelength+length(tvar{1});
                  end
               else
                  truelength=1;
               end

            else
               truelength=length(varinfo);
            end
            %This is a check to stop the rows loop.  If it reaches the
            %start of the next block it will have less numbers
            if (truelength)~=(length(tsteps)+1)
               if strncmp(tline,' --------------------------------------',39);
                  totalblock=block;
                  block=0;
                  rows=0;
               else
                  rows=0;
               end
            else
               rows=rows+1;

            end
         end
         if block~=0
            block=block+1;
         end

      end

   end


end
[lvarname,~]=size(varname);
for i=1:lvarname
   for j=1:totalblock
      if ~strcmp(varname{i,j},varname{i,1})

         error('varnames don''t match')
      end

   end
```

```
    end
    varname=varname(:,1);
elseif sType=='S' && rType=='Z' && type=='s'
    while ~feof(fid2)
        tline=fgetl(fid2);
        match=strfind(tline,'Summary of the potential surface scan');
        %If at the right location in file continue
        if ~isempty(match)
            tline=fgetl(fid2);
            ttext=textscan(tline,'%s');
            varname=ttext{1}(2:end-1);
            tline=fgetl(fid2);
            Nsteps=0;
            searching=1;
            tline=fgetl(fid2);
            while searching==1

                %make the format for textscan
                format='%u %f ';
                for i=1:scanVarNum
                    format=[format '%f '];
                end
                Nsteps=Nsteps+1;
                tnum=textscan(tline,format);
                var(Nsteps,1:scanVarNum)=cell2mat(tnum(2:1+scanVarNum));
                energy(Nsteps)=tnum{end};
                tline=fgetl(fid2);
                tstr=textscan(tline,'%s');
                if strcmp(tstr{1}(1),'----')
                    searching=0;
                end
            end
        end

    end

elseif rType=='M' && type=='s'
    Nsteps=0;
    Nenergy=0;
    while ~feof(fid2)
        tline=fgetl(fid2);
        match1=strfind(tline,'-- Stationary point found.');
        match2=strfind(tline,'-- Number of steps exceeded');
        match4=strfind(tline,'Standard orientation:');
        match5=strfind(tline,'Input orientation:');
        if Nsteps==0 && (~isempty(match4) || ~isempty(match5))
            Nsteps=Nsteps+1;
            tline=fgetl(fid2);
            tline=fgetl(fid2);
```

```
        tline=fgetl(fid2);
        tline=fgetl(fid2);
        ttext=textscan(fid2,'%u %u %u %f %f %f',nAtoms);
         [tx,ty,tz]=reOrient(ttext{4},ttext{5},ttext{6});
%           tx=ttext{4};
%           ty=ttext{5};
%           tz=ttext{6};
        var(:,Nsteps,1)=tx;
        var(:,Nsteps,2)=ty;
        var(:,Nsteps,3)=tz;
    end
    match5=strfind(tline,'Input orientation:');
    if ~isempty(match5) && Nsteps~=0
       flook=ftell(fid2)-50;

    end
    %If at the right location in file continue
    if ~isempty(match1) || ~isempty(match2)
        tline=fgetl(fid2);
        running=1;
        fstart=ftell(fid2);
        Nsteps=Nsteps+1;
        fseek(fid2,flook,-1);
        while running
            match=strfind(tline,'Standard orientation:');
            match6=strfind(tline,'Input orientation:');
            if (~isempty(match) || ~isempty(match6))
                tline=fgetl(fid2);
                tline=fgetl(fid2);
                tline=fgetl(fid2);
                tline=fgetl(fid2);
                ttext=textscan(fid2,'%u %u %u %f %f %f',nAtoms);
                [tx,ty,tz]=reOrient(ttext{4},ttext{5},ttext{6});
%                   tx=ttext{4};
%                   ty=ttext{5};
%                   tz=ttext{6};
                var(:,Nsteps,1)=tx;
                var(:,Nsteps,2)=ty;
                var(:,Nsteps,3)=tz;
                running=0;
                fseek(fid2,fstart,-1);
            end
            tline=fgetl(fid2);
        end
    end
    match3=strfind(tline,'EIGENVALUES --');
    if ~isempty(match3)
        ttext=textscan(tline,'%s');
        tenergy=textscan(ttext{1}{3},'%f');
```

```
         if Nenergy==0;
            energy=tenergy{1};
            Nenergy=1;
         else
            energy=[energy;tenergy{1}];
         end
      end

   end
   Nsteps=Nsteps-1;
   varname='none';
elseif rType=='Z' && type=='f'
   Nsteps=0;
   while ~feof(fid2)
      tline=fgetl(fid2);
      match1=strfind(tline,'SCF Done:');
      match2=strfind(tline,'-- Stationary point found.');
      match3=strfind(tline,'-- Number of steps exceeded');
      if ~isempty(match1)
        temp=textscan(tline,'%s %s %s %s %f %s %s %s %s');
        tempEnergy=temp{5};
      end

      if ~isempty(match2) || ~isempty(match3)
         Nsteps=Nsteps+1;
         energy(Nsteps)=tempEnergy;
         if ~isempty(match2)
            skip=7;
         else
            skip=8;
         end
         for i=1:skip
           temp=fgetl(fid2);
         end
         go=true;
         row=0;
         while go
            row=row+1;
            text=textscan(temp,'%s %s %f %s %s %f %s');
            varname(row,Nsteps)=text{2};
            var(row,Nsteps)=text{3};
            temp=fgetl(fid2);
            match4=strfind(temp,'---------------------------------');
            if ~isempty(match4)
               go=false;
            end
         end
      end
   end
```

```
    [lvarname,~]=size(varname);
    for i=1:lvarname
        for j=1:Nsteps
            if ~strcmp(varname{i,j},varname{i,1})

                error('varnames don''t match')
            end

        end
    end
    varname=varname(:,1);
end
end

    function [x,y,z]=reOrient(xin,yin,zin)
        %Reorients in a z-matrix type fashion.
        %Center first atom at zero
        x1=xin(1);
        y1=yin(1);
        z1=zin(1);
        nAtoms=length(xin);
        for i=1:nAtoms
            x(i)=xin(i)-x1;
            y(i)=yin(i)-y1;
            z(i)=zin(i)-z1;
        end
        th1=acos(z(2)/sqrt(x(2)^2+z(2)^2));
        if x(2)>0
            th1=-1*th1;
        end
        Ry=[cos(th1) 0 sin(th1);0 1 0;-sin(th1) 0 cos(th1)];
        for i=2:nAtoms
            rot=Ry*[x(i);y(i);z(i)];
            x(i)=rot(1);
            y(i)=rot(2);
            z(i)=rot(3);
        end
        th2=atan(y(2)/z(2));
        Rx=[1 0 0;0 cos(th2) -sin(th2); 0 sin(th2) cos(th2)];
        for i=2:nAtoms

            rot=Rx*[x(i);y(i);z(i)];
            x(i)=rot(1);
            y(i)=rot(2);
            z(i)=rot(3);
        end
        th3=atan(x(3)/y(3));
        if y(3)<0
            th3=th3+pi;
```

```
      end
      Rz=[cos(th3) -sin(th3) 0;sin(th3) cos(th3) 0;0 0 1];
      for i=2:nAtoms
         rot=Rz*[x(i);y(i);z(i)];
         x(i)=rot(1);
         y(i)=rot(2);
         z(i)=rot(3);
      end


   end

%% Converting Bond-Angle-Torsion to Anchored Cartesian coordinates
% This document is a tutorial for a set of MATLAB scripts for converting
% given BAT coordinates of a molecule to anchored cartesian coordinates.
% See Figure 1 of J. Chem. Phys. 127, 024107 _2007_ for a description of
% BAT coordinates
%
% <html>
% <img vspace="1" hspace="1" src="../cyclohexane.PNG">
% </html>
%
%%
function [conform] = genConfBATConn( bond, angle , torsion , bondconn ,  angleconn , torsionconn , b , a , t , Nref )
% function [conform] = genConfBATConn( bond, angle , torsion , bondconn ,
% angleconn , torsionconn , b , a , t , Nref )
%
% Converts BAT coordinates to Cartesian coordinates using connectivity
% matrix
%
%  - phase torsion angles implemented
%
% Input:
%   bond , angle , torsion = 2-D matrices with conformations stored
%   row-wise
%   angleconn , bondconn , torsionconn = connectivity matrices
%   Nref  = Number of conformations to convert; default is all conformations
%
% Output:
%   conform = 2-D matrix with each row of the form
%           [x1 y1 z1 x2 y2 z2 .... xNatom  yNatom zNatom  ]
%          where Natom = number of atoms
%
% Dependencies:
%   bat2xyz.m
%
% Last updated:
%       05 Jan 2009 - created
%
```

```
%% Overview
% The various steps of the method are demonstrated using all-atom Cyclohexane as the test system.
% It contains 18 atoms - 6 carbons and 12 hydrogens which correspond to
% 3*18-6 = 48 internal coordinates consisting of 17 bonds, 16 angles and 15 torsions.
%
% Click <http://www.chemicalphysics.umd.edu/~ssomani/html/coord2pdbWname.html here>
% to download a zip file containing required files.
%
% In following sections, file names and matlab variables are in |this
% font|.
%
%% Connectivity Matrix
% The set of BAT coordinates are not unique and are specified by the
% connectivity matrices.
% load |cyclohexaneConn.mat| to import the connectivity data structure
%
% The connectivity is defined in terms of the atom numbers in the pdb file
% (see |cyclohexaneOrig.pdb|). Thus atom 1 is c1, atom 2 is c2 .. atom18 is h18.
%
% Bond connectivity is contained in matrix bondconn which has 17 rows - one
% for each bond. The first two numbers in each row are the atom numbers corresponding to the bond.
% The third column is irrelevant for this tutorial. The fourth column gives the corresponding column
% number in matrix bonds which contains values of this bond in different
% conformations.
%
% In addition to |bondconn|, function |genConfBATConn| requires another
% data structure |b| which contains information about the columns of the
% |bondconn| matrix. For this tutorial only |b.SampleIdCol| need to be set which here is 4
% indicating the 4th column of |bondconn| matrix
%
% Angle connectivity matrix |angleconn| and data structure |a| are
% analogous to bonds. Now first three columns of |angleconn| contain the
% atom numbers forming the angle. Again, only cols 1:3 and 5 of
% |angleconn| and |a.SampleIdCol| are relevant here.
%
% Torsions are defined by |torsionconn| and |t|.
% Cols [1:4 6] of |torsionconn| and |t.SampleIdCol| required.
%
%% BAT input data
% load |BATinput.mat| to import BAT coordinates of 10 conformations in the pdb
% trajectory file |cyclohexaneOrig.pdb|.
%  |bonds| is 10x17 matrix with each row containing the 17 bond lengths of
%  corresponding pdb structure in |cyclohexaneOrig.pdb|
%  Similarly, |angles| and |torsions| matrices contain the angle and
%  torsion values in radians.
%
%
%% Conversion command
```

```
% |[conform] = genConfBATConn(bonds,angles,torsions,bondconn,angleconn,torsionconn,b,a,t);|
%
% |conform| contains the converted cartesian coordinateis for each
% atom. Each row contains one conformation with entries as
%
% $$[x_1 \ y_1 \ z_1 \ x_2 \ y_2 \ z_2 \ ... \ x_{18} \ y_{18} \ z_{18}]$$
%
% For the current case it contains 10 rows - one for each conformation.
%
%% Create pdb trajectory of reconstructed frames
% The cartesian coordinates for the 10 conformations in |conform| can be
% used to write a pdb trajectory file as described
% <http://www.chemicalphysics.umd.edu/~ssomani/html/coord2pdbWname.html
% here>.
%
% |load atomNameCyclohexane.mat| for atom name, and
% |load molNameCyclohexane.mat|  for molecule name to use in pdb file.
%
% |coord2pdbWname(conform,'cyclohexaneRecons',-1,atomName,molName)| then creates the
% pdb trajectory file |reconsCyclohexane.pdb|.
%
% Note that due to way BAT coordinate system is set up, for each
% conformation atom h7 is placed on the origin, atom c1 is on the x-axis
% and atom c2 is in the x-y plane.
%
% In other words, we from all have removed six rigid body translational and
% rotational degrees of freedom.
%
%% VMD check
% To verify if the conversion was done correctly compare the original
% trajectory |cyclohexaneOrig.pdb| with reconstructed
% |cyclohexaneRecons.pdb| one in VMD 1.8.6
%
% To superimpose the two trajectories:
%
%  1. goto VMD Main -> Extensions -> Analysis -> RMSD Trajectory Tool
%
%  2. replace 'protein' by 'all'
%
%  3. click 'Add All'
%
%  4. click 'Align'
%
% If everything went well, the two corresponding frames should overlap exactly!

%----------------
% set number of conformations
if nargin == 9
   Nref = size(torsion,1);
```

```
end
if Nref < 0 || Nref > size(torsion,1)
   Nref = size(torsion,1);
end

% set number of atoms
D = size(torsionconn, 1) ;% 3 N - 6 - 3
Natom = D + 3    ;

disp(sprintf('%s conformations of %s atom molecule will be generated',num2str(Nref),num2str(Natom)))

conform = zeros(Nref, 3*Natom)  ;

%-------------------
for iconf = 1:Nref
   conformt = zeros(1,3*Natom)  ;

   %atom indices from first row of torsionconn
%     a1 = torsionconn(1,1) ;
%     a2 = torsionconn(1,2) ;
%     a3 = torsionconn(1,3) ;
   %Modified by D. Edwards
   a1=bondconn(1,1);
   a2=bondconn(1,2);
   a3=bondconn(2,2);

   % x y z of first atom
   crd1 = [ 0 0 0 ]' ;
   conformt = putXYZ( conformt , a1 , crd1) ;

   % second atom
   [bval] = getBval(bond, bondconn, b , [ a1  a2 ] , iconf ) ;

   % x y z of second atom on x-axis
   crd2 = [ bval 0 0 ]' ;
   conformt = putXYZ( conformt , a2 , crd2) ;
   % x y z of third atom in x-y plane
   [bval] = getBval(bond, bondconn, b , [ a2  a3 ] , iconf )  ;  % second bond
   aval   = getAval(angle , angleconn, a , [ a1 a2 a3] , iconf ); % first angle
   crd3 = [ crd2(1) + bval*cos(pi-aval)  crd2(2) + bval*sin(pi+aval) 0 ]' ;
   conformt = putXYZ( conformt , a3 , crd3) ;
   % first three atoms done

   % LOOP over torsionconn to set other atoms
   for j=1:D
      a1 = torsionconn(j,1)  ;
      a2 = torsionconn(j,2)  ;
      a3 = torsionconn(j,3)  ;
      a4 = torsionconn(j,4)  ;
```

```
      bval = getBval(bond, bondconn, b , [ a3  a4 ] , iconf ) ;
      aval = getAval(angle , angleconn, a , [ a2 a3 a4] , iconf ) ;
      tval = getTval(torsion , torsionconn, t, [ a1 a2 a3 a4] , iconf ) ;

      if bval < 0
         bval = getBval(bond, bondconn, b , [ a4  a3 ] , iconf ) ;
         if bval < 0
            disp('genConfBATConn.m: bond absent from conn matrix')
            pause
         end
      end
      if aval < 0
         aval = getAval(angle , angleconn, a , [ a4 a3 a2] , iconf ) ;
         if aval < 0
            disp('genConfBATConn.m: angle absent from conn matrix')
            pause
         end
      end

      % compute coordinates of next atom
      r1 = getXYZ( conformt, a1 ) ;
      r2 = getXYZ( conformt, a2 ) ;
      r3 = getXYZ( conformt, a3 ) ;

      r4 = bat2xyz(r1,r2,r3,bval,aval,tval) ;
      conformt = putXYZ(conformt , a4 ,r4) ;
   end   %  for j=1:D
   % end of loop over torsions

   conform(iconf, :) = conformt ;

   if ~mod(iconf,1000)
      disp(sprintf('genConfBATConn.m: conformation number = %s',num2str(iconf))) ;
   end

end % for iconf = 1:Nref
disp('genConfBATConn.m: All Done')


%%%%%%%%%%%%END OF MAIN%%%%%%%%%%%%%%%%%%%%%%
function conform = putXYZ( inconform , a1 , crdDum)
%
   xi  = 3*(a1-1) + 1 ;
   yi  = 3*(a1-1) + 2 ;
   zi  = 3*(a1-1) + 3 ;
   conform = inconform ;
   conform( xi ) = crdDum(1) ;
   conform( yi ) = crdDum(2) ;
```

```
   conform( zi ) = crdDum(3) ;

%--------------------------
function [crdDum] = getXYZ( conform , a1 )
% crdDum = 3x1 column vector
   xi  = 3*(a1-1) + 1 ;
   yi  = 3*(a1-1) + 2 ;
   zi  = 3*(a1-1) + 3 ;
   crdDum = [ 0 0 0 ]' ;

   crdDum(1) = conform( xi ) ;
   crdDum(2) = conform( yi ) ;
   crdDum(3) = conform( zi ) ;
%-------------------------------
function [bval] = getBval(bond, bondconn, bhead , ind, iconf )
% returns the row id of bondconn such that the row is [ ind1 ind2 ... ]

a = find( bondconn(:,1) == ind(1) )  ;
b = find( bondconn(:,2) == ind(2) )  ;

bRow =  intersect( a , b ) ;
bval = -1 ;

if isempty( bRow )
   return
else
   % if active take value from input 'bond'
   % else set to topology values contained in conn file

   sampleid = bondconn( bRow , bhead.SampleIdCol ) ;
   if sampleid > 0
      bval = bond(iconf, sampleid ) ;     % active dof
   else
      bval = bondconn( bRow , bhead.TopIdCol ) ;    % fixed dof
   end
end



%------------------------------
function [aval] = getAval(angle , angleconn, ahead, ind , iconf )
% returns the angle value of conformation iconf
% corresponding to angle ind1-ind2-ind3 if the sampled id in angleconn is
% positive
% returns -1 if angle not found in conn matrix

aa = find( angleconn(:,1) == ind(1) ) ;
bb = find( angleconn(:,2) == ind(2) ) ;
cc = find( angleconn(:,3) == ind(3) ) ;
```

```
aRow = intersect( intersect( aa , bb ) , cc ) ;

aval = -1 ;
if isempty( aRow )
   return
else
   sampleid = angleconn( aRow , ahead.SampleIdCol ) ;
   if sampleid >0
      aval = angle( iconf, sampleid ) ;   % active dof
   else
      aval = angleconn( aRow , ahead.TopIdCol )  ;      % fixed
   end
end
%-------------------------------

function [tval] = getTval(torsion , torsionconn, thead, ind , iconf )
% returns the torsion value of conformation iconf corresponding
% to torsion ind1-ind2-ind3-ind4 if the sampled id in torsionconn is positive
%
% returns -1 if torsion not found in conn matrix

a = find( torsionconn(:,1) == ind(1) ) ;
b = find( torsionconn(:,2) == ind(2) ) ;
c = find( torsionconn(:,3) == ind(3) ) ;
d = find( torsionconn(:,4) == ind(4) ) ;

% find the number common to sets a, b, c and d
% if the torsion is present in the conn matrix only one number will be
% returned
tRow = intersect( intersect( intersect( a , b ) , c ) , d) ;

tval = -1 ;

if isempty(tRow)
   return
else
   Ntorsion = size(a,1) ;

   sampleid = torsionconn( tRow , thead.SampleIdCol ) ;

   if sampleid >0
      tval = torsion( iconf, sampleid ) ;   % active dof
   else
      if abs(sampleid) > Ntorsion
         tval = torsionconn( tRow , thead.TopIdCol )  ;      % fixed
      else % phase angle
         phaseof = abs(sampleid) ;
         tvalphase = torsion( iconf, phaseof ) ;
```

```
         tval = tvalphase +  pi ;
         if tval > 2*pi
            tval = tval - 2*pi ;
         end
      end
   end
end

%----bat2xyz begins-------------------------
function [crd4] = bat2xyz(crd1 , crd2 ,crd3,r,t,p)
% bat2xyz takes cartesian coords for three atoms (crd1,crd2,crd3),
%  and a distance (r), an angle (t for theta) and a dihedral (p for phi)
%  and computes the cartesian coords (crd4) for the fourth atom.
%
%  NB: the conditionals dealing with rotation axes that are already
%  on a Cartesian axis are not exhaustive... one might obtain
%  a NaN result from this code if bonds are precisely on-axis,
%  or if the planes defined by angles are precisely on-axis.
%
% Input:
%   crd1 , crd2 , crd3 are 3x1 column vectors
%   t and p are in radians
% Usage:
%         x y z
% crd1 = [ 0 0 0 ]' ; crd2 = [ 1 0 0 ]' ; crd3 = [ 1 1 0 ]' ;
% r    = 1         ;  t   = pi/2       ; p    = pi/2       ;
% [crd4] =  bat2xyz(crd1 , crd2 ,crd3,r,t,p)
%crd4 =
%   1.00000000000000
%   1.00000000000000
%   1.00000000000000
%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
TOL = 1e-3 ;
TOL1= 1e-5 ;

bn1 = crd2-crd1 ;
bn2 = crd3-crd2 ;

%1) place atom 4 along vector joining atoms 2 and 3:
sumBN2 = sum(bn2.^2)    ;
factor = r/sqrt(sumBN2) ;

crd4 = crd3 + bn2 * factor ;

% 2) rotate coords of atom 4 about axis defined
% by cross product of vectors joining 1-2 and 2-3:
ax = cross(bn1,bn2) ;
```

```
% vector to be rotated is r3-r4:
wrk = (crd4-crd3)   ;

% construct rotation matrix:
%   first, construct matrix that will rotate the cross-product axis to the
%   z-axis; accomplish this by expressing it in spherical coords
%   rel to r2:

  if ( abs(ax(1)) < TOL && abs(ax(2)) < TOL )
     phi = 0 ;
     if (ax(3)<0)
       theta = pi ;
     else
       theta = 0  ;
     end

  else
     rax= sqrt(sum(ax.^2)) ;

     theta = acos(ax(3)/rax) ;

     if (sin(theta)==0)
       theta = theta + TOL1 ;
     end

     cosphi = ax(1)/(rax*sin(theta)) ;
     sinphi = ax(2)/(rax*sin(theta)) ;

     while (abs(cosphi) > 1),
       cosphi = cosphi* (1-TOL1) ;
     end

     phi = acos(cosphi) ;
     if (sinphi<0)
        phi = 2*pi - phi ;
     end
  end  % if (abs(ax(1)) < TOL && abs(ax(2)) < TOL)

%c   construct matrices to set ibond2 on z axis rel to ibond1, and then rotate back
   [rot1,rot2]=make_matrix1b(theta,phi)  ;

%c   operate rot1 on working vector (r3-r4)
%    call matrix_multb(rot1,wrk(1),wrk(2),wrk(3))

  wrk = rot1 * wrk ;

%c   now working vector is in coords with
%c   cross-product axis vector along z-axis; apply a rotation
```

```
%c   of pi-t to make the r2-r3-r4 angle = r4

%c   make z-rotation matrix:
  ang = pi - t ;
  rot3 = make_matrix2b(ang) ;

%c   apply the z-rotation rot3 to the working vector:
  wrk = rot3 * wrk ;

%c   reverse the coordinate transformation to put
%c   the working vector back into its original coordinates:
   wrk = rot2*wrk ;

%%%%%%%%%%%%%%%% DIHEDRAL %%%%%%%%%%%%%%%%%%%%%%%%%
% c 3) now do a similar procedure to set the dihedral angle
% c of atom 4 around the 2-3 bond; here bn2 takes the place
% c of the cross-product, ax. We continue using the wrk vector.

   rax2=0  ;

   if ( abs(bn2(1)) < TOL && abs(bn2(2)) < TOL )
     phi = 0. ;
     if (bn2(3) < 0 )
       theta = pi ;
     else
       theta = 0 ;
     end
   else
     rax = sqrt(sum(bn2.^2)) ;

     theta = acos(bn2(3)/rax) ;
%      if (sin(theta) < TOL1 )    % original
     if (sin(theta) == 0 )
       theta = theta + TOL1 ;
     end

     cosphi = bn2(1)/(rax*sin(theta)) ;
     sinphi = bn2(2)/(rax*sin(theta)) ;

     while (abs(cosphi)>1),
        cosphi = cosphi*(1-TOL1) ;
     end

     phi = acos(cosphi) ;

     if (sinphi < 0)
        phi = 2*pi - phi ;
     end
   end
```

```
%c   construct matrices to set bn2 on z-axis, and then to rotate back:
     [rot1,rot2] = make_matrix1b(theta,phi) ;
%c   operate rot1 on working vector (r3-r4)
     wrk = rot1*wrk ;
%c create z-rot matrix for dihedral:
     rot3 = make_matrix2b(p) ;
%c   apply the z-rotation rot3 to the working vector:
     wrk = rot3*wrk ;
%c   reverse the coordinate transformation to put
%c   the working vector back into its original coordinates:
     wrk = rot2*wrk ;
%c   add r3 back to wrk to restore the correct origin of coordinates:
    crd4 = wrk + crd3 ;


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%         END OF bat2xyz                              %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

function [vecout] = cross(vec1,vec2)
% cross product of two 3-D vector
     vecout(1) = vec1(2)*vec2(3) - vec1(3)*vec2(2)  ;
     vecout(2) = vec1(3)*vec2(1) - vec1(1)*vec2(3)  ;
     vecout(3) = vec1(1)*vec2(2) - vec1(2)*vec2(1)  ;

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [rot1,rot2]=make_matrix1b(theta,phi)
% make rotation matrices
%
rtheta = [ cos(-theta)   0   sin(-theta)  ;
          0          1        0     ;
        -sin(-theta)   0   cos(-theta)  ] ;

rphi  = [  cos(phi)    sin(phi)    0    ;
        -sin(phi)    cos(phi)    0    ;
          0           0       1      ] ;

rot1 = rtheta*rphi ; % order is important ! ssomani

rrtheta = [ cos(theta)   0   sin(theta)  ;
          0          1        0     ;
        -sin(theta)    0   cos(theta)    ] ;

rrphi  = [  cos(-phi)    sin(-phi)    0   ;
        -sin(-phi)    cos(-phi)     0   ;
          0           0       1       ] ;

rot2 = rrphi*rrtheta ;
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

function rot3 = make_matrix2b(phi)
% make z rotation matrix.

rot3 = [ cos(phi)   -sin(phi)  0 ;
        sin(phi)    cos(phi)  0 ;
        0            0      1   ] ;


%----bat2xyz ends-------------------------







function val=getVarValue(namList,varList,seekVar)
for i=1:length(namList)
   if strcmp(namList{i},seekVar)
      val=varList(i);
      break;
   end
end


end





function cartCoord=writeFiles(atom,IBond,BondVar,Iangle,AngleVar,idih,DihVar,...
   NumAtoms,stepsize,Nsteps,var,varname,energyunits,name,fileDir,varI,...
   rType,scanVarNum)
import RelaxedScanParsing.getVarValue;
if rType=='Z'
   var=[var varI'];
   %Create the z-matrix file
   fid3=fopen(fullfile(fileDir,'Zout.xyz'),'w+');
   for i=1:Nsteps+1
      for j=1:(2+NumAtoms)
         if j==1
            fprintf(fid3,'%u\n',NumAtoms);
         elseif j==2
            if i==(Nsteps+1)
               fprintf(fid3,'Initial geometry for optimization');
            else
               fprintf(fid3,'On Step: %u\n',i);
            end
```

```
        elseif j==3
            fprintf(fid3,'%s \n',upper(atom{j-2}));
        elseif j==4
            tbond=getVarValue(varname,var(:,i),BondVar{j-3});
            fprintf(fid3,'%s %u %f\n',upper(atom{j-2}),IBond(j-3),...
                tbond);
            bondconn(j-3,:)=[IBond(j-3),(j-2),(j-3),(j-3)];
            bond(i,j-3)=tbond;
        elseif j==5
            tbond=getVarValue(varname,var(:,i),BondVar{j-3});
            tangle=getVarValue(varname,var(:,i),AngleVar{j-4});
            fprintf(fid3,'%s %u %f %u %f\n',upper(atom{j-2}),IBond(j-3),...
                tbond,Iangle(j-4),tangle);
            bondconn(j-3,:)=[IBond(j-3),(j-2),(j-3),(j-3)];
            angleconn(j-4,:)=[Iangle(j-4),IBond(j-3),j-2,j-4,j-4];
            bond(i,j-3)=tbond;
            angle(i,j-4)=tangle;
        else
            tbond=getVarValue(varname,var(:,i),BondVar{j-3});
            tangle=getVarValue(varname,var(:,i),AngleVar{j-4});
            tdih=getVarValue(varname,var(:,i),DihVar{j-5});
            fprintf(fid3,'%s %u %f %u %f %u %f\n',upper(atom{j-2}),IBond(j-3),...
                tbond,Iangle(j-4),tangle,idih(j-5),tdih);
            bondconn(j-3,:)=[IBond(j-3),(j-2),(j-3),(j-3)];
            angleconn(j-4,:)=[Iangle(j-4),IBond(j-3),j-2,j-4,j-4];
            dihconn(j-5,:)=[idih(j-5),Iangle(j-4),IBond(j-3),j-2,j-5,j-5];
            bond(i,j-3)=tbond;
            angle(i,j-4)=tangle;
            dih(i,j-5)=tdih;
        end
    end

end


if isequal(sort(dihconn(1,1:2)),sort(bondconn(1,1:2)))
    cas=1;
elseif isequal(sort(dihconn(1,1:2)),sort(bondconn(2,1:2)))
    cas=2;
else
    cas=3;
    %error('The bond and dih connectivity matrix don''t match')
end

if cas==1
    if ~isequal(dihconn(1,1:2),bondconn(1,1:2))
        temp=bondconn(1,2);
        bondconn(1,2)=bondconn(1,1);
```

```
         bondconn(1,1)=temp;
      end
   elseif cas==2
      if ~isequal(dihconn(1,1:2),bondconn(2,1:2))
         temp=bondconn(2,2);
         bondconn(2,2)=bondconn(2,1);
         bondconn(2,1)=temp;
      end
   elseif cas==3
      disp(['In writeFiles, error at line 76, connectivity not working']);
         disp('try and reorder the list of z-matrix coordinates.');
    %  keyboard  This temporary measure seemed to work for CH4
    %  dissociation.
      temp=bondconn(1,2);
         bondconn(1,2)=bondconn(1,1);
         bondconn(1,1)=temp;

   end

   %Transform z-matrix coordinates to cartesian.  Using the genConfBATConn
   %program.  I found it on file exchange.  It isn't the greatest.  The arrays
   %and connectivity information needs to be organized just right or it won't
   %work.  But I believe I have sorted it out.
   a=struct('MDIdCol',4,'SampleIdCol',5,'TopIdCol',6);
   b=struct('MDIdCol',3,'SampleIdCol',4,'TopIdCol',5);
   t=struct('MDIdCol',5,'SampleIdCol',6,'TopIdCol',6);

   cartCoord=RelaxedScanParsing.genConfBATConn(bond,angle*pi/180,...
      dih*pi/180,bondconn,angleconn,dihconn,b,a,t);
   fclose(fid3);
end

if rType=='M'
   [r,c,d]=size(var);
   for i=1:c
      for j=1:r
         cartCoord(i,(j-1)*3+1)=var(j,i,1);
         cartCoord(i,(j-1)*3+2)=var(j,i,2);
         cartCoord(i,(j-1)*3+3)=var(j,i,3);
      end
   end
   cartCoord=[cartCoord(2:end,:);cartCoord(1,:)];
end
%Write the lam.dat file
fid5=fopen(fullfile(fileDir,'lamm.dat'),'w+');
[~,nam,~]=fileparts(name);
fprintf(fid5,'%s \n',nam);
fprintf(fid5,'Autogenerated from matlab,File: %s\n',name);
fprintf(fid5,'%u\n',NumAtoms);
```

```
fprintf(fid5,'%f %u %f    !Check that they are correct\n',0,Nsteps,stepsize);
for i=1:NumAtoms
   fprintf(fid5,'%f\n',getMass(atom{i}));
end
for i =1:Nsteps
   for j=1:NumAtoms
      fprintf(fid5,' %f %f %f\n',cartCoord(i,(j-1)*3+1),...
         cartCoord(i,(j-1)*3+2),cartCoord(i,(j-1)*3+3));
   end
   fprintf(fid5,'\n');
end
fprintf(fid5,'Another comment line\n');
for i=1:Nsteps
   fprintf(fid5,'%f %f\n',(i-1)*stepsize,energyunits(i,2));
end


fclose(fid5);

   function m=getMass(atom)
      if upper(atom)=='C'
         m=12;
      elseif upper(atom)=='H'
         m=1;
      elseif upper(atom)=='O'
         m=16;
      elseif upper(atom)=='X'
         m=3;
      end
   end
end


function lnDeg=runLamm(fileDir)
%getCARTCOORD- runs lamm.exe and reads in the results.
system(fullfile(fileDir,'lamm.exe'));
fid6=fopen(fullfile(fileDir,'lamm.out'));
stars=0;
while ~feof(fid6)
   tline=fgetl(fid6);
   if ~isempty(tline)
      tstr=textscan(tline,'%s');

      if strcmp(tstr{1}{1},'INDEX') || stars~=0

         tline=textscan(fid6,'%u %f %f %f %f %f');

         if stars==0
            lnDeg=tline{5};
```

```
            else
               InDeg=[InDeg;tline{5}];
            end
            if length(tline{4})~=length(tline{5})
               stars=stars+1;
               InDeg=[InDeg;0];
            else
               totalstars=stars;
               stars=0;
            end

        end
    end
end
fclose(fid6);


function [phi,xn,angle,sol]= MichaelLS(x,domain,n,phi)
%MICHAELLS Summary of this function goes here
%   Detailed explanation goes here
for i=1:length(x)
    for j=1:n
        if j==1
            A(i,j)=1;
        else
            A(i,j)=cos((j-1)*(phi+domain(i)));
        end
    end

end
xn=A\x;
angle=domain(1):(domain(end)-domain(1))/1000:domain(end);
sol=xn(1);
for i=2:n
    sol=sol+xn(i)*cos((i-1)*(angle+phi));
end




end
```