THE EXPERIMENTAL AND THEORETICAL DETERMINATION OF COMBINATORIAL KINETIC ISOTOPE EFFECTS FOR MECHANISTIC ANALYSIS

A Dissertation

by

CHAD F. CHRISTIAN

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

May 2007

Major Subject: Chemistry

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Approved by:

Chair of Committee,	Daniel A. Singleton
Committee Members,	David E. Bergbreiter
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	Andy C. LiWang
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ABSTRACT

The Experimental and Theoretical Determination of Combinatorial Kinetic Isotope Effects for Mechanistic Analysis. (May 2007)

Chad F. Christian, B.A., Texas A&M University

Chair of Advisory Committee: Dr. Daniel A. Singleton

Unfortunately, chemists can never experimentally unravel a full reaction pathway. Even our ability to define key aspects of mechanisms, such as short-lived intermediates and the even more ephemeral transition states, is quite limited, requiring subtle experiments and subtle interpretations. Arguably the most important knowledge to be gained about the mechanism of a reaction is the structure and geometry of the transition state at the rate-limiting step, as this is where a reaction's rate and selectivity are generally decided. The Singleton group has developed a methodology for predicting the combinatorial kinetic isotope effects (KIEs) at every atomic position, typically carbon or hydrogen, at natural abundance. A combination of experimental isotope effects and density functional theory (DFT) calculations has greatly aided our ability to predict and understand a reaction's pathway and transition state geometries. Precise application of this method has allowed for the mechanistic investigation of a myriad of bioorganic, organic, and organometallic reactions. The technique has been applied in the analysis of the catalytic borylation of arenes via C-H bond activation, dynamic effects in the enyne allene cyclization, palladium catalyzed allylic alkylation, the nature of proton transfer in orotate decarboxylase, and the epoxidation of enones with t-butyl hydroperoxide.

DEDICATION

To Grandmama and Honey

ACKNOWLEDGMENTS

I would like to thank my advisor, Dr. Singleton, for his guidance, patience, and support throughout my tenure as a graduate student under his tutelage.

I would like to thank my committee members, Dr. Bergbreiter, Dr. Raushel, and Dr. LiWang for their time and direction.

A special thanks to the past and current Singleton group members that I have provided me a fruitful arena for learning and discussion; I am indebted to their friendship and encouragement. I am thankful for the many friends, acquaintances, and experiences that have had so far in my career.

Last, and most important, I have to thank my family who have always supported and encouraged me.

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CHAPTER I

INTRODUCTION

Purpose

Chemists have the ability to relatively easily determine the products of a reaction and define the reaction's thermodynamics, kinetics, and selectivity. These directly observable properties are important but the understanding of what happens in chemical reactions also requires a knowledge of *how* it works, that is, the reaction's mechanism. Ideally, chemists would like to be able to follow a molecule along the reaction pathway through all of the short lived reactive intermediates and transition states involved in the mechanism. Armed with such complete knowledge of the reaction pathway, chemists would be able to deduce the rationales underlying the diverse experimental observations of reactions. Unfortunately, chemists can never experimentally unravel a full reaction pathway. Even our ability to define key aspects of mechanisms, such as short-lived intermediates and the even more ephemeral transition states, is quite limited, requiring subtle experiments and subtle interpretations. Nonetheless, obtaining such knowledge is a central goal of physical organic chemistry, because the insight obtained can allow the rational control of reactions and inspire the rational design of new reactions.

This dissertation follows the style and format of *The Journal of the American Chemical Society*.

Arguably the most important knowledge to be gained about the mechanism of a reaction is the structure and geometry of the transition state at the rate-limiting step, as this is where a reaction's rate and selectivity are generally decided. The Singleton group studies at the atomic level the changes in bonding and/or hybridization at the rate-limiting step of a reaction by looking at the small changes in the rates of reactions that occur on isotopic substitution. These *kinetic isotope effects* (KIEs) have been developed and established as an effective tool in probing the rate-determining step of a reaction.[1,2,3,4] Most of the studies in this dissertation will make use of KIEs, including the development of novel methodology used in the determination of KIEs and its application in several important organic reactions.[5] Sometimes, however, even a complete knowledge of the transition states and intermediates in a mechanism is not enough to understand how a reaction works or its selectivity. In such cases, chemistry must fall back on a full consideration of a mechanistic pathway, including the positions and momenta of atoms. These *dynamics* considerations are conventionally ignored but will play an important role in this dissertation.

Fundamental Origin of Kinetic Isotope Effects

The simplest change that can be made in a chemical reaction without greatly affecting the molecular structure, the chemical environment, and the potential energy surface of a reaction is isotopic substitution, (e.g. D for H, ^{13}C for ^{12}C, ect.). Isotopologues, for example XH and XD, follow an identical pathway on a reaction potential energy surface, but one can observe differences in the rate constants, eq 1-1

and 1-2. The effect on the ratio of the rate constants for the two chemically identical components that only differ by their isotopic composition represents the KIE (eq 1-3).[6]

$$XH + Y \xrightarrow{k_H} X + YH \qquad (1\text{-}1)$$

$$XD + Y \xrightarrow{k_D} X + YD \qquad (1\text{-}2)$$

$$KIE = \frac{k_H}{k_D} \qquad (1\text{-}3)$$

Isotope effects arise mainly from the effect of isotopic substitution on changes in zero-point energies (ZPEs) as a reaction proceeds from starting material to the transition state (Figure 1-1). It should be noted factors other than ZPE are found to play a role in KIEs when full conventional transition state theory is considered, but ZPE is usually the major factor.

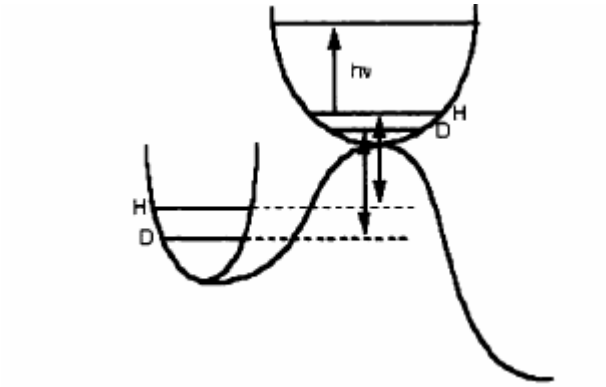


Figure 1-1. The origin of a kinetic isotope effect arises from a difference in the ZPE of the reacting isotopomers as a reaction proceeds from starting material to the transition state.

Classically, the vibrational modes of molecules are treated like a harmonic oscillator, for which the vibrational frequency, υ, can be determined (eq 1-4).[7] Isotopic substitutions do not alter the electronic structure of a molecule which makes the force constants, k, for the reacting isotopomers the same. Any difference that arises is due to the change in the mass, m, and its effect on the vibrational frequencies.

$$\upsilon = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \qquad (1\text{-}4)$$

The quantum-mechanical treatment of the frequencies for the vibrational modes leads to the energy, E, in eq 1-5.

$$E = (n + 1/2)\, h\upsilon \qquad n = 0, 1, 2, ... \qquad (1\text{-}5)$$

This energy is measured from the lowest point in a potential energy curve. Because a molecule always retains some energy when n=0, the lowest possible energy lies at a level ½hυ above the minimum of the well (eq 1-6).

$$ZPE = 1/2\ h\upsilon \qquad (1\text{-}6)$$

Simple math and previously described assumptions provide that the ZPE is inversely proportional to the square root of the mass (eq 1-7).

$$ZPE = \sqrt{\frac{1}{m}} \qquad (1\text{-}7)$$

Therefore, the ZPE is always lower for molecules containing heavier isotopes than molecules containing lighter isotopes. The difference in ZPE between the two will depend on the detailed structure of the molecule and will in general change as a structure changes from starting material to transition state. This model is used to rationalize the observed trends in KIEs.

Isotope effects are categorized as either primary isotope effects or secondary isotope effects. A primary KIE involves the loss of a stretching frequency as a vibrational mode becomes a translational motion over the potential energy surface. Primary isotope effects occur when a σ-bond is being broken or formed in the rate-determining step (rds), with typical values of between 2-7 for k_H/k_D and 1.01-1.05 for k_{12C}/k_{13C}. Secondary isotope effects arise from changes in the force constants for an atom that is not undergoing σ-bond breaking or formation as a reaction proceeds from ground state to transition state. Because a secondary KIE involves only small changes in the stretching or bending frequencies, the values are small. Secondary KIEs can either be classified as normal (>1) or inverse (<1) with values between 0.7-1.4 for k_H/k_D and 0.99-1.01 for k_{12C}/k_{13C}. A normal secondary KIE is generally observed for hydrogen / deuterium atoms attached to a reactive center that is undergoing a hybridization change from sp^3 to sp^2; inverse secondary KIEs are observed for the corresponding case where hybridization changes from sp^2 to sp^3. Normal secondary KIEs are also generally

observed at atoms undergoing a weakening of their bonds in the transition state, while inverse secondary can result from crowding of an atom at the transition state. From such simple rules, KIEs can be interpreted qualitatively to provide valuable information about the nature of atoms being transferred and/or the geometry of transition state for the rate-limiting step. In addition, KIEs can also be calculated in detail from the combination of theoretical calculations and conventional transition state theory, and this can allow a more quantitative interpretation of KIEs.

Methodology for Determining Kinetic Isotope Effects

For the reasons described above, kinetic isotope effects are a powerful tool for studying reaction mechanisms, but the precise and accurate measurement of KIEs can be difficult. Commonly, isotope effects are measured either non-competitively or competitively.

Non-competitive KIEs are determined by separately measuring the rate constants for a reaction for unlabeled material and isotopically labeled material, with the ratio of these two rate constants yielding the KIE, eq 1-3. This is simple in principle but there are notable obstacles in practice, including, the tedious and difficult synthesis of isotopically labeling substrates, the challenge of precisely and accurately measuring the absolute kinetics for a reaction, and the difficulty of controlling and maintaining identical reaction conditions for separate reaction vessels.

Methods that competitively determine isotope effects alleviate some of the limitations associated with non-competitive measurements. First, because both isotopic substrates are in the same reaction flask, they are subjected to the same reaction

conditions. Qualitatively the unlabeled and labeled will react identically, but quantitatively they should react at different rates. As a reaction proceeds toward completion, the product becomes enriched in the faster reacting isotopomer while the reactants become enriched in the slower reacting isotopomer. The KIE can then be calculated from the change in the isotopic composition and an accurate measurement of the percent conversion. This method is often preferred because it limits experimental errors.

Competitive measurements require the accurate and precise measurement of the ratio of labeled and unlabeled material. Three techniques are commonly employed, scintillation counting, isotopic mass spectrometry, and NMR methodology. The last of these is employed and developed further in this dissertation.

NMR spectra exhibit separate peaks for each non-equivalent position in a molecule and the size of the peaks is proportional to the amount of the particular isotope being examined at each position. Because NMR is nucleus-specific, it can be used to look at trace nuclei in the presence of large amounts of alterntive isotopes. For almost two decades, it has been recognized that these properties of NMR allow its use to determine deuterium kinetic isotopic effects at natural abundance, at least in special cases.[8]

In 1995, the Singleton group reported a general methodology for the simultaneous determination of KIEs at natural abundance.[5] This method takes advantage of nature's labeling of all substrates to a certain percentage, and avoids the laborious synthesis of labeling substrates. Conveniently, it allows for the combinatorial determination of ^{2}H and ^{13}C KIEs at every atomic position within a molecule very effeciently and precisely.

The Singleton methodology takes advantage of the previously discussed idea that as a reaction proceeds the product will become enriched in faster reacting isotopomers and the starting material will become enriched in slower reacting isotopomers. After taking the reaction to a high conversion (usually >70%), the unreacted isotopically enriched starting material is recovered and purified. High precision NMR spectra of identically prepared samples are obtained for the enriched starting material and compared to a standard sample containing starting material of the same lot that has not been exposed to the reaction conditions. An atom whose isotopic composition is assumed not to be changing over the course of the reaction, KIE=1, and is distant from the reaction center is typically chosen as the internal standard. The changes in isotopic composition of the other atoms are obtained from comparing changes in the integration to that of the internal standard. By NMR methods, the relative isotopic composition (R/R_O) is determined by calculating the ratio of the average integrations. The KIE can then be calculated from R/R_O and the fractional conversion.

Experimental Kinetic Isotope Effects

Standard studies measuring competitive intermolecular KIEs assume that two isotopic molecules **A** and **B** with concentration a and b undergo identical irreversible reactions,[6] then the reaction rates can be expressed as eq 1-8 and 1-9 and the ratio of the rate constants is expressed in eq 1-10.

$$A_{(1)} + B \xrightarrow{k_1} P_{(1)}$$

$$A_{(2)} + B \xrightarrow{k_1} P_{(2)}$$

$$-\frac{da_1}{dt} = k_1 a_1 b \tag{1-8}$$

$$-\frac{da_2}{dt} = k_2 a_2 b \tag{1-9}$$

$$\frac{k_1}{k_2} = \frac{\log\left(\frac{a_1}{a_1^{\,0}}\right)}{\log\left(\frac{a_2}{a_2^{\,0}}\right)} \tag{1-10}$$

The fractional conversion, F, is introduced and defined into the ratio of rates when $a_1/a_1^{\,0} = 1\text{-}F_1$ and $a_2/a_2^{\,0} = 1\text{-}F_2$. Substitution of the terms in eq 1-10 yields eq 1-11, and taking the natural log and rearranging gives eq 1-12.

$$\frac{k_1}{k_2} = \frac{\log(1\text{-}F_1)}{\log(1\text{-}F_2)} \tag{1-11}$$

$$F_2 = 1 - (1\text{-}F_1)^{k_2/k_1} \tag{1-12}$$

From an experimental analysis the direct ratio of the isotopic composition can be expressed as $a_2^{\,0}/a_1^{\,0} = R_0$ and $a_2/a_1 = R$. Substitution of the terms into and solving eqs 1-

10 and 1-11 affords eqs 1-13 and 1-14. Simple rearrangement affords the term used in the calculation of experimental KIE (eq 1-15).

$$\frac{k_1}{k_2} = \frac{\log (1\text{-}F_1)}{\log [(1\text{-}F_1)R/R_0]} \tag{1-13}$$

$$R/R_0 = (1\text{-}F)^{(1/KIE\text{-}1)} \tag{1-14}$$

$$KIE_{calcd} = \frac{\ln(1 - F)}{\ln[(1 - F)R/R_0]} \tag{1-15}$$

In most competitive KIE measurements, the isotopic ratio is small and F_1 can be replaced by the overall conversion F with a negligible effect on the KIE. Error analysis of eq 1-13 indicates that the uncertainty in the KIE decreases significantly as F increases, in spite of the relatively low precision of NMR integrations.[5] This is because the changes in isotope composition in recovered starting material can greatly exceed the size of the isotope effect. Figure 1-2 illustrates the relationship between the isotopic ratio, R/R_0, and the fractional conversion, F.

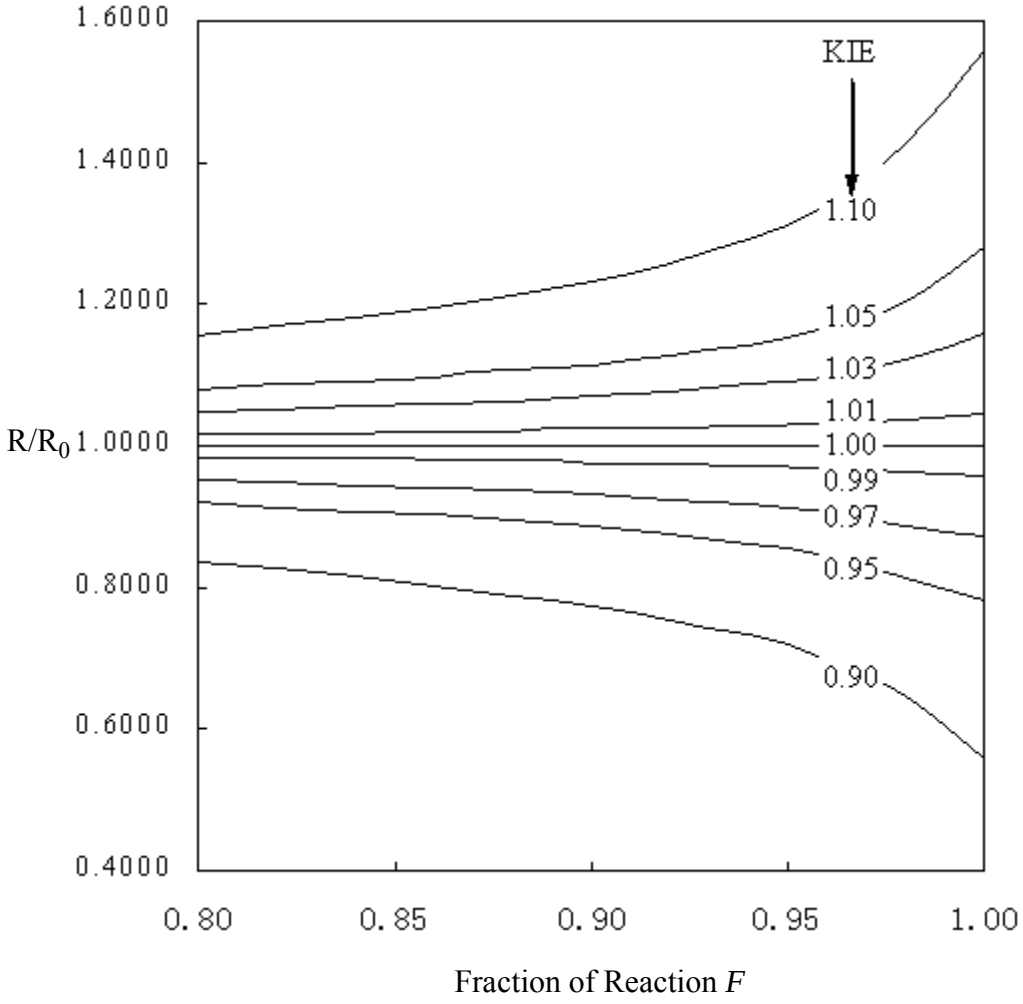


Figure 1-2. Illustrates the relationship between the isotopic ratio, R/R_0, and the fractional conversion, F, and their effect on the KIE.

Predicting Kinetic Isotope Effects

The ability to computationally explore complex reaction mechanisms is improving rapidly. Applying density functional theory calculations in combination with experimental KIEs provides a powerful tool in elucidating a reaction path. Theoretical calculations can now be applied to reasonably large systems which not only allow for the

detailed exploration of a reaction mechanism, but also a quantitative interpretation of the experimental isotope effects.

Kinetic isotope effects for each transition state located along a reaction path can be predicted from the scaled vibrational frequencies[9] by apply conventional transition state theory using a method described by Bigeleisen and Mayer.[10] Conventional transition state theory makes no allowance for tunneling, and the prediction of KIEs is improved by including a one-dimensional tunneling correction (eqs 1-16 – 1-18).[11] Such predictions have proven highly accurate in reactions not involving hydrogen transfer, as long as the calculation accurately depicts the mechanism and the transition state geometries.[2]

$$(S_2/S_1)\, f_{GS} = \prod_{i}^{3N-6} \left\{ \frac{u_{i\,(2)}}{u_{i\,(1)}} \times \frac{\mathrm{EXP}[(1/2)\, u_{i\,(1)}]}{\mathrm{EXP}[(1/2)\, u_{i\,(2)}]} \times \frac{1-\mathrm{EXP}(-u_{i\,(1)})}{1-\mathrm{EXP}(-u_{i\,(2)})} \right\} \qquad (1\text{-}16)$$

$$(S_2/S_1)\, f_{TS} = \prod_{i}^{3N^{\ddagger}-6} \left\{ \frac{u_{i}^{\ddagger}{}_{(2)}}{u_{i(1)}} \times \frac{\mathrm{EXP}[(1/2)\, u_{i}^{\ddagger}{}_{(1)}]}{\mathrm{EXP}[(1/2)\, u_{i(2)}]} \times \frac{1-\mathrm{EXP}(-u_{i}^{\ddagger}{}_{(1)})}{1-\mathrm{EXP}(-u_{i(2)})} \right\} \qquad (1\text{-}17)$$

$$\mathrm{KIE}_{TST} = \frac{\nu^{\ddagger}_{L\,(1)}}{\nu^{\ddagger}_{L\,(2)}} \times \frac{(S_2/S_1)\, f_{GS}}{(S_2/S_1)\, f_{TS}} \qquad (1\text{-}18)$$

where $u_i = h\upsilon_i/kT$

υ_i = frequency of the i^{th} vibrational mode

k: Boltzmann constant

h: Planck's constant

T: temperature in Kelvin

f: force constant

Conclusion

Despite the simplicity in the approach, transition state theory can be effectively and accurately applied in the prediction of isotope effects. The Singleton group has effectively used a combination of experimental KIEs and computational theory as an extremely powerful tool in mechanistic investigations. This dissertation focuses on applying the above described theories and methodology to obtain a qualitative and quantitative picture of the transition state for the rate-limiting step. This aid will provide valuable clues in determining a reaction's path.

CHAPTER II

ISOTOPE EFFECTS AND THE NATURE OF SUBSTRATE SELECTIVITY IN THE IRIDIUM CATALYZED BORYLATION OF ARYL C-H BONDS

Introduction

Carbon-hydrogen bonds are the most ubiquitous in Nature. The selective functionalization of inert C-H bonds is a long standing goal with far reaching implications. Hydrocarbons are the major constituent of petroleum feedstock, but currently there lacks efficient processes for their direct conversion into more valuable chemical commodities. Our fundamental understanding of the limited chemical reactivity of C-H bonds can be attributed to their high bond energies, low acidity, and low basicity. Despite the difficulty in cleaving inactivated C-H bonds, relative to carbon-halogen bonds, they are not completely inert.

The selective functionalization of C—H bonds is attractive owing to their ubiquity in organic molecules. This was recognized as early as 1834, when Mitscherlich reported on nitrations of substituted benzenes.[12] Indeed, the rules of electrophilic aromatic substitution that are taught today were established in the early 20th century.[13] Nevertheless, significant challenges in the functionalization of aromatic C—H bonds remain despite important advances, such as nucleophilic aromatic substitution and

directed ortho metalation.[14,15] The development of new processes that complement existing methods are critical because functionalized aromatic compounds pervade chemistry, biology, and materials science.

Nature has formulated a process for the direct oxidation of hydrocarbons. Enzymes known as monooxygenases, such as methane monooxygenase (MMO)[16] and cytochrome P450 monooxygenase (P450),[17] have attracted attention because of their ability to oxidize saturated hydrocarbons. Despite intense study on the mechanisms of MMO and P450, agreement is limited as to the definitive mechanistic details. However, iron is known to play a critical role in the enzyme's catalysis, which has led to the intense study of structural and fuctional mimics performing similar processes.[18]

Transformations of alkanes have been limited to radical processes in the gas and solution phase, until recently. The activation of C-H bonds by transition metal complexes has been a major goal in organometallic chemistry, and over the past 20 years, metal-mediated C-H activation has emerged.[19] While C-H activation is requisite for generating species with M-C bonds, catalytic examples that further elaborate the M-C bond selectively are limited.[20,21,22,23]

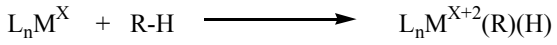
The role of transition metals in the elaboration of C—H bonds has developed more recently.[24] While Chatt reported the first C—H oxidative addition to a transition metal in 1965,[25] the implications for aromatic C—H functionalization were not evident until later when Ittel et al. reported the oxidation addition of toluene to low valent iron.[26] Specifically, they found the activation of toluene's aromatic C—H bonds to be strongly preferred over the weaker benzylic C—H bonds. In terms of regioselectivity, meta and

para aryl C—H insertion products formed in a 2:1 ratio. The absence of ortho activation and the statistical mixture of meta and para isomers suggested that the regiochemistry of C—H insertion was sterically determined. This selectivity was particularly significant since it complemented electrophilic aromatic substitution and directed ortho metalation whose regioselectivities have electronic origins.

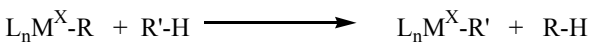
Despite numerous examples of sterically directed C—H insertion that followed Ittel's work, it was not until 1998, when Berry disclosed Rh-catalyzed silylation of *m*-xylene at the 5–position, that this feature was deployed in a catalytic system.[27] Unfortunately, the substrate scope in this system was limited.[28]

The fundamental mechanistic processes for C-H bond activation have been studied extensively and are well developed in many stoichiometric reactions. Several pathways for the activation of C-H bonds have been postulated and studied (Figure 2-1), including (i) oxidative addition of R-H to the transition metal,[29] (ii) σ bond metathesis between M-R' and R-H,[30] (iii) 1,2-addition of R-H to M=X (X=O, NR, CR_2) [31] (iv) electrophilic activation of M-X (X=halide, hydroxide, triflate, ect.) and R-H to generate M-R and HX, and (v) metalloradical activation.[32]

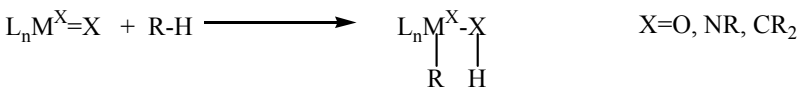
Oxadative Addition



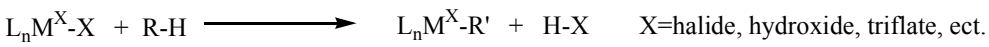
Sigma-bond Metathesis



1,2 Addition



Electrophilic Activation



Metalloradical Activation

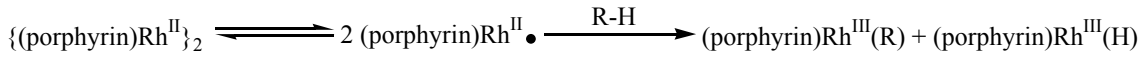
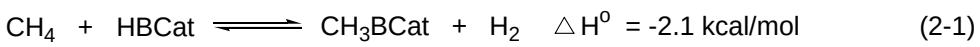
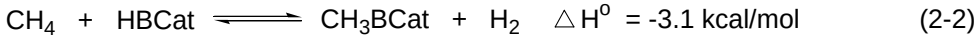


Figure 2-1. Several of the proposed pathways for the activation of C-H bonds.

Despite the tremendous progress with stoichiometric activations, the challenge to develop catalytic systems that could activate and selective functionalize C-H bonds for practical applications remained a "Holy Grail". In 1994, Hartwig *et al.* computationally determined the bond dissociation energies (BDEs) for a series of boranes.[33] From the calculated BDEs for B-H, C-H, and B-C bonds, the synthesis of alkyl boronic esters directly from boranes and alkanes should be thermodynamically feasible because the transformation is essentially thermoneutral (eq 2-1).



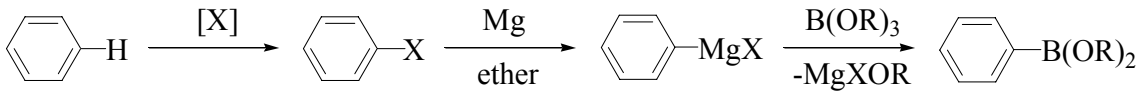
(2-1)



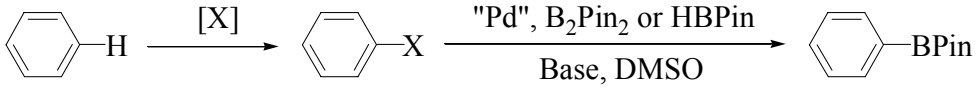
(2-2)

Applications utilizing boronic acids or esters in Miyaura-Suzuki cross-coupling are expansive and demonstrate the catalytic significance of eq 2-1 and eq 2-2.[34] Typically, alkylboron or arylboron reagents are synthesized in multistep processes (Figure 2-2).

Traditional Method



Suzuki *et al.*



Direct Borylation

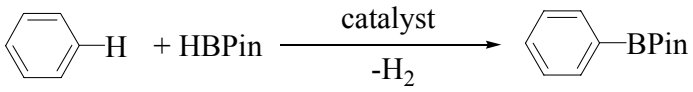


Figure 2-2. Methods for synthesizing arylboranes.

A substantial advance in recent years has been the development of the direct borylations of hydrocarbons. Borylations have been mediated by iron,[35,36,37] ruthenium,[35] tungsten,[35] manganese,[37] molybdenum, rhenium,[37,38] rhodium,[39,40,41,42] and iridium[39,43,44,45,46,47,48,49] complexes, and efficient catalytic systems have been developed. This diversity of metal complexes and the versatility of the products suggest that a very rich chemistry of these reactions is emerging.

In 1999, Smith and coworkers reported a thermal, Ir-catalyzed conversion of benzene and pinacolborane (HBPin) to phenylpinacolatoborane (PhBPin) and

dihydrogen.[43] Smith *et al.* discovered substantial amounts of arylborone products produced from solvent activation while investigating the stoichiometric B-C bond formation of pre-catalyst Cp*Ir(PMe_3)(Ph)(H) and HBPin in C_6D_6.[43] Subsequent characterization and synthesis of the active organometallic borane complex, Cp*Ir(PMe_3)(BPin)(H), led to development of the first catalytic borylation of arenes. Intrigued by Marder's synthesis of of (η^6-arene)Ir($BCat)_3$ from (Ind)Ir(cod) in HBCat in arene solvents,[50] led to Smith *et al.* developing an analogous route that is catalytically viable and quantitatively forms arylboranes.[44] The reaction exhibits excellent chemoselectivity and interesting regioselctivity trends.[48] The borylation does not follow traditional electrophilic aromatic substitution patterns. Mono-substituted arenes yield a mixture of ortho, meta, and para regioisomers; interestingly, meta substitution is favored. The borylations seem to be sterically directed.[51] These direct borylations have allowed for the simple synthesis of usually difficult arylboranes that can be used in the production of more complex structures.[44]

Although the initial catalytic system was inefficient, it was nevertheless the first thermal conversion of its type. Subsequent work showing that chemoselectivities in Ir-catalyzed transformations[40] were superior to those arising from a seemingly more efficient Rh system[39] provided the impetus to identify the catalytically relevant species in the Ir catalytic manifold. In 2002, Smith and coworkers reported the results of these efforts, which strongly implicated Ir^{III} phosphinoboryl complexes as the species responsible for catalysis.[44] Now generated from much more efficient precatalysts, the bisphosphine[44] and closely related dipyridyl Ir species[46] are efficient and compatible

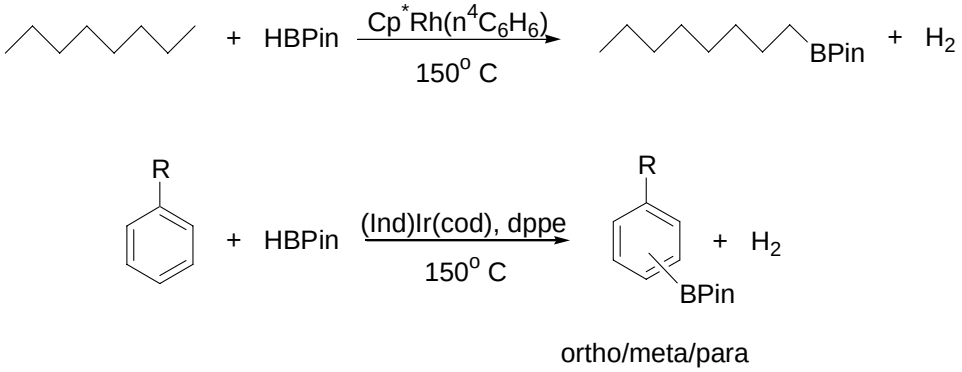
with a broad range of functional groups. Consequently, Ir-catalyzed borylation is emerging as a practical means of functionalizing sp^2-hybridized C—H bonds in aromatic and heteroaromatic molecules.[44,46,47,48,52,53,54,55,56,57,58,59]

The unique features of Ir-catalyzed borylations make the quest for a detailed understanding of its mechanism an important one. To date the most thorough computational study is the one reported by Sakaki and co-workers,[60] and the most detailed mechanistic study is that recently disclosed by Hartwig and co-workers.[61] Though these two studies agree on certain common features, there are points of computational and experimental dissonance. For example, Sakaki's computed barrier for the C—H insertion is nearly 10 kcal/mol higher than the barrier Hartwig estimates from his experimental data.

Further features of Ir-mediated borylations have yet to be addressed. For instance, even though steric effects dominate, electronic effects can contribute significantly to regioselectivities. Understanding the origins of these selectivities is critical to designing improved catalysts for the functionalization of more advanced substrates. For this reason, we have undertaken a unified computational and experimental approach to shed additional light on the underlying mechanism. In particular, we have focused on computationally evaluating ^{13}C and ^{2}H isotope effects and regioselectivities for mono-substituted benzenes, determined experimentally, in the context of potential mechanisms for Ir-mediated C—H functionalizations. This contribution is based on the findings from this study.

A critical issue in the ultimate utility of catalytic borylations is the understanding and control of selectivity. In some ways, these reactions are surprisingly selective, for example in specifically borylating methyl groups of alkanes. However, borylations of arenes are surprisingly unselective, generating mixtures of *ortho, meta,* and *para* isomers from mono-substituted arenes (Scheme 2-2).[46] One might expect C-H activation in arenes to be in essence an electrophilic process, but the regioselectivity differs greatly from conventional electrophilic aromatic substitutions. A detailed mechanistic understanding of selectivity in these reactions has been lacking.

Scheme 2-2



Examples of catalytic reactions that will selective functionalize the terminal position of a linear alkane have been limited to the photochemical and thermal production of alkylboranes.[38,42] The thermal reaction between n-octane and pinacolborane (HBpin) catalyzed by either iridium or rhodium transition metal complex exploits the regiospecific borylation of n-alkane methyl groups to afford a terminal alkylboronate ester. Interestingly, the linear product is not the result of an isomerization

from initially formed internal alkylboronate ester, but the steric preference for formation of a linear transition state metal-alkyl complex.[39,62,63]

Despite the importance of the iridium-catalyzed aryl borylation, the mechanism and the structure of the active catalytic species remains unknown. Several mechanistic proposals have been suggested, but none with fruitful evidence as to the catalytic cycle or the nature of selectivity for the C-H activation.[44] Several groups agree that C-H bond activation is rate-limiting, but their ^{2}H isotope effects are difficult to interpret.[35,44] A more quantitative and qualitative picture of the transition state for the rate-determining step will confirm or disprove previous postulates. Determining ^{13}C KIEs should alleviate isotopic scrambling and allow for the determination of the catalytic cycle as well as understanding the nature of the selectivity for C-H activation.

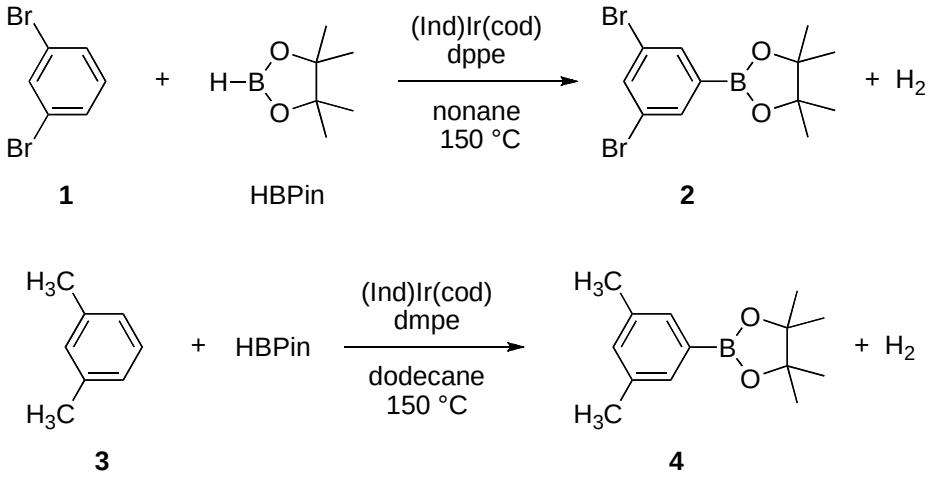
We describe here a study of the mechanism of iridium-catalyzed borylation of arenes with pinacolborane (HBpin) using a combination of kinetic isotope effects (KIEs) and DFT calculations. The results delineate a surprising rate-limiting step and provide insight into the nature of selectivity in these reactions.

Results

Experimental

Experimental ^{13}C Kinetic Isotope Effects. The measurement of high-precision and high-accuracy kinetic isotope effects by a competition reaction typically requires a comparison of product from a reaction taken to partial conversion with product from a clean reaction taken to complete conversion, or else a comparison of starting material

from a reaction taken to high conversion with original starting material. Because many C-H activation reactions require a large excess of reactant, with the products subject to further conversions in reactions taken to high conversion, many such reactions, particularly including borylations, are not readily amendable to best-quality isotope effect measurements. However, the selective borylations of arenes catalyzed by iridium complexes work well in this regard. For example, the borylation of 1,3-dibromobenzene (**1**) with pinacolborane (HBPin) using (Ind)Ir(cod)/dppe as catalyst precursor occurs cleanly in nonane at 150 °C and affords the borylarene **2** as the only observable product. *m*-Xylene (**3**) is less reactive and subject to reaction at the benzylic methyl groups, but its borylation to afford **5** can still be taken to over 70% conversion with only ≈5% reaction at the methyl groups.[64]



The complete set of ^{13}C kinetic isotope effects for the borylations **1** and **3** were determined at natural abundance by NMR methodology. Two borylations of **1** employing 2 mol % of (Ind)Ir(cod), 2 mol % of dppe, and 1.5 eq of HBPin were taken to 75 and 73.5% conversion at 150 °C. The unreacted **1** was recovered after an aqueous

workup followed by fractional distillation, then analyzed by ^{13}C NMR. Changes in isotopic composition relative to the original **1** were determined using the aromatic *para* carbon as a standard, assuming that its isotopic composition does not change. From the changes in isotopic composition, the ^{13}C KIEs were calculated as previously described.[5] An analogous process was applied in a reaction of **3** taken to 73% conversion.

The isotope effects obtained are summarized in Figure 1. The Ind(Ir)(cod) catalyzed borylation with **1** and **3** exhibits a substantial ^{13}C KIE at the *meta* aryl carbon and negligible KIEs at the remaining aromatic ring carbons. The large isotope effect at the *meta* aryl carbon qualitatively suggests a substantial bond breaking or bond formation to this carbon in the rate-limiting step. In fact, the ^{13}C KIEs by themselves would not qualitatively delineate between C-H bond breaking or C-B bond formation. The isotope effects observed for the (Ind)Ir(cod) catalyzed borylation with **1** and **3** are within experimental error of another suggesting a similar transition state geometry.

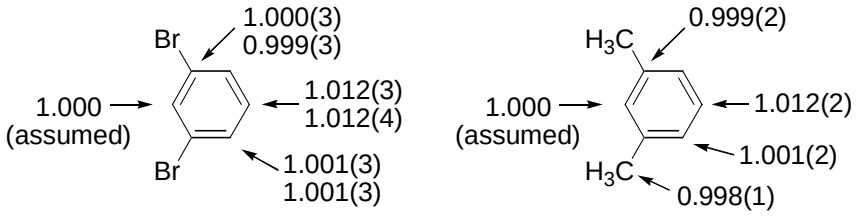
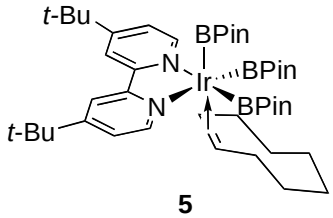


Figure 2-3. ^{13}C Kinetic isotope effects (k_{12C}/k_{13C}, 150 °C) for borylations of **1** and **3** with pinacolborane using (Ind)Ir(cod)/dppe as catalyst precursor. Numbers in parentheses are 95% confidence limits for the last digit.

H/D KIEs and H/D Exchange. Ishiyama, Miyaura, and Hartwig have reported H/D KIEs for both stoichiometric and catalytic borylations mediated by the bipyridine-

ligated iridium trisboryl complex **5**, based on both competition reactions (C_6H_6 versus C_6D_6 or *o*-$C_6H_4Cl_2$ versus *o*-$C_6D_4Cl_2$) or absolute kinetics (*o*-$C_6H_4Cl_2$ versus *o*-$C_6D_4Cl_2$).[46,61] All of the H/D KIEs observed have been within a range associated with primary hydrogen isotope effects, suggesting rate-limiting cleavage of the aryl C-H bond. However, the variability of the observed KIEs has been notable: 2.0 ± 0.4 for a *o*-$C_6H_4Cl_2$ / *o*-$C_6D_4Cl_2$ competition reaction, 3.3 ± 0.6 for a *o*-$C_6H_4Cl_2$ / *o*-$C_6D_4Cl_2$ absolute kinetics, and ranging from 3.6 ± 0.2 to 5.0 ± 0.4 for catalytic and stoichiometric reactions of **5** with C_6H_6 / C_6D_6. Such a large variation in the KIEs is unusual and suggests experimental or mechanistic complexities. Our results will define two such complexities.



5

The H/D KIEs here have been measured in several ways, using (Ind)Ir(cod)[65] (**6**) / dmpe, **6** / 2 PMe_3, or (MesH)Ir(Bpin)$_3$[66] (**7**) / 2 PMe_3 as pre-catalysts in catalytic reactions of HBPin or using *fac*-(PMe_3)$_3$Ir(Bpin)$_3$[66] (**8**) in stoichiometric thermolysis reactions. In all cases, the borylation reaction was carried out at 150 °C using excess arene as solvent. The experiments using PMe_3 as the phosphine co-ligand under catalytic conditions were undertaken to facilitate comparison with the stoichiometric reaction employing the fully characterized complex **8**. Both intermolecular and intramolecular KIEs were measured, the former using a 1:1 mixture of C_6H_6 and C_6D_6,

and the latter using 1,3,5-trideuterobenzene. Intermolecular KIEs are the measure of the impact of isotopic substitution on the overall reactivity of a molecule, reflecting the transition state for the first irreversible step undergone by the arene substrate in a catalytic reaction. Intramolecular KIEs reflect the relative facility of two branches of a mechanism that are equivalent, except for isotopic substitution. As such, intramolecular KIEs characterize the selectivity-determining step in a reaction, the step determining regioselectivity in the current case. When the intermolecular and intramolecular KIEs are both determined at the same transition state, the two should correspond in a logical fashion, though they will not necessarily be equal due to secondary isotope effects.

The results are summarized in Table 1. In each case the H/D KIE is substantial and consistent with a primary KIE resulting from rate-limiting and selectivity-determining C-H bond cleavage. The large observed KIE in borylations of C_6H_6 / C_6D_6 argue against rate-determining arene coordination, which Jones found to be the case for C–H activations mediated by Rh(I) intermediates.[67] The similar KIEs for borylations in 1,3,5-trideuterobenzene corroborate this conclusion – if arene coordination was even partially rate limiting, it would be expected that the intramolecular KIE would be larger than the intermolecular KIE. The general similarity of the KIEs observed in the stoichiometric reactions of **8** with those observed in the catalytic reactions supports is consistent with a common active species in C–H activation.

However, two trends in the magnitude of the KIEs should be noted. The first is that the H/D KIEs with the dmpe and PMe_3 are all smaller than those observed in

reactions of **5** with C_6H_6 / C_6D_6. The second is that the intramolecular KIEs observed using 1,3,5-trideuterobenzene are all somewhat smaller than the intermolecular KIEs observed using C_6H_6 / C_6D_6.

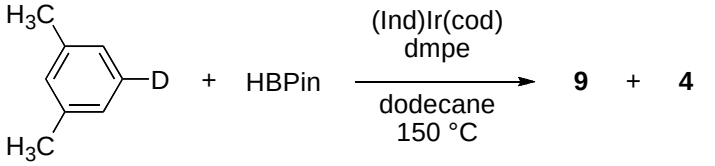
Table 2-1. Intermolecular and intramolecular H/D KIEs for borylation reactions at 150 °C.

Conditions	Substrate[a]	KIE
0.02 (Ind)Ir(COD) (**6**) : 0.02 dmpe : 1 HBPin	1:1 C_6H_6 / C_6D_6	2.37±0.10
0.02 (Ind)Ir(COD) (**6**) : 0.04 PMe_3 : 1 HBPin	1:1 C_6H_6 / C_6D_6	2.28[b]
	1,3,5-$C_6D_3H_3$	1.94[c]
0.02 (MesH)Ir(Bpin)$_3$ (**7**) : 0.04 PMe_3 : 1 HBPin	1:1 C_6H_6 / C_6D_6	2.29[b]
	1,3,5-$C_6D_3H_3$	2.06[c]
fac-(PMe_3)$_3$Ir(Bpin)$_3$ (**8**)	1:1 C_6H_6 / C_6D_6	2.53[b]
	1,3,5-$C_6D_3H_3$	1.93[c]

[a]The substrate was used in a 15- to 22-fold excess versus the HBPin for the catalytic reactions and used in a 140-fold excess versus the *fac*-(PMe_3)$_3$Ir(Bpin)$_3$ for stoichiometric thermolysis. [b]The intermolecular KIE measurements were based the ratio of the baseline-separated peaks for C_6H_5Bpin and C_6D_5Bpin in gas chromatographic analysis. [c]The intramolecular KIE measurements were based on ^{1}H NMR integrations for the aromatic hydrogens in the crude mixture of $C_6D_3H_2$BPin and $C_6D_2H_3$BPin.

A complicating factor in the observation of H/D KIEs in these reactions was brought to light in an attempt to measure the isotope effect for borylation of *m*-xylene. *m*-Xylene-5-d (**9**) with ≈80% deuterium at C5 was prepared by forming the Grignard

reagent from 5-bromo-*m*-xylene, followed by quenching with D_2O. This material was borylated to 40-50% conversion using (Ind)Ir(cod)/dmpe in dodecane at 150 °C, followed by NMR analysis of the unreacted **9**. Surprisingly, the deuterium incorporation in the recovered **9** was consistently *less* than that in the original **9**. If a normal primary isotope effect were operative, it might be expected that the deuterium incorporation would increase in recovered **9**. The observed decrease would thus suggest a difficultly rationalized inverse isotope effect. A better explanation for this observation is that the borylation is accompanied by competitive H/D exchange with the HBPin. In a kinetic simulation that assumes that the borylation and H/D exchange have identical rate laws (except for rate constants) and assumes an H/D KIE of 2.3 for borylation, the observed decrease in deuterium incorporation can be modeled if H/D exchange is 8 – 15 times slower than borylation.



9	starting %D in **9**	%conversion	final %D in **9**
	82.1	42.5	77.2
	82.6	46.0	77.1
	81.0	44.9	78.0

H/D exchange under these reaction conditions was verified in a study of the borylation of pure C_6D_6. In a reaction employing 2 mol % (Ind)Ir(Cod) / dmpe versus HBPin with excess (26 equiv) C_6D_6 taken to 80% conversion of HBPin at 150 °C, NMR analysis of the reaction mixture revealed that 17% of the H in the original HBPin was present as C_6D_5H, and that the ratio of DBPin to HBPin was 3:1. The exchange increases at further borylation conversion – at 93% conversion of the HBPin, 20% of the

H in the original HBPin was present as C_6D_5H and the ratio of DBPin to HBPin was 6.7:1. In a kinetic simulation of these results, the observed C_6D_5H and DBPin / HBPin ratio could be modeled with H/D exchange roughly 2 – 10 times slower than borylation (the best-fit value depends on the unknown DBPin / HBPin reactivity isotope effect).

The experimental complexity of competitive H/D exchange may account for some of the variability in the other H/D KIE measurements. Because the attempted measurement of the KIE with **9** depended on analysis of recovered starting material and because only one deuterium was present, this reaction was highly sensitive to H/D exchange. The KIE measurements with C_6H_6 / C_6D_6 are much less sensitive to exchange, as they depend on product analysis and this analysis cannot distinguish between C_6D_5BPin and C_6D_4HBPin. The measurement with 1,3,5-trideuterobenzene is somewhat more sensitive to exchange than the C_6H_6 / C_6D_6 experiment because H/D exchange in either product or starting material can affect the NMR analysis of the apparent products ratios. Under any circumstances, the operation of competitive H/D exchange will have to be considered in the mechanistic analysis of these reactions.

Theoretical Calculations

Theoretical Calculations. The reaction pathway for the iridium catalyzed borylation was studied in B3LYP calculations employing a SDD basis set and effective core potential on iridium and a 6-31G** basis set on all remaining atoms. Calculated energies associated with the catalytic cycle are presented here in two ways, either as potential energy with a zero-point energy correction (E +zpe) or as a free energy estimate including an estimated relative entropy. Previous work has supported the

ability of these calculations to adequately predict ground-state structures and reasonable mechanistic pathways for transition metal boryl complexes.[68,69,70,71] The accuracy of these calculations to predict the transition state structures for the iridium catalyzed borylations will be gauged by comparison of the theoretically predicted and experimental isotope effects. Several mechanistic pathways for the iridium-catalyzed borylation of benzene were modeled, but only the cycles that accurately predict the KIEs and are energetically viable will be discussed here.

Smith[44] proposed a mechanism based upon Marder's[42a] synthesis of (η^6–arene)Ir(BCat)$_3$ (Cat=ortho-catecholate) from (Ind)Ir(COD). Initial meachanistic studies excluded a simple phosphine dissociative pathway which narrowed possible active catalytic cycles to loss of Cp (Figure 2-4).

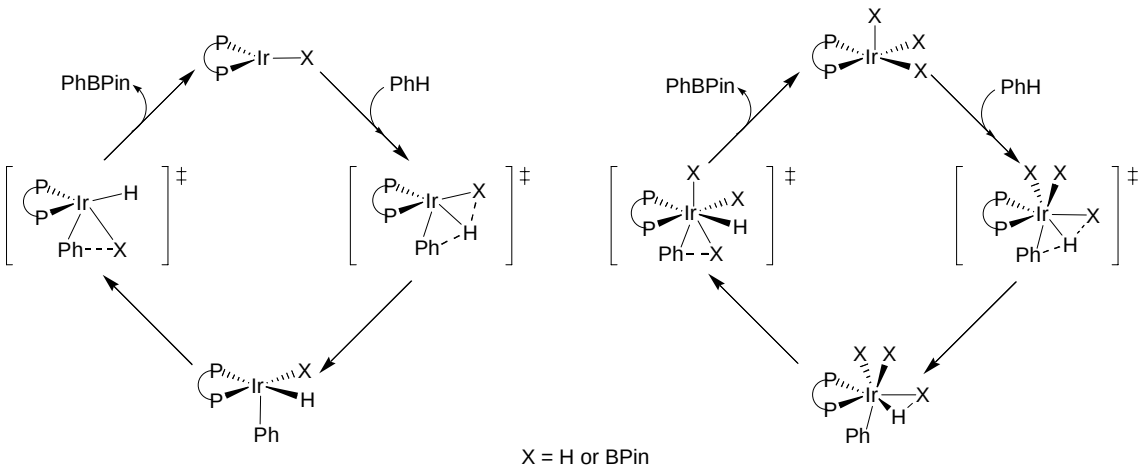
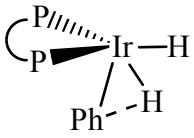
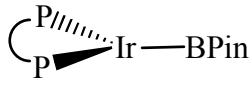
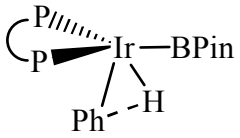
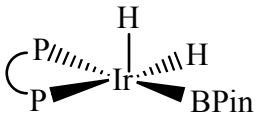
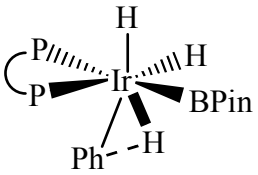
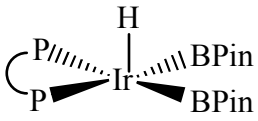
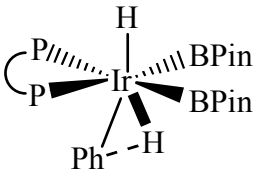


Figure 2-4. Proposed catalytic cycles.

Initially we began modeling the Ir (I-III) cycle, until it was discovered that the iridium tris-BPin was catalytically viable. Table 2-2 briefly summarizes some of the Ir (I)/Ir(III) and Ir(III/Ir(V) catalysts that were explored along with their corresponding

relative energies and KIEs. Eventhough the calculational models mostly discussed here involve (dmpe) or (bpy) and the tris-BPin, it is our hypothesis that (dmpe)Ir(BPin)$_2$(H) or (dmpe)Ir(BPin)(H)$_2$ may be involved in the catalytic cycle. The two species involvement in the reaction is being explored, and we believe they are directly responsible for the experimentally observed deuterium exchange.

Table 2-2. Active catalyts explored for C-H activation.

Initial Catalyst	C-H Activation TS	Relative Energies	Calculated KIE
		zpe = 9.12 $\Delta G_{423} = 8.60$	^{13}C KIE = 1.017 $k_H/k_D = 3.218$
		zpe = 9.70 $\Delta G_{423} = 9.59$	^{13}C KIE = 1.016 $k_H/k_D = 3.230$
		zpe = 12.48 $\Delta G_{423} = 15.97$	^{13}C KIE = 1.017 $k_H/k_D = 3.232$
		zpe = 14.37 $\Delta G_{423} = 16.70$	^{13}C KIE = 1.016 $k_H/k_D = 3.241$

The calculational model reactions here were chosen to be reasonably complete, including the use of bypyridine as a model for the ligand in reactions employing dtbpy and dmpe as the ligand or model ligand for reactions employing dmpe, dppe, or PMe_3 as

ligand. The parent 1,3,2-dioxaborolane, HBeg (eg (ethyleneglycolato) = OCH_2CH_2O), was used as a model for HBPin, except as noted. A variety of catalytic cycles were explored, including Ir(I)/Ir(III) cycles and Ir(III)/Ir(V) cycles with various substituent on the iridium – important aspects of the cycles judged non-experimentally relevance are given in the Appendix. The cycles described here involve iridium coordinated to a chelating ligand (dmpe or bpy in the calculations) and three BPins (three 1,3,2-dioxaborolanes in the calculations), as in **10** and **20**, as a key intermediate. Such cycles have received substantial support from the mechanistic work of Hartwig and coworkers, and will be found here to be consistent with our experimental studies in a variety of ways. Extensive effort was made to broadly explore the stereochemical diversity of possible minima and transition structures for the catalytic cycle. However, the conformational complexity of the cycles, particularly with dmpe as ligand, required some selection of conformations considered energetically competitive. For example, a total of five transition structures were located for C-H activation in the reaction of **10** with benzene, all within 2 kcal/mol of the best structure **11**. A great many more possibilities might be envisioned, arising from the cant of the chelating dmpe and possible orientations and arrangements of the Beg ligands and the incoming benzene versus the dmpe, but these possibilities were excluded based either on observations with the five located structures or based on model studies employing $H_2PCH_2CH_2PH_2$ as ligand. The discussion here will focus on the key structures for the lowest-energy catalytic cycle – higher-energy structures and mechanistically minor stationary points are given in the Appendix.

The preferred structure for (dmpe)Ir(Beg)$_3$ is the square pyramidal **10** (Figure 2). The empty axial site of **10** is not electrophilic – a complex of benzene at this site was located (see the Appendix) but it was extremely loose with an Ir—C distance of 3.44 Å. At a complexation energy of –4.6 kcal/mol (E + zpe), it is questionable whether such a complex is a real minimum on a free energy surface. The C-H activation step faces the highest barrier in the catalytic cycle at 19.7 kcal/mol (E + zpe). The transition structure **11** for C-H activation is quite late with a nearly complete broken C-H bond (at 1.68 Å) and essentially fully formed C-Ir and H-Ir bonds. The C-H activation is not a simple oxidative addition leading to a heptacoordinate Ir(V) intermediate, but is better described as a metal-assisted σ-bond metathesis involving a hydrogen transfer from carbon to boron to afford the η2-HBeg structure **12**.

The reductive elimination of PhBeg from **12** might be envisioned as occurring directly by C-B bond formation with the equatorial Beg ligand, but this would require either formation of an Ir(I) η2-HBeg intermediate or full oxidative addition of the η2-HBeg. The latter occurred in a search for such a transition structure, but the barrier was high (25.7 kcal/mol) and considerable ligand reorganization is involved (the transition structure itself, in the Appendix, resembles structure **23** in the bpy cycle below). Instead, reductive elimination occurs via transition structure **13** for rotation of the equatorial η2-HBeg ligand. This places the boron of the η2-HBeg ligand near the phenyl group. After this rotation, there is no barrier to formation of the PhBeg, so that the transition structure for "reductive elimination" is best understood as simply the

transition structure for ligand rotation. Loss of PhBeg (via a very weak complex – see the Appendix) leads to (dmpe)Ir(H)$(Beg)_2$ **14**.

The regeneration of **10** from **14** starts with axial coordination of HBeg to afford the η2-HBeg complex **15**. Ligand reorganization can then occur in an intriguing fashion involving transfer of a Beg group from an axial hydride to an equatorial hydride with simultaneous rotation of the transient equatorial η2-HBeg structure via transition structure **16**. No local minimum can be located for a equatorial η2-HBeg complex unless the boron atom of the η2-HBeg is rotated away from the axial hydrogen. The process affords the equatorial η2-HBeg complex **17**. Transfer of a hydrogen from HBeg to the axial hydride via transition structure **18** affords axial η2-H_2 complex **19**. Loss of H_2 from **19** reforms **10**. There is no potential energy saddle point associated with the loss of H_2, but an approximate canonical variational transition was located and is shown in the Appendix.

The most striking feature of the calculated catalytic cycle with dmpe as ligand is the absence of clear Ir(V) intermediates. Instead, the catalytic cycle proceeds by a series of η2 Ir(III) intermediates, though some of the transition states interconverting these intermediates may interestingly be described as Ir(V). The rate-limiting C-H activation transition structure **11** is of this type. It is notable for the isotope effect analysis below that the rotational transition structure **13** is only modestly lower in energy than **11**, particularly in the estimated free energy, so that this transition structure is predicted to be partially rate limiting.

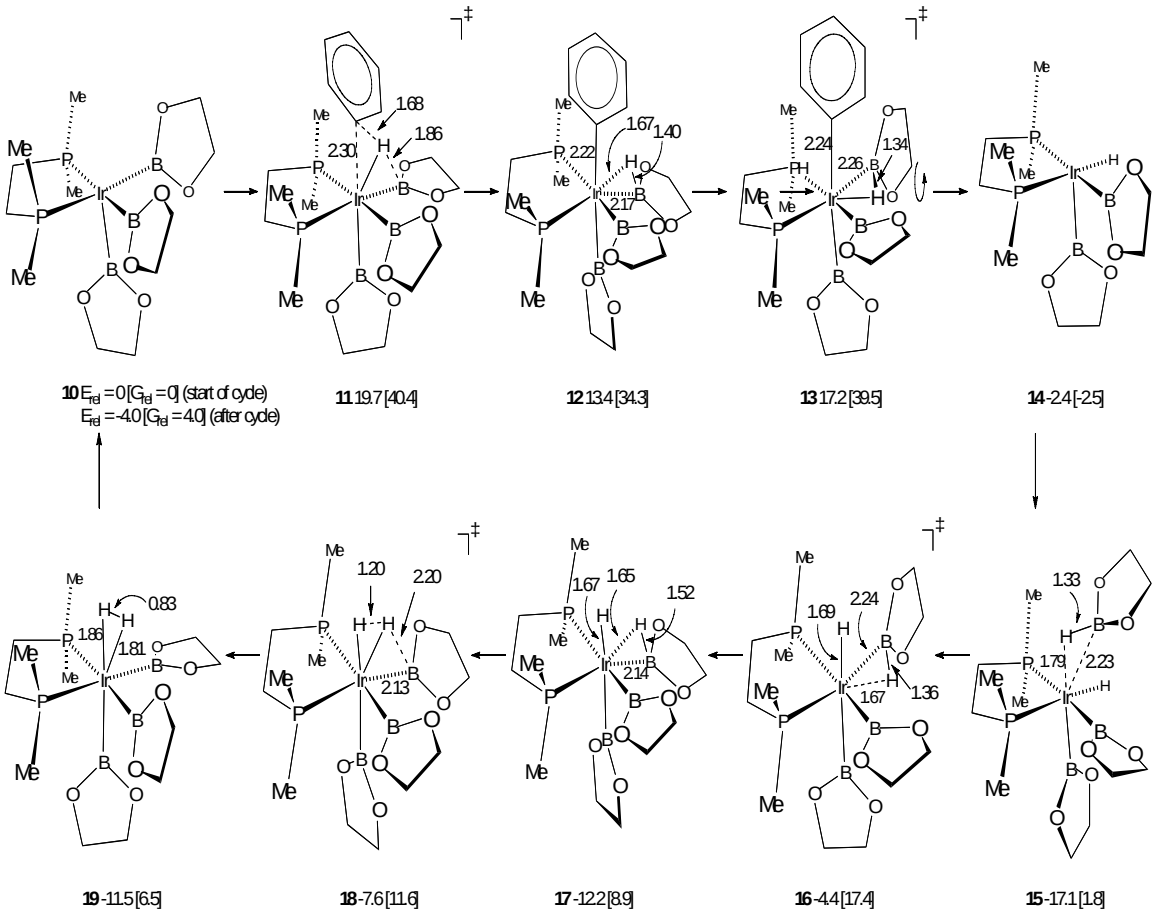


Figure 2-5. Key structures and energies (kcal/mol, relative to **10** and free starting materials) in the calculated catalytic cycle for the borylation of benzene via (dmpe)Ir(Beg)$_3$. Higher-energy stereoisomers and minor stationary points are given in the Appendix.

The calculated catalytic cycle via (bpy)Ir(Beg)$_3$ (Figure 2-6) differs from that previously described in the thorough work of Sakaki in some ways, but eight of the twelve key structures are effectively identical to those reported by Sakaki. The cycle will be discussed here tersely as a background for comparison with experimental observations. In contrast to the dmpe cycle, the bpy cycle is predicted to involve

intermediates best described as Ir(V). Thus, the C-H activation transition structure **21**, while similar to **11**, leads to Ir(V) intermediate **22**. This appears to be true even when the full steric requirements of the BPin ligand are taken into account – optimization of the dodecamethyl [$(BPin)_3$] analog of **22** retained the Ir(V) structure with a B--H distance of 1.64 Å (see the Appendix). No minimum could be located for the corresponding η2-HBPin structure, even in the dodecamethyl analog. Sakaki had reported that reductive elimination of PhBeg occurs by a transition structure equivalent to **25**, but prior to **25** there is a significant barrier for ligand reorganization, occurring via transition structure **23**. Once the ligands are arranged correctly as in intermediate **24**, reductive elimination affording PhBeg and **26** is nearly barrierless. The pathway for reformation of **20** from **26** requires formation of the Sakaki $Ir(Beg)_3(H)(H)(bpy)$ intermediate **29** followed by formation of the axial η2-H_2 complex **31** and loss of H_2, but the formation of **29** is complicated. It was previously reported that this occurs via a process resembling the conversion of **15** to **17**, with an equatorial η2-HBeg in the key transition structure (see the Appendix). However, the reorganization of **27** to **29** has a 11.8 kcal/mol lower barrier via transition structure **28**, which is analogous to **23** in the reductive elimination process.

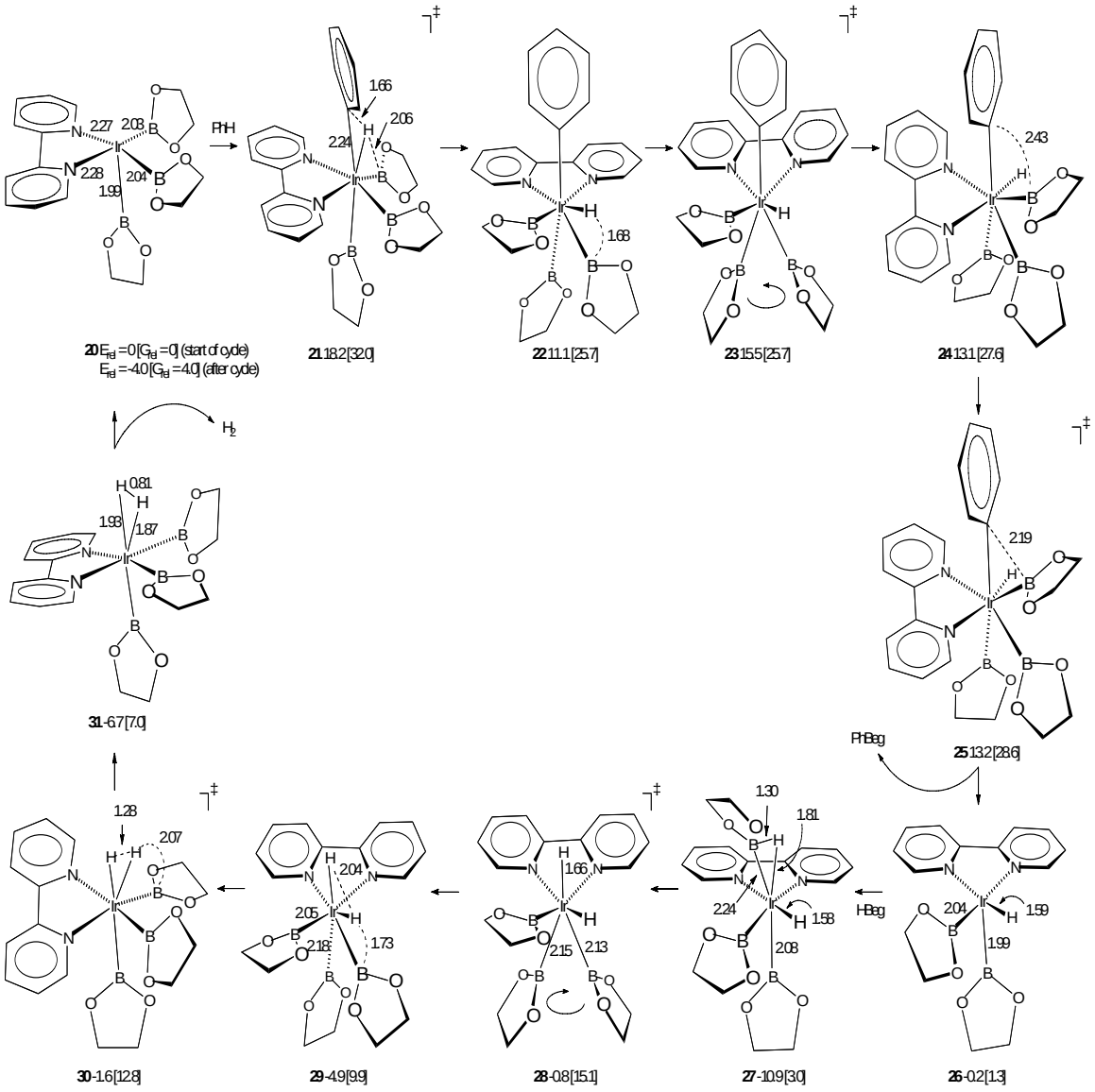


Figure 2-6. Key structures and energies (kcal/mol) in the calculated catalytic cycle for the borylation of benzene via (bpy)Ir(Beg)$_3$. Higher-energy stereoisomers and minor stationary points are given in the Appendix.

Predicted Isotope Effects. For comparison with the experimental ^{13}C KIEs for borylation of **1** and **4** along with the diverse deuterium KIEs observed in other measurements, the ^{13}C and deuterium KIEs were predicted for the borylation of benzene

based on transition structures **12** and **14**. The KIEs associated with these transition structures were predicted from the scaled theoretical vibrational frequencies[72] using conventional transition state theory by the method of Bigeleisen and Mayer.[73] For ^{13}C KIEs, tunneling corrections were applied using the one-dimensional infinite parabolic barrier model.[74] Such KIE predictions have proven highly accurate in reactions not involving hydrogen transfer, so long as the calculation accurately depicts the mechanism and transition state geometry.[2] Due to the difficulty of accurately predicting the effect of tunneling on deuterium KIEs, no tunneling correction was used for the deuterium KIE predictions. Tunneling generally increases deuterium KIEs, so the deuterium KIEs here will be considered as lower-bound predictions for the calculated transition structures.

The results are summarized in Figure 2-7. The ^{13}C KIE predicted for the C_1 position of the C-H activation transition structure **12**, at 1.017, is somewhat larger than the experimental values with **1** and **4** of 1.012. In addition, the lower-bound prediction of the deuterium KIE based on transition structure **12** is higher than the 1.9 – 2.5 range observed using either **7** / 2 PMe_3 or **8** / 2 PMe_3 in catalytic reactions or using **9** in stoichiometric thermolysis reactions. The predicted ^{13}C KIE of 1.013 for C_1 of transition structure **14** seems surprisingly large since this carbon is undergoing no bonding change in **14**, but is understandable since the C_1-Ir bond is much weaker than the aromatic C_1-H bond in the starting material. Similarly, the deuterium KIE for **14** may seem large since **14** is undergoing a stereochemical reorganization, not a hydrogen transfer, but the KIE may be understood from the weakness of the H-Ir bond in **14** compared to the starting aromatic C_1-H bond. Overall, transition structure **14** leads to a

better fit with experiment. However, due to the difficulty of predicting the impact of tunneling on the deuterium KIE for **14**, it is uncertain whether **14** can account for the magnitude of the experimental deuterium KIE.

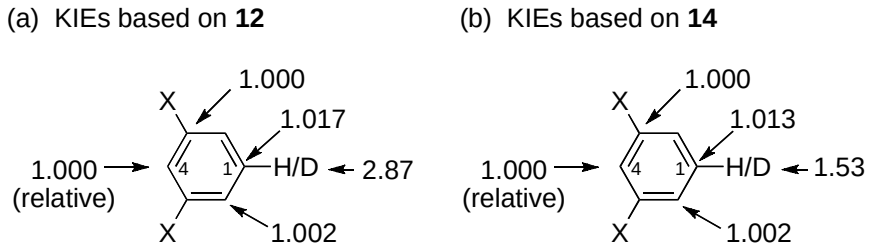


Figure 2-7. Predicted ^{13}C (k_{12C}/k_{13C}) and deuterium (k_H/k_D) kinetic isotope effects at 150 °C. The group X is hydrogen in the calculational structures, compared to bromine or methyl groups in the experimental systems. To facilitate comparison with the experimental ^{13}C KIEs, the predicted ^{13}C KIEs have been adjusted to be relative to C_4. The predicted deuterium KIEs are absolute values and do not include a tunneling correction. (a) Isotope effects based on transition structure **12**. (b) Isotope effects based on transition structure **14**.

Calculated versus Experimental Regioselectivity in Borylations of Arenes. The calculated barriers and regioselectivities for the borylation of arenes were compared with either new or literature experimental selectivities for a series of reactions. On the calculational side, this involved locating various C-H activation transition structures, treating the C-H activation step as fully rate-limiting and selectivity determining. With dmpe as ligand, this process was complicated by the combination of regioisomeric and stereoisomeric transition states – there would be at least 25 possible transition structures for C-H activation of each mono-substituted arene. Only those structures considered potentially energetically competitive were explored, and eleven, eleven, and nine structures were located for C-H activation of toluene, anisole, and chlorobenzene, respectively. For calculating the regioselectivity with dmpe as ligand, only the lowest-

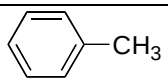
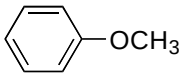
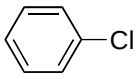
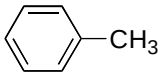
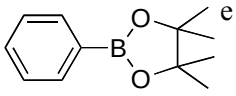
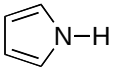
energy transition structure for *para* reaction was considered along with the two lowest-energy transition structures for *meta* reaction. The situation is stereochemically simpler with bpy as ligand and only a single *para* transition structure and two *meta* transition structures were located for each reaction. Complete structures are given in the Appendix. For comparison with the calculational dmpe ligand, some experimental selectivities that had been previously determined with PMe_3 or dppe as ligand were redetermined using dmpe as ligand in reactions employing (Ind)Ir(cod) as precatalysts.

The results are summarized in Table 2-2. The selectivities were calculated in two ways, either based on the E + zpe or based on the estimated free-energy barrier (including entropy). It is not clear which of these should be more accurate – reality obviously includes entropy but the real entropy differences between the quite similar regioisomeric transition structures are likely to be smaller than the random error introduced by including a questionably accurate entropy estimate based on the harmonic frequencies. The predictions based on free-energy are sometimes slightly better and sometimes slightly worse, but overall the two sets of predicted selectivities are quite similar.

The agreement between the calculated and experimental regioselectivities is striking. The greatest error in the relative barriers for *para* versus *meta* substitution was 0.3 kcal/mol in the case of borylation of PhBin (calculationally, PhBeg), and even in this case the calculations correctly predict the energetic preference for *para* substitution. The calculated barriers also fit with the experimental observation that alkyl groups decrease reactivity while BPin or halogen substituents increase reactivity. Finally, the

heteroaromatic pyrrole is predicted to be highly reactive, and experimentally the borylation of pyrrole is complete within a few minutes at room temperature.

Table 2-3. Calculated and experimental regioselectivity in borylations of arenes.

Arene	Catalyst and Conditions	$\Delta E^{\ddagger}$ [$\Delta G^{\ddagger}$] of TS's[a]	Calc'd Selectivity	Observed Selectivity
	(Ind)Ir(COD) dmpe, 150 °C	para: 19.8 [38.5] meta: 19.8 [38.4] meta': 20.1 [39.2] ortho: 26.2 [47.5]	p:m:o 38:62:0 [38:62:0][c]	p:m:o 32:67:1
	(Ind)Ir(COD) dmpe, 150 °C	para: 20.0 [40.5] meta: 19.2 [40.0] meta': 19.9 [40.5] ortho: 20.8 [42.3]	p:m:o 17:70:13[b] [24:70:6][c]	p:m:o 19:76:5
	(Ind)Ir(COD) dmpe, 150 °C	para: 18.4 [38.6] meta: 17.8 [38.4] meta': 18.3 [38.1]	p:m 22:78 [24:76][c]	p:m 23:77
	[Ir(OMe)(COD)]$_2$ dtbpy, 25 °C	para: 18.4 [31.7] meta: 18.5 [31.8] meta': 18.5 [32.1 ortho: 23.3 [36.9]	p:m:o 36:64:0[b] [43:57:0][c]	p:m:o 31:69:0[d]
	[Ir(OMe)(COD)]$_2$ dtbpy, 25 °C	para: 17.8 [31.4] meta: 18.3 [31.4] meta': 18.3 [32.1]	p:m 51:49[b] [44:56][c]	p:m 64:36[f]
	[Ir(OMe)(COD)]$_2$ dtbpy, 25 °C	2-: 12.6 [27.9] 3-: 17.1 [31.2]	2-:3- 99.9:0.1	2-:3- 100:0
	150 °C		99.1:0.9	99.8:0.2

[a]Barriers are B3LYP with an SDD basis set on Ir and a 6-31G** basis set on the remaining atoms, including zpe, in kcal/mol. Estimated activation free-energies are shown in brackets. [b]Calculated selectivities have allowed for an assumed factor of 2 entropy effect on the ortho reactions. [c]Calculated from the estimated relative free energies. [d]Taken from ref 46. [e]In calculations PhBeg was used as the model. [f]Taken from ref 52.

Discussion

For a catalytic reaction, the observed KIEs may not necessarily reflect the rate-limiting or turnover-limiting step in the catalytic cycle. However, the KIEs should reflect the first *irreversible* step between free substrate and the product. Qualitatively, the ^{13}C KIE (~1.012) at the *meta* position indicates that a bonding change is occurring at this position. Typically one would expect the processes discernable, but in this case the results seem ambiguous. The interpretation of these experimental results is difficult because of the minuscule difference between the theoretically predicted ^{13}C KIE for C-H activation (1.016) and reductive elimination of aryl borane (1.013). Further complicating the interpretation of this result is the magnitude of the experimental deuterium KIE (1.9-2.5), that indicates that a C-H bond may be undergoing a bonding a change at the rate limiting step, and the experimentally observed deuterium exchange.

Numerous studies have concluded that C-H activation is rate limiting, and typically the large deuterium KIEs (3.5-5) reported have supported this conclusion. But, if the mechanism for this borylation were similar, then one would expect the experimental deuterium KIEs to be similar in magnitude to the results described previously. For example, several of Hartwig's results strongly support rate-limiting C-H activation with bpy, and the computational results reported here support this overall conclusion.[61] So why are the experimental deuterium KIEs for the Ir bisphosphine complexes notably smaller in magnitude?

Several results indicate that mixed rate-limiting steps are involved. First, recall in Figure 2-5 that transition structure **13** is ~0.9 kcal/mol lower in energy than **11**. This

is within the errors of the calculation, and since no attempt was made to find the global minimum for either structure due to the numerous rotational isomers, it is difficult to discern which if not both of transition structures could be contributing to the KIE. If there were mixed rate-limiting steps then that could explain the lower observed ^{13}C KIE from what is predicted for C-H activation (KIE=1.016). Additionally, if the deuterium KIE is corrected for the rate of exchange, the maximum observed value is still significantly smaller than what is predicted (k_H/k_D=3.5). A simple comparison of the Ir bpy and dmpe structures one can rationalize the observed deuterium exchange as simply arising from the large difference in steric encumbrance.

Sterics alone cannot explain the preferred *meta* selectivity. Even if C-H activation is rate-limiting, the origin of selectivity can be best understood from the fully formed Ir-C bond that is formed during C-H activation. Since Ir is less electronegative than H, explains why substituent effects in these reactions are limited and do not follow the expected regioselectivy of simple aromatic substitutions. Why then is there a rate enhancement with electron withdrawing groups (EWG) if substituent effects are limited? This is best understood as a polarity effect. Since Ir is less electronegative than H, EWG is going to favor and stabilize a C-Ir bond over a C-H bond. All of the substituent effects arise not from π effects, but purely arise through σ effects. Interestingly, using both transition structures **11** and **13** one can statistically predict the observed experimental selectivity! This observation can be further attributed to the small differences in polarity for C-H and Ir-C bond, which is further explains the rate enhancement and regiochemical preference at the *meta* position.

Conclusions

The experimental ^{13}C and deuterium KIE were determined for the Ir(dmpe) catalyzed borylation of arenes. Qualitatively the KIEs appear to be too small for the rate-limiting step of the borylation to be purely C-H activation, and the theoretically predicted energies and KIEs support this conclusion. The observed deuterium KIE value 1.9-2.5 is relatively small for a primary H/D KIE where are C-H bond is being broken, and it appears inconsistent with the predicted value of ~3.5 based upon **11**. From the isotope effect alone one can not rule out a mixture of **11** and **13** influencing the magnitude of the deuterium KIE. The simplest interpretation of the isotope effects is that the reaction has mixed rate-limiting steps that contribute to the observed KIEs.

CHAPTER III

"CONCERTED" TRANSITION STATE, STEPWISE MECHANISM. DYNAMICS EFFECTS IN C^2 – C^6 ENYNE ALLENE CYCLIZATIONS*

Introduction

Reaction mechanisms are often qualitatively described in the context of transition-state theory and illustrated with a two dimensional potential energy diagram. The curve in a potential energy diagram represents a reaction's lowest-energy path from reactants to products. Such diagrams make clear the differences in reactivity and selectivity associated with reaction barriers between reactants, transition states, intermediates, and products. Despite, transition-state theory's well-recognized complications and limitations, such as tunneling, recrossing, and variational transition-state theory, it is widely used in the interpretation of experimental evidence.

Transition-state theory implicitly assumes that a reaction's selectivity arises from the intrinsic barriers associated with separate transition states (Figure 3-1).

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* Reproduced with permission from "**"**Concerted" Transition State, Stepwise Mechanism. Dynamics Effects in C^2 – C^6 Enyne Allene Cyclizations**"** by Bekele, T; Christian, C. F.; Lipton, M. A.; Singleton, D. A., **2005**, *J. Am. Chem. Soc.*. Copyright 2005 American Chemical Society.

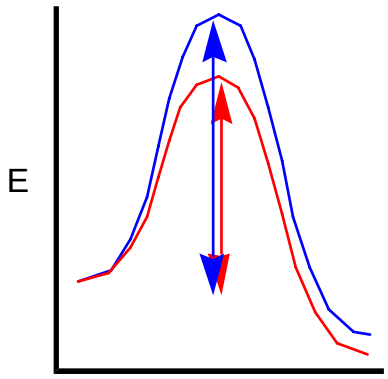


Figure 3-1. The potential energy diagram illustrates transition state theory's description for predicting a reaction's selectivity.

This assumption fails when product selectivity is determined by dynamics where rates are affected by a non-statistical recrossing. Selectivity is then determined by the random motions inherent to any molecule. Illustrated in Figure 3-2, as a reaction proceeds in three dimensional space along the potential energy surface from a single transition state down the minimum energy path it reaches a col where the pathway bifurcates leading to the non-statistical distribution of separate products.

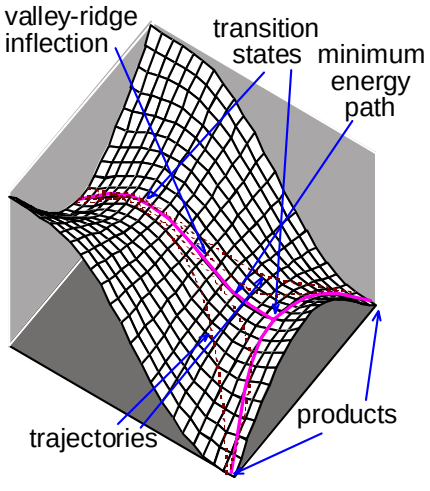


Figure 3-2. Three dimensional energy surface illustrating the premise of dynamics.

When exploring a potential energy surface of a reaction it is important to understand the stationary points, a point on the potential energy surface where the partial first derivatives of the potential energy with respect to all geometrical coordinates is simultaneously zero. Two topological features on the potential energy surface correspond to stationary points, transition states (maxima) and intermediates or products (minima). Typically, the potential energy surface near the transition state usually follows the steepest path of descent to a single reactant in one direction or a single product or intermediate in the other. But occasionally a transition state geometry is shared by more than one of the reactants or products creating a valley ridge inflection (VRI) point on the potential energy surface.[75] At the valley ridge inflection point the partial second derivative is equal to zero, and is located adjacent to two transition states. On a potential energy surface with a VRI, reactants that pass through the rate-determining transition state can descent into two distinguishable products without barrier, despite there being an energetic barrier for interconversion of one product to another. Transition state theory is unable to accurately predict the observed product ratio and the dynamic trajectories must be studied in reactions that have a valley ridge inflection point on the potential energy surface.

When the surface is symmetrical, the minimum energy path (MEP) bifurcates to afford an equal product ratio. However, when the pathway is asymmetric, the minimum energy path may not bifurcate, but there still will be trajectories that lead to each product. Figure 3-3 illustrates a symmetrical and unsymmetrical potential energy surface.

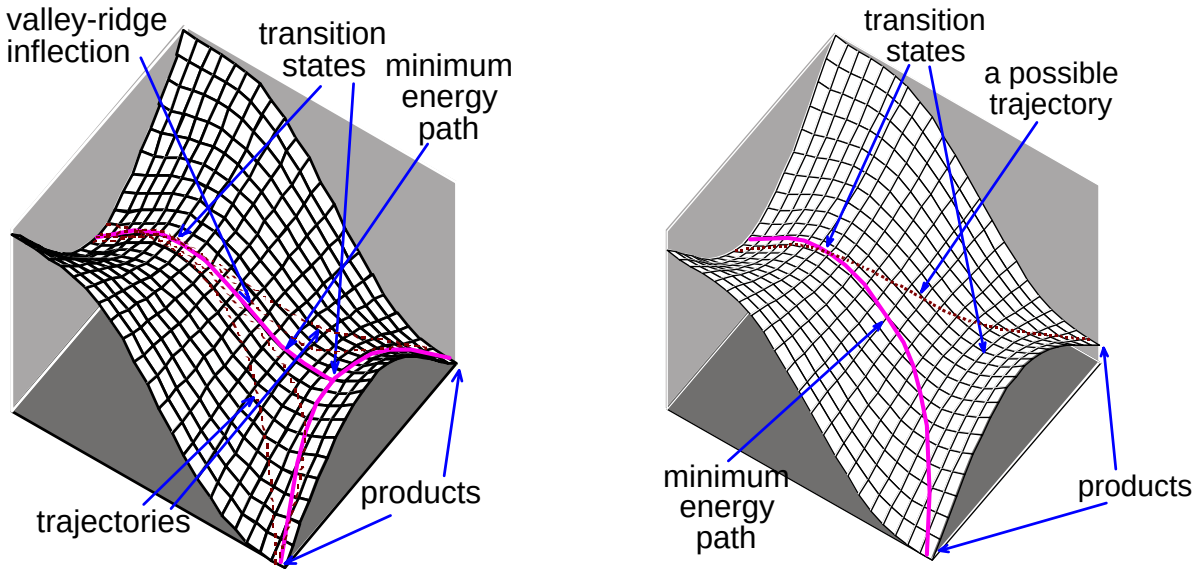


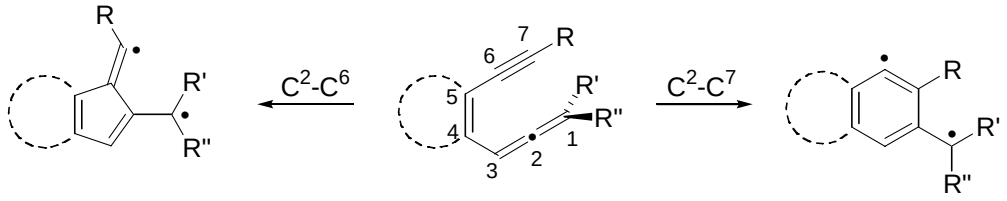
Figure 3-3. Bifurcating surfaces in which dynamic effects would control selectivity. (a) The surface is symmetrical and the MEP bifurcates at a second transition state. Real trajectories would tend to diverge from the MEP in the area of the VRI. (b) The surface is unsymmetrical and the MEP does not bifurcate. However, some possible trajectories afford a product not on the MEP.

There are numerous examples of dynamic effects in the gas phase and in symmetrical systems where symmetry is broken after the transition state.[76] Reactions that are unsymmetrical are the most interesting, but there are very few examples and little is understood.

The C^2-C^6 (Schmittel) / ene cyclization of enyne-allenes was studied by a combination of kinetic isotope effects, theoretical calculations, and dynamics trajectories. The formation of reactive diradical intermediates in the thermal cyclizations of enediynes and enyne-allenes is both fundamentally intriguing and biologically momentous.[77,78] Myers[79] and Saito[80] showed that enyne-allenes (**1**) undergo thermal C^2-C^7 cyclizations to afford α,3-tolyl diradicals (**2**), and this is thought to be the key step in

the biological activation of neocarzinostatin A.[78b] The ability of simple reactants to form such highly reactive intermediates is usually attributed to the aromaticity gained on cyclization. Schmittel, however, established a second reaction motif for enyne-allenes in which C^2-C^6 cyclization affords products apparently derived from fulvenyl diradicals (**3**).[81,82,83] This cyclization gains no aromaticity but is still promoted by the formation of a strong sp^2–sp^2 sigma bond from sp-hybridized carbons. The Schmittel cyclization motif has proven valuable in synthesis and has received extensive interest.[84]

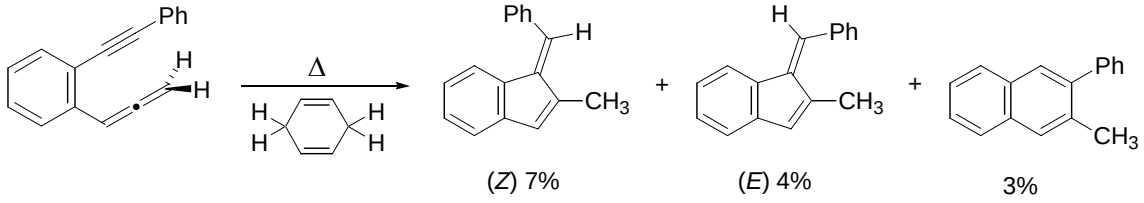
Scheme 3-1



3 **1** **2**

Evidence for the intermediacy of a diradical in the C^2-C^6 cyclization of enyne-allenes has included trapping with 1,4-cyclohexadiene[83] (Scheme 3-2) as well as the observation of double stranded DNA cleavage by structures known to undergo the Schmittel-type cyclization. Schmittel found that changing solvent polarity did not affect the rate of reaction or product ratios, leading him to rule out zwitterionic intermediates.

Scheme 3-2

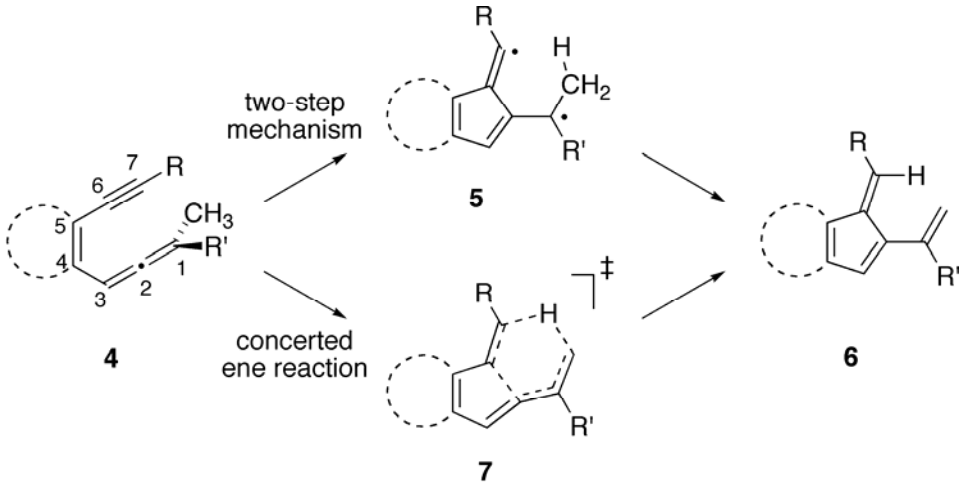


Theoretical studies on the cyclization of the parent (*Z*)-1,2,4-heptatrien-6-yne have supported a diradical mechanism for the C^2-C^6 cyclization.[85] In this system the C^2-C^7 cyclization is predicted to be favored over C^2-C^6 by approximately 10 kcal/mol, consistent with the experimental observation of exclusive C^2-C^7 cyclization.[86] The C^2-C^6 cyclization is predicted to be relatively favored by benzannulation,[87] and it is also favored by bulky terminal substituents and radical stabilizing groups at C^7. Studies in one of our laboratories have demonstrated an interesting acceleration of the C^2-C^6 cyclization by oxyanion substituents.[88]

When the enyne-allene is substituted by an alkyl group at C^1, the ultimate product of the C^2-C^6 cyclization has undergone hydrogen transfer from the alkyl substituent to C^7 and the overall conversion is formally an ene reaction (Scheme 3-3). The ene reaction is allowed as a concerted pericyclic process, but as a whole, ene reactions have been notably mechanistically diverse. Concerted mechanisms have been experimentally supported often,[89,90] yet many ene reactions have been found to involve more complex mechanisms.[90,91,92] The mechanism of any given ene reaction may be considered uncertain in the absence of evidence, but the mechanistic ambiguity of these reactions of enyne-allenes seems particularly interesting. In this case, the two-step mechanism

involving a diradical intermediate is imminently credible based on the chemistry in Scheme 3-2. In a theoretical study by Engels, the two-step and concerted mechanisms were predicted to have nearly equal free energies of activation.[93] Engels suggested that the two mechanisms could be distinguished using kinetic isotope effects, as have been applied to many ene reactions.

Scheme 3-3



The energetic similarity of concerted and two-step mechanisms in these reactions raises fundamental issues. By the Thornton hypothesis,[94] when the intermediate for a potential two-step mechanism is low in energy, the transition state for the corresponding concerted process should geometrically approach the stepwise process. As the intermediate goes lower in energy, the concerted mechanism ultimately transitions into the stepwise pathway. However, the nature of mechanisms at the concerted / stepwise boundary is not well understood. Should such reactions involve a mixture of

mechanisms?[95] What is the effect of intrinsic entropic differences between a two-step mechanism and a more organized concerted process?

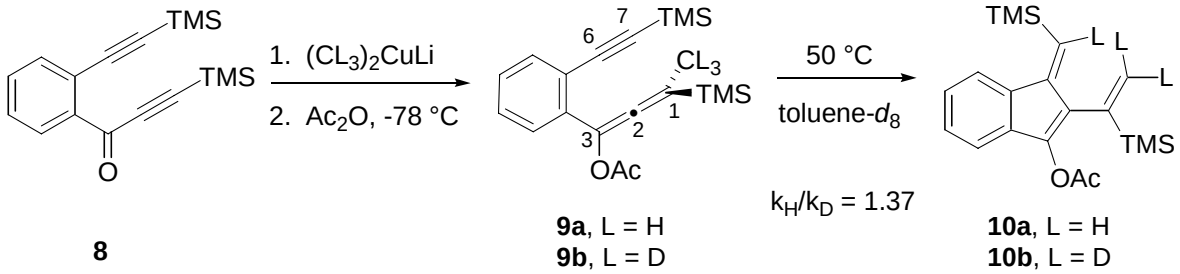
We describe here a combined experimental and theoretical study of the C^2-C^6 / ene cyclization of enyne-allenes, a reaction with a mechanism at the concerted / stepwise boundary. We find that this reaction is not well-described by either concerted or two-step labels, and that the consideration of dynamic effects is necessary to understand the nature of these intriguing reactions.

Results

Experimental

Experimental Kinetic Isotope Effects. The allenol acetate **9** was chosen for study owing to its clean conversion to the cyclized product **10** at a moderate temperature and rate. Both the unlabeled substrate **9a** and the deuterium labeled **9b** were prepared by the addition of the appropriate Gilman reagent to the acetylenic ketone **8** by a previously reported procedure.[88] The deuterium incorporation in **9b** prepared in this way is >98% based on ^{1}H NMR analysis.

Scheme 3-4



8

9a, L = H
9b, L = D

10a, L = H
10b, L = D

The cyclization of **8** in toluene-d_8 at 50 °C was conveniently followed by ^{1}H NMR. The conversion of **9a** versus time was consistent with a first-order process over

the course of the reaction with a half-life of ≈9000 s, and first-order kinetics were assumed in rate-constant determinations. The conversion of **9** to **10** was monitored by the intensity of characteristic aromatic signals for each relative to the residual methyl signal of toluene-d_8 used as an internal standard. The signals corresponding to the acetate and TMS groups were unsuitable due to peak overlap. ^{1}H NMR spectra were collected at 30-minute intervals until no further change in relative peak heights was observable, and the resulting data were fit directly as a first-order process. The isotope effect for the reaction was determined from both the disappearance of **9** and appearance of **10** in two reactions each for labeled and unlabeled materials, affording a total of four measurements with an average k_{CH3}/k_{CD3} of 1.43 and a standard deviation of 0.12. This standard deviation may underestimate the uncertainty in k_H/k_D because only two completely independent reactions are involved.

This isotope effect will be discussed in more detail below, but we note here that the k_H/k_D is smaller than normally observed in concerted ene reactions.[89d,90a,91g,2f] However, the k_H/k_D is qualitatively too large to support a stepwise ene process. This is in line with the idea that the mechanism is near the concerted / stepwise boundary.

Theoretical Calculations

Theoretical Pathways from 9. Engels has previously reported extensive careful calculations on the C^2-C^6 cyclization of a series of enyne-allenes capable of undergoing the overall ene conversion.[93] The focus here is in two areas – the reaction of the experimental system **9** and a more detailed study of a model system. The results of these

studies suggested a more complex picture of the reaction mechanism than would conventionally be considered.

Three possible pathways for the C^2-C^6 cyclization of **9** were explored in restricted and unrestricted B3LYP calculations employing a 6-31G(d,p) basis set (Figure 3-3). The first is direct formation of **10** by a concerted process. Transition structure **11**‡ was located for this conversion, and the predicted barrier of 23.8 kcal/mol is well consistent with a reaction that proceeds in a few hours at 50 °C. (The predicted half-life at 50 °C after inclusion of an entropy estimate based on the unscaled harmonic frequencies is a fortuitous 8900 s.) The second possible pathway is cyclization of **9** with an "inward" rotation of the methyl group on C^1 to afford diradical **12**. Intramolecular hydrogen transfer in **12** could then afford product **10** via transition structure **13**‡. As will be considered in greater detail below, no transition structure could be located for the formation of **12** from **9**. The third possible pathway is cyclization of **9** with an "outward" rotation of the methyl group on C^1 to afford diradical **15** via transition structure **14**‡. This cyclization has the effect of running together the two trimethylsilyl groups and is rather sterically encumbered. As a result, the predicted barrier for this cyclization is 8.8 kcal/mol above that for the ene pathway. Based on this result and the absence of experimental support for long-lived diradicals in this reaction,[88] this pathway is unlikely to be experimentally relevant.

It should be noted that the predicted energies of **12** and **15** are dubious due to spin contamination ($\langle S^2 \rangle$ is 0.43, 0.09, 0.04, and 0.47 for **12**, **13**‡, **14**‡, and **15**, respectively). The diradical energies will be considered further for a model reaction. Structure **11**‡ was

identical for restricted and unrestricted calculations and its wavefunction was spin-unrestricted stable.

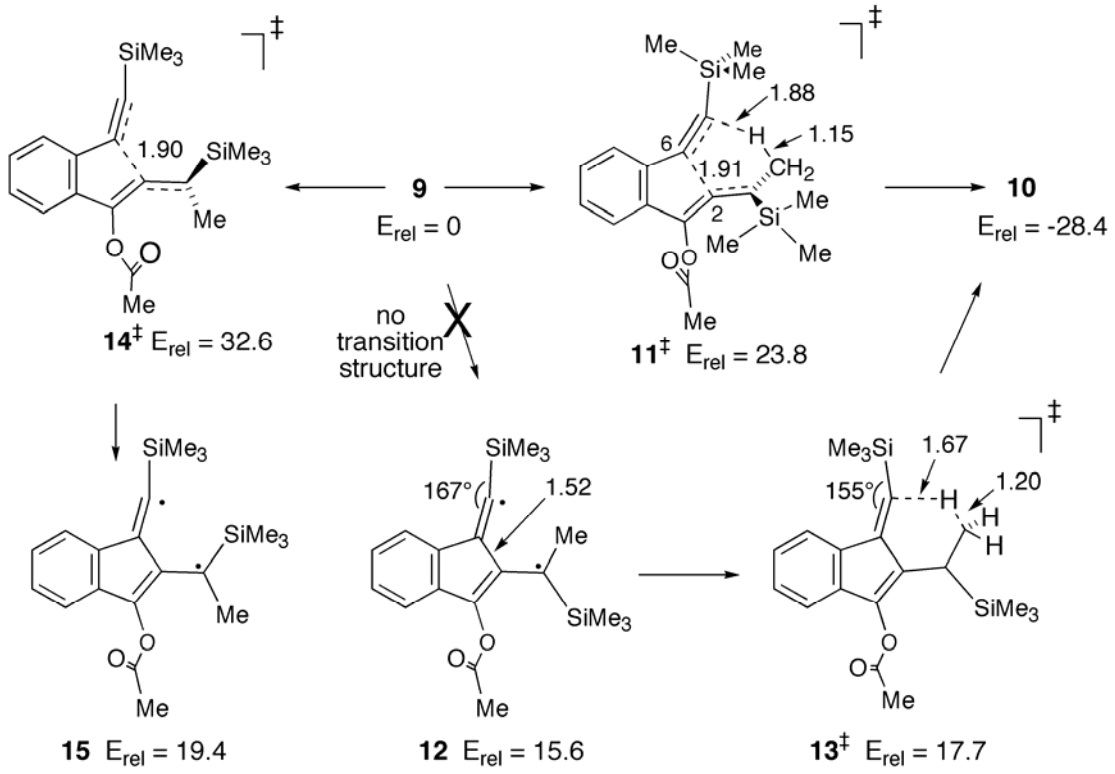


Figure 3-4. Predicted pathways for the cyclization of **9** in (U)B3LYP/6-31G(d,p) calculations. Structures **12**, **13**‡, **14**‡, and **15** were obtained using unrestricted calculations, while the remaining structures were identical in restricted and unrestricted calculations. Relative energies are in kcal/mol and include zpe.

All attempts to locate a transition structure for formation of **12** failed, using both restricted and unrestricted calculations. Instead, the saddle-point searches invariably converged on **11**. This is in agreement with the observations of Musch and Engels, who reported for a similar cyclization that a transition structure for formation of a diradical could not be located when the C^7 methyl group twists toward the alkyne.[93] An attempt

to locate a transition structure for formation of **12** in UBPW91/6-31G(d,p) calculations also converged instead on a transition structure similar to **11**‡.

How could there be no transition structure for formation of **12**? Both **11**‡ and a hypothetical transition structure for formation of **12** would involve formation of the C^2-C^6 bond, and the difference between the two is that **11**‡ also involves hydrogen transfer. However, the degree to which hydrogen transfer has progressed in **11**‡ is very minor – the breaking C–H bond is only slightly elongated compared to **9**. As a result, the structure of **11**‡ is very close to that expected for a transition structure forming **12**. Rather than involving two separate transition structures with extremely similar geometries, it appears that the stepwise and concerted pathways have merged in the single transition structure **11**‡. The significance of this observation will be explored in more detail after the interpretation of the experimental kinetic isotope effect is considered.

Predicted Isotope Effects. To aid in interpreting the experimental H/D isotope effect, predicted isotope effects based on transition structures **11**‡ and **14**‡ were calculated. These predictions used the scaled theoretical vibrational frequencies[9] in conventional transition state theory by the method of Bigeleisen and Mayer.[10] For the secondary H/D isotope effect associated with transition structure **14**‡, a tunneling correction was applied using a one-dimensional infinite parabolic barrier model.[11] No tunneling correction was applied for the prediction of the primary H/D isotope effect associated with transition structure **11**‡, and the resulting prediction is likely a lower

bound compared to a complete treatment of tunneling and variational transition state effects (impractical in this case).

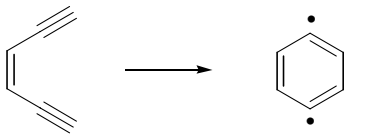
The idea behind the prediction of an isotope effect for transition structure **14**‡ is that **14**‡ may serve as a surrogate for a transition structure that would lead to diradical **12**. The predicted k_{CH3}/k_{CD3} at 50 °C for **14**‡ is 1.06. This is slightly greater than unity because the adjacent radical character in **14**‡ has the effect of weakening the C-H bonds in the methyl group on C^1, but this prediction is much smaller than the experimental isotope effect. This appears to exclude rate-limiting formation of the diradical, but for reasons that will soon be clear, we opt for a more careful wording: the experimental isotope effect is inconsistent with a predominant rate-limiting transition state involving C^2-C^6 ring closure without partial C–H bond breakage.

The predicted k_{CH3}/k_{CD3} based on **11**‡ is 1.54. Qualitatively, both this predicted isotope effect and the experimental isotope effect of ≈1.43 are in the realm of very small primary isotope effects. The difference is perhaps small enough to ignore – the experimental isotope effect is consistent with the qualitative nature of **11**‡ in which C–H bond breakage has progressed to a minimal extent. However, it is enlightening for the discussion later to consider possible origins for the difference between the experimental and predicted isotope effects. Aside from experimental error, the simplest explanation is inaccuracy in **11**‡. In this regard, the smaller observed isotope effect suggests that the progress of C–H bond breaking in the experimental transition state is less than in **11**‡.

An alternative, more complex, explanation is that the observed isotope effect represents a mixture of concerted and two-step mechanisms. These two possibilities are

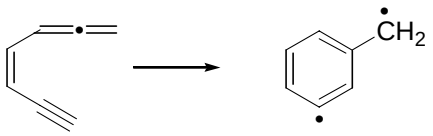
distinct in classical physical organic terms, but the difference will be less well defined when dynamics are considered below.

Theoretical Pathways in a Model Reaction. In order to explore the C^2-C^6 / ene cyclization in more detail and with higher-level calculations, the model cyclization of **16** was studied. Stationary-point geometries for the reaction path were optimized in restricted or unrestricted B3LYP calculations employing a 6-311+G(d,p) basis set. Single-point energies were then computed using Brueckner orbitals including double excitations and a perturbative estimate of triple excitations (BD(T)),[96] employing a 6-31+G(d,p) basis set. An unrestricted wavefunction was employed for diradical structures; for other structures the difference between unrestricted and restricted BD(T) results was negligible. The applicability and accuracy of this calculational approach was supported by studies of the thermodynamics of cyclizations of *cis*-hex-3-en-1,5-diyne to *p*-benzyne (1) and hepta-1,2,4-trien-6-yne to α,3-didehydrotoluene (2), which can be compared with reported experimental data.[97,98] In both cases, the predicted cyclization energies [(U)BD(T)//6-31+G(d,p)//(U)B3LYP/6-311+G(d,p) + thermal correction for 25 °C] are within the uncertainty of the experimental values.



(1)

ΔH_{expt} = 8.5 ± 1.0 kcal/mol (ref 25)
ΔH_{calcd} = 8.5 kcal/mol



(2)

ΔH_{expt} = -15 ± 4 kcal/mol (ref 26)
ΔH_{calcd} = -11.6 kcal/mol

The results for the cyclization of **16** are summarized in Figure 3-4. Transition structure **17**‡ was located for the concerted formation of product **18** from **16**. This structure is similar to **11**‡, with substantial C^2-C^6 bond formation but little progress in the hydrogen transfer from the methyl group on C^1 to C^7. As was the case for **9**, no transition structure could be located for formation of diradical **19** from **16**. Our search for such a transition structure included imposing constraints to preclude hydrogen transfer in the transition structure. Invariably, when the constraints were removed, the transition structure converged to **17**‡. An attempt to locate a transition structure for formation of **19** in MP2/6-31G(d,p) calculations also converged instead on a transition structure similar to **17**‡. Two transition structures for the formation of *E*-*Z* isomers of **19** were located, and these are shown in the appendix. Since our focus is on the energy surface in the area of **17**‡, **19**, and **20**‡ as a model for the experimental reaction of **9** and the energy surface in the area of **11**‡, **12**, and **13**‡, we did not explore the likely-favored C^2-C^7 cyclization of **16**.

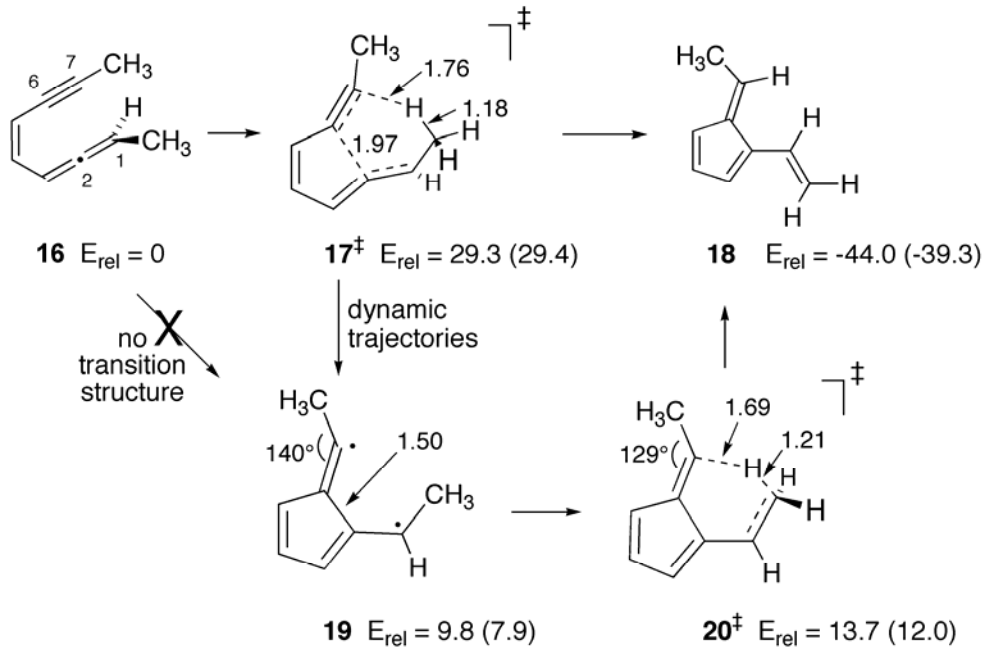


Figure 3-5. Predicted pathways for the cyclization of **16**. Structures **19** and **20**‡ were obtained using unrestricted calculations. The relative energies (kcal/mol) shown are (U)BD(T)/6-31+G(d,p)//B3LYP/6-311+G(d,p) + zpe. Relative (U)B3LYP/6-31G(d,p) energies are shown in parentheses for comparison.

Figure 3-4 also shows how the BD(T)/6-31+G(d,p)//(U)B3LYP/6-311+G(d,p) energies compare with those obtained for **16**–**20** in (U)B3LYP/6-31G(d,p) calculations (the calculations used for **9**–**15**, and for dynamics below). The DFT approach performs well in predicting the reaction barrier, as previously suggested by the comparison with experiment, but slightly overestimates the stability of diradical **19**. This is unsurprising as **19** is subject to spin contamination ((<S^2> = 0.28). The barrier for product formation from **19** is estimated reasonably. Overall, the DFT calculations appear to reproduce the key features of the energy surface.

Dynamics. The fascinating common feature in the C^2-C^6 cyclization of **9** and the model **16** is the absence of a separate transition state for formation of diradicals **12** and

19. This observation is reminiscent of recent discussions in the literature, by one of us and by others, of reactions in which a single initial transition state can lead to two separate products.[92,99,100,101] We hypothesized that the energy surface in these cyclizations has the qualitative features shown in Figure 3-5. From the rate-limiting transition structures **11**‡ or **17**‡, the steepest-descent path in mass-weighted coordinates (the "minimum energy path") affords the ene product. A standard theoretical analysis would thus conclude that the ene reaction occurs in a concerted fashion. However, continued formation of the new C^2-C^6 bond from **11**‡ or **17**‡ without concomitant hydrogen transfer could lead in a downhill process to **12** or **19**. It was thus possible that trajectories passing through the "concerted" ene transition state could lead to the diradical intermediate. In such a situation, whether a significant proportion of the reaction involves a stepwise process, and the competition between concerted and stepwise mechanisms, becomes a question of dynamics.

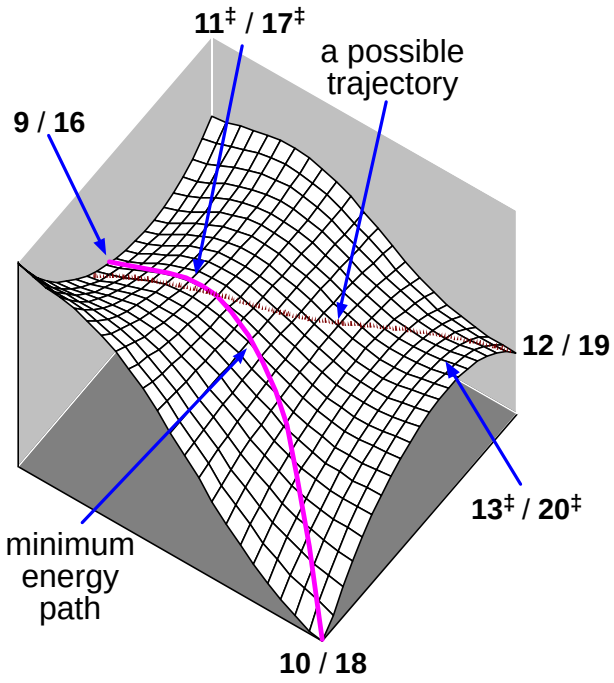


Figure 3-6. Qualitative energy surface for the cyclizations of **9** and **16**.

To study this issue, **17**‡ was used as the starting point for quasiclassical direct dynamics trajectories on the UB3LYP/6-31G(d,p) surface. With all atomic motions freely variable, the trajectories were initialized by giving each vibrational mode a random sign for its initial velocity, along with an initial energy based on a random Boltzmann sampling of vibrational levels appropriate for 323.15 K, including zero point energy. The mode associated with the imaginary frequency was treated as a translation and given a Boltzmann sampling of translational energy "forward" over the col. Two processes were explored for assigning the starting atomic positions. In the first, the geometry of **17**‡ was used as the starting point, forcing all trajectories to go through **17**‡ exactly. In the second, the starting atomic positions on the potential energy ridge in the area of **17**‡ were randomized using a linear sampling of possible harmonic classical displacements for each normal mode, adjusting the kinetic energy for each mode

accordingly. The two processes ultimately gave similar results. Forces were calculated directly at the UB3LYP/6-31G(d,p) level at each point, and employing a Verlet algorithm, 1-fs steps were taken until either the ene product **18** was formed (defined by a C^2-C^6 distance < 1.5 Å with a C^7-H distance < 1.1 Å) or diradical **19** was formed (defined by a C^2-C^6 distance < 1.5 Å with the C^7-H distance increased to > 2.1 Å). The median time for product formation was 30 fs, and all trajectories were complete within 85 fs. With such short simulation times, the effect of intramolecular vibrational energy redistribution[102] should be minimal. A graph of C^2-C^6 versus C^7-H distances for some typical dynamics trajectories is shown in Figure 4.

The results were striking. Although the minimum energy path from **17**‡ smoothly affords **18**, 29 out of 101 trajectories afforded diradical **19**. Five of the 29 trajectories entering the area of **19** were followed for an additional 100 fs, but none of these went on to **18**. It thus appears that *an intermediate is formed in a substantial portion of trajectories proceeding via the transition structure for the concerted ene reaction.* These intermediate diradicals would ultimately go on to **18**, but since the barrier (via **20**‡) is substantial, the time scale for the simulation is insufficient to observe this transformation.

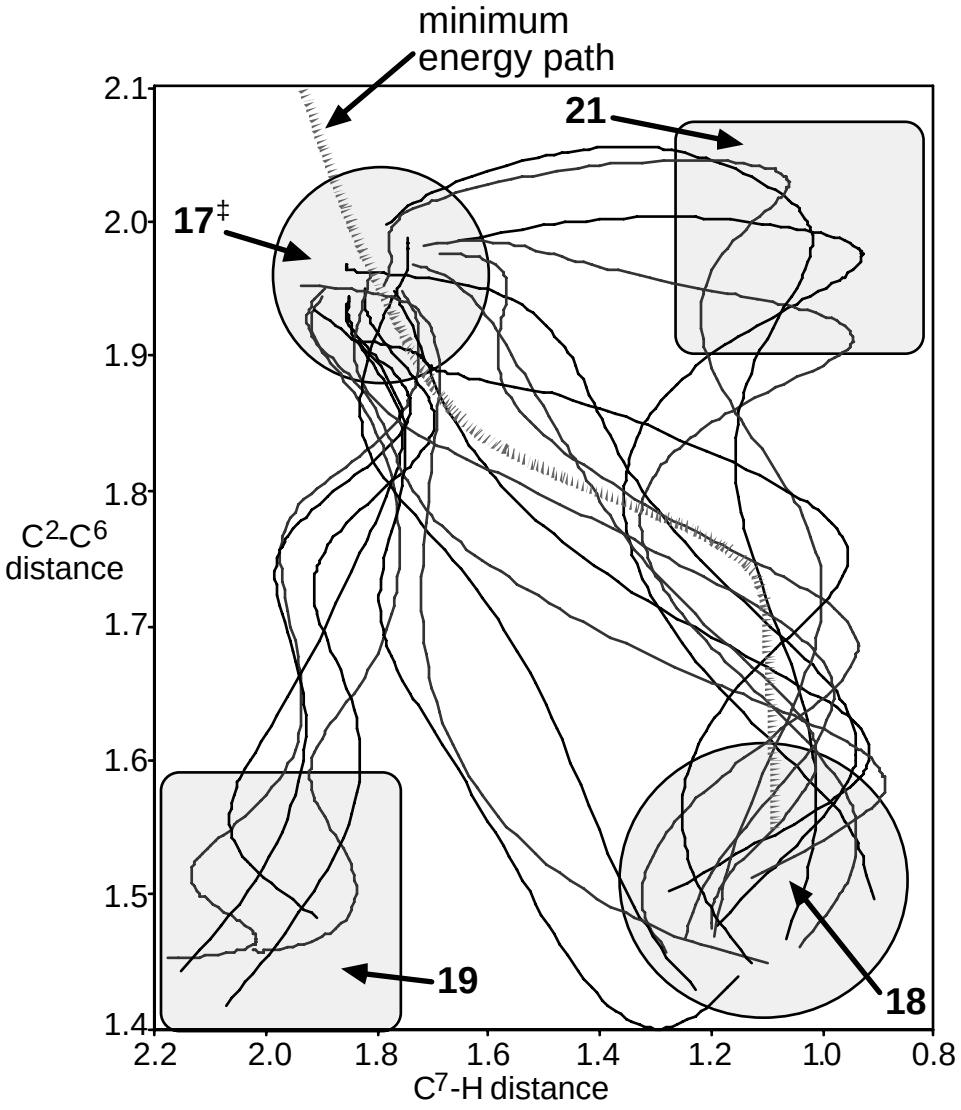
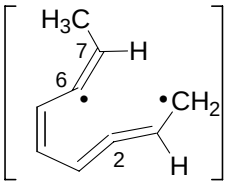


Figure 3-7. Graph of C^2-C^6 versus C^7-H distances for selected dynamics trajectories starting from **17**‡, along with the steepest-descent pathway through **17** is mass-weighted coordinates (the minimum energy path).

A second remarkable observation was that many trajectories underwent rapid hydrogen transfer to C^7 without simultaneous C^2-C^6 bond formation. Out of 101 trajectories, 29 saw the C^7-H distance decrease to < 1.1 Å while the C^2-C^6 distance was still > 1.8 Å. Seven trajectories had the C^7-H distance decrease to < 1.1 Å while the C^2-

C^6 distance increased to > 2.0 Å. Such trajectories pass through a geometry resembling structure **21**. No potential-energy minimum associated with this structure could be located, and all of the trajectories go on rapidly to **18**. The intervention of structures resembling **21** thus has no outward consequence. Nonetheless, the surprising prevalence of trajectories through the area of **21** would seem to impact the conception of asynchronicity in pericyclic reactions. Structure $\mathbf{17}^{\ddagger}$ would be described as highly asynchronous, with the C^2-C^6 bond formation preceding hydrogen transition, but despite this, *many trajectories complete the hydrogen transfer first*.



21

Discussion

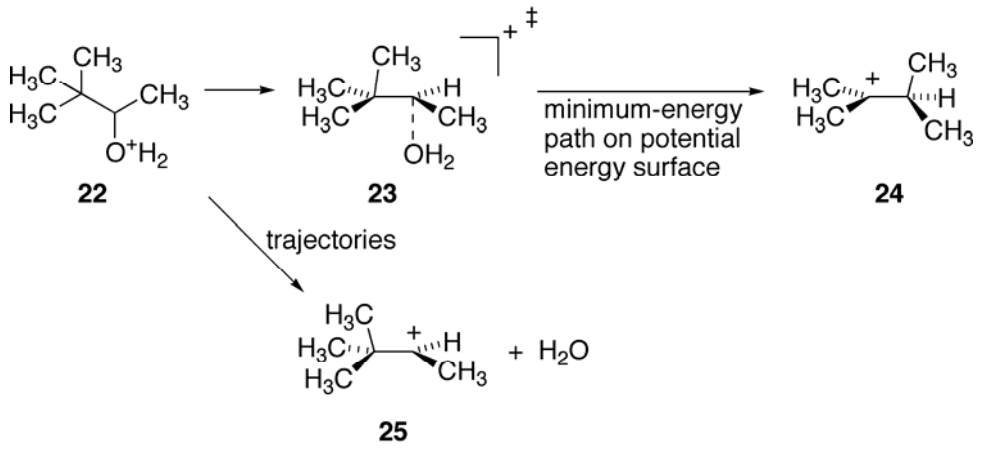
Within conventional physical organic chemistry, much has been made of the distinction between concerted and stepwise mechanisms for reactions with multiple bonding changes. This is seemingly a well-defined problem – concerted mechanisms occur by a pathway involving a single transition state and no intermediate, while a stepwise mechanism passes through at least two transition states with an intervening intermediate. The steps of a stepwise mechanism are always conceivably kinetically distinguishable, that is, separately influenceable. A concerted mechanism, in contrast, has a single kinetic barrier, and any factor that influences product formation or

selectivity must equivalently influence starting material disappearance. A sufficiently detailed characterization of a reaction's transition state, whether it be experimental (substituent effects, isotope effects, entropy of activation, volume of activation, spectroscopic observation, etc.) or theoretical, is considered adequate to distinguish between stepwise and concerted mechanisms, at least in principle. The possibility that a mixture of separate stepwise and concerted mechanisms can be operative is well recognized, but this adds no essential complication. The borderline between stepwise and concerted mechanisms is classically straightforward – does the mechanistic pathway involve an intermediate, or does it not?

Dynamic effects complicate the situation. Carpenter and others have discussed extensively the situation in which dynamic trajectories pass through the area of an intermediate without equilibration of vibrational energy.[103,104,105] As a result, the product selectivity doesn't reflect the presence of an intermediate or the presence of a second kinetically distinguishable step. In effect, the mechanistic pathway follows the energy surface of a stepwise mechanism but the reaction "acts" concerted in observables, for example in stereochemistry.

Recent work by Yamataka, Aida, and Dupuis has further complicated the distinction between stepwise and concerted mechanisms.[106] In theoretical calculations on the ionization of **22**, the minimum-energy path on the potential energy surface passes through transition structure **23** to afford the tertiary cation **24**. In this conversion, loss of the water leaving group and methyl-group rearrangement occur in a concerted fashion. However, dynamics simulations found that most trajectories at 400 K afforded initially

the secondary cation **25**. This cation is not "connected" to the starting material by a minimum-energy path, but can be formed readily by a process that simply breaks the C—O bond without concurrent methyl rearrangement. In effect, the reaction proceeds by a stepwise process while a classical analysis would predict a concerted process. A thermodynamic interpretation of this observation is that, in contrast to the potential energy surface, the canonical variational transition state on the free-energy surface leads to the secondary cation.



22 **23** **24** **25**

The results here suggest a new wrinkle on the impact of dynamics on the idea of stepwise versus concerted mechanisms, a wrinkle that is potentially widespread. The observed kinetic isotope effect and the calculational results both support the idea that the C^2-C^6 / ene cyclization of **9** is near the stepwise/concerted boundary. It might be envisioned that in such cases, separate stepwise and concerted mechanisms could be competitive. Here, such a competition cannot be ruled out from the experimental isotope effect alone, but the calculations support a merging of the stepwise and concerted pathways as far as the rate-limiting transition state. Under these circumstances, experimental mechanistic probes of this transition state would appear to implicate an

exclusively concerted reaction. Going on from this transition state, however, an intermediate may or may not be formed, depending on the dynamics of individual trajectories. The intermediate could in principle be trapped or detected, implicating the stepwise mechanism. Kinetic observations and trapping experiments would appear contradictory.

It is enlightening to qualitatively consider the ene reactions of **9** or **16** within the context of a More O'Ferrall-Jencks diagram (Figure 3-5).[107] Ene reaction mechanisms can be very complicated, but here we restrict our consideration to having carbon-carbon bond formation and hydrogen transfer as the dominant dimensions for the More O'Ferrall-Jencks diagram.[89a] Because the overall reaction is exothermic, it would be expected that the transition state would be relatively early, and since the diradical intermediate after carbon-carbon bond formation is relatively stable (as evidenced by the chemistry of Scheme I), the transition state should be shifted toward the edge of the diagram, as shown. This is consistent with the predicted transition structures **11**‡ and **17**‡, as well as the experimental isotope effect with **9**. The normal qualitative understanding of these reactions would then be based on a smooth reaction path passing through the transition state. However, a broad range of structures are energetically downhill from the transition state, and it is possible for trajectories to depart drastically from the qualitative reaction path. This can include reaching an intermediate in the corner of the More O'Ferrall-Jencks diagram that is not on the reaction path.

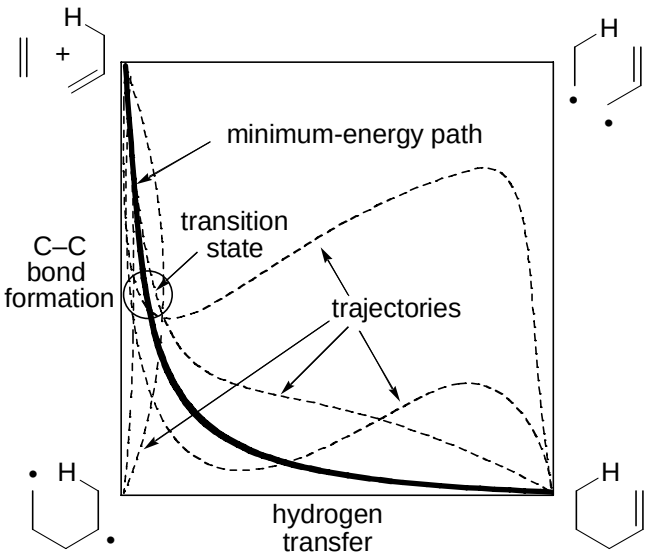


Figure 3-8. More O'Ferrall-Jencks diagram for ene reactions. The approximate minimum-energy path expected for reaction of **9** or **16** is shown as a solid bold line. Possible qualitative trajectories are shown as dotted lines.

The concept of a reaction path between starting material and product is fundamental in the chemistry paradigm. In the absence of bifurcations, such paths can be mathematically well-defined, the common definition as the steepest-descent path in mass-weighted coordinates being only one example out of many possibilities. It is of course well understood that real trajectories do not follow exactly the reaction path. However, qualitative discussions of reaction mechanisms implicitly assume the existence of a path that is chemically representative of the ensemble of trajectories connecting starting material and product. The technical justification for this view is that trajectories should tend to regress toward a minimum-energy path. However, such regression will not necessarily overcome the thermal divergence of trajectories, outside of the bottleneck area of a transition state. When trajectories vary sufficiently, no single

reaction path can adequately describe the mechanism. This appears to be the case for the current reaction.

It is fascinating to consider the possible applicability of the ideas here in other pericyclic reactions. Many cycloadditions, for example, have been predicted to occur by concerted processes through highly asynchronous transition states. In many such cases, both the cycloaddition product and the intermediate for a stepwise cycloaddition may be downhill from the rate-limiting transition state.[108] If so, trajectories passing through the "concerted transition state" could conceivably lead to intermediates in substantial amounts. A theoretical study that merely characterized the stationary points and minimum-energy paths in a mechanism could not resolve whether intermediates were formed, no matter how accurate the calculation. Notably, kinetic mechanistic probes of such reactions would be completely incapable of deciding whether intermediates were formed. Stereochemical and trapping probes could still be applied, though the conventional limitations of such probes have been discussed extensively[109] and, as described above, dynamic effects can make stepwise mechanisms appear stereochemically concerted.[103,104a-c,110] It should be of considerable interest to explore the degree to which such dynamic effects complicate diverse pericyclic mechanisms.

Conclusions

The KIE (k_{CH3}/k_{CD3}) for the C^2-C^6 / ene cyclization of **9** is approximately 1.43. This appears qualitatively too large to be a secondary isotope effect for formation of a diradical, and the theoretically predicted KIE based on diradical-forming **14**‡ supports

this conclusion. The 1.43 value is very small for a primary H/D KIE, but it appears roughly consistent with the predicted isotope effect of 1.54 based on **11**‡. From the observed isotope effect alone, we cannot rule out a mixture of standard concerted and two-step mechanisms. However, the theoretical calculations do not support a conventional mixture of mechanisms, and the simplest interpretation of the isotope effect is that the ene reaction involves a highly asynchronous transition state, near the concerted / stepwise boundary, in which hydrogen transfer has progressed to a minimal extent.

No transition structure could be located for formation of diradical **12** from **9** or diradical **19** from **16**. The initial geometry changes associated with these stepwise processes would be expected to be very similar to those for the highly asynchronous concerted mechanism, and the stepwise and concerted pathways have apparently merged as far as the rate-limiting transition structures. From these structures, the minimum-energy path leads to the ene product, but it is also downhill to the diradical intermediates.

Quasiclassical direct dynamics trajectories emanating from **17**‡ vary greatly. Although **17**‡ would normally be considered the transition state for a concerted reaction, many trajectories lead to an intermediate. A large alternative portion of the trajectories complete hydrogen transfer before full carbon-carbon bond formation, in contrast to what would be expected from the asynchronicity of the transition structure. The *single* minimum-energy path from starting material to product does not adequately describe the mechanism.

The ideas of transition state theory and reaction paths are so entwined in the mechanistic understanding of chemistry that they limit the questions that may be asked regarding a mechanism and the answers that may arise from mechanistic studies. When a reaction involves multiple bonding changes, a standard question has been whether the bonding changes occur by a stepwise or concerted pathway. When the question is asked this way, the only possible answers are that the reaction proceeds by a concerted pathway, or by a stepwise pathway, or by a mixture of the two separate pathways. Advances in the understanding of dynamic effects in mechanisms[92,99,103,104,105,106] have shown that the question of concerted versus stepwise is too simple, and that the answer to the question may be very complicated indeed. The consideration of a possible role for dynamic effects, even for complex reactions in solution, should be incorporated into the mechanistic chemistry paradigm.

CHAPTER IV

ISOTOPE EFFECTS AND THE MECHANISM OF PALLADIUM-CATALYZED ALLYLIC ALKYLATION*

Introduction

The carbon-carbon (C-C) bond represents the "foundation" of organic chemistry. Developing methodologies for the inter- and intra-molecular formation of carbon-carbon bonds remains fundamentally intriguing. The carbonyl group represents one of the more important functional groups for the formation of C-C bonds, but alkenes represent an attractive isoelectronic alternative.

Several organometallic complexes catalyze the nucleophilic or electrophilic formation of new C-C bonds with allylic functionalities.[111] Allylic carbonates, esters, and halides react *in situ* with metal complexes to generate a π-allylorganometallic complexes. In 1965, Tsuji *et al.* reported the addition of carbon nucleophiles (malonates, acetoacetates, and enamines) to π-allylpalladium complexes providing a new synthetic strategy for carbon-carbon bond formation. The mildness of the allylic alkylation reaction conditions and their broad chemoselectivity has allowed the application of these reactions to diverse complex structures.[112] Highly enantioselective

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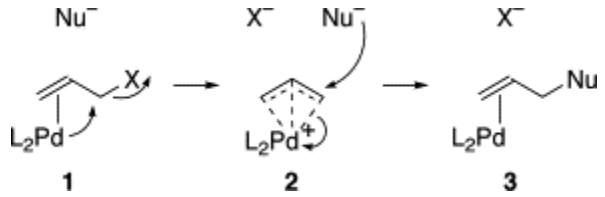
allylations have now emerged as a powerful tool in the synthesis of optically active products.[113]

Much is known in general terms about the mechanism of Pd-catalyzed allylations. Under most reaction conditions, the products are the result of a double-inversion process, consistent with an S_N2-like nucleophilic displacement of the leaving group by Pd, followed by a second displacement of Pd by an incoming nucleophile. The support for initial formation of a η^2-Pd π-complex **1** and the intermediacy of a η^3-Pd π-allyl complex **2** is extensive (Scheme 4-1). However, a more detailed knowledge of the selectivity-determining transition states would aid in addressing subtle selectivity issues, as would allow, for example, the design of new ligands for enantioselective reactions. The theoretical study of these reactions can in principle provide such detail.[114] However, this is a challenging reaction for theory, as most experimental reactions involve key steps that either generate or annihilate ions. This problem has been addressed using both solvent models and neutral nucleophiles/leaving groups,[114] but the experimental relevance of the results is often difficult to judge.

Scheme 4-1



The mechanism of the Pd-catalyzed allylic alkylation was studied using a combination of theoretical calculations and experimental kinetic isotope effects (KIES). The KIEs not only provide a qualitative view of the rate-limiting transition state but also

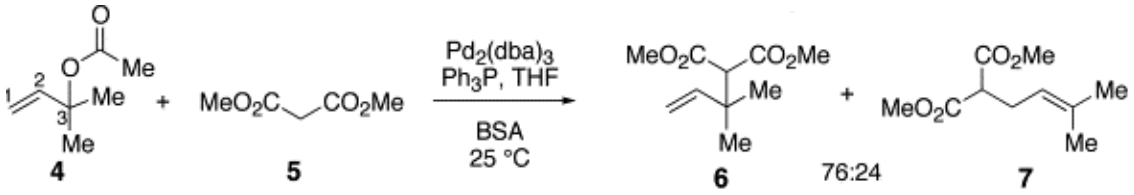
allow us to assess the accuracy of calculational models. The combination of theory and experiment supports a transition state that is η^2-like and S_N1-like in character, providing insight into the nature of selectivity in these reactions.

Results

Experimental

Experimental Kinetic Isotope Effects. The allylic alkylation reaction of dimethylallyl acetate (**4**) with dimethyl malonate (**5**) was chosen for study because it is a prototypical example and allylations via the intermediate 3-methylbutenyl palladium complexes have been well-studied previously (Scheme 4-2).[115] The reaction of **4** with **5** at 25 °C in THF was catalyzed by a combination of $Pd_2(dba)_3$ and triphenylphosphine (≈3 equiv phosphine per Pd), using *O*,*N*-bis(trimethylsilyl)acetamide (BSA) as base. Under these conditions, a 76:24 mixture of substitution products **6** and **7** is formed in nearly quantitative yield over the course of a few hours. The preference for nucleophilic attack at the more substituted allylic carbon in this particular reaction is in line with most previous observations.[115] Andersson and Bäckvall have reported that these products can equilibrate under certain conditions,[115e] but no significant equilibration could be observed under the mild conditions here. Allylic isomerization of **4** to afford 1-acetoxy-3-methyl-2-butene was observable but it was very slow (≈2.5% in recovered **4** after 71% conversion).

Scheme 4-2



The ^{13}C KIEs of **4** were determined by NMR methodology at natural abundance.[2,5] Two reactions of **4** at 25 °C were taken to 71% and 75% conversion, and the starting **4** was recovered by an extractive workup followed by fractional distillation. The recovered **4** was analyzed by ^{13}C NMR along with standard samples that had not been subjected to the reaction conditions. The change in isotopic composition in each position was determined relative to the methyl carbons of the dimethylallyl group, with the assumption that isotopic fractionation in these carbons was negligible. From the changes in isotopic composition, the KIEs were calculated as previously described.[5]

The results from six separate determinations on the two independent reactions are summarized in Figure 1. A very large ^{13}C KIE of ≈1.037 was observed at the tertiary carbon C3 of **4**, indicative of this carbon undergoing a substantial bonding change in the transition state for the rate limiting step. Very small normal isotope ^{13}C KIEs were observed at C1 and C2. These small KIEs are consistent with π-complexation to the olefin during the rate-limiting step, but suggest that these carbons are not undergoing a significant bonding change. Overall, the KIEs appear qualitatively consistent with rate-limiting C–O bond cleavage ionizing the acetoxy group in a η^2-Pd complex.

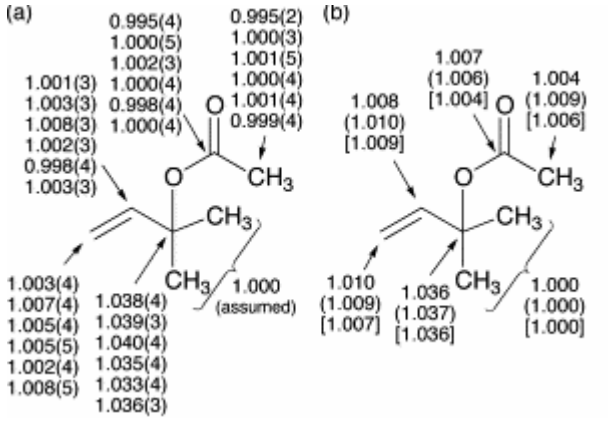


Figure 4-1. (a) Experimental ^{13}C KIEs (k_{12C}/k_{13C}) for the allylic alkylation reaction of **4** with **5** at 25 °C. The top three KIEs in each group arise from the 75%-conversion reaction. Standard deviations ($n = 6$) are shown in parentheses. (b) Predicted ^{13}C KIEs for three calculational models. Plain numbers are based on transition structure **10**, numbers in parentheses are based on transition structure **12**, and numbers in brackets are based on transition structure **13**.

If ionization of the acetoxy group were reversible, followed by rate-limiting nucleophilic attack on the η^3-Pd π-allyl complex, then the isotope effects at C3 versus C1 would reflect the 76:24 product mixture. The low KIE averaging 1.005 at C1 does not seem consistent with this scenario. Together with the low amount of allylic isomerization of **4** observed, the results do not support reversibility of ionization as the major mechanistic pathway.

Theoretical Calculations

Theoretical Calculations and Predicted Kinetic Isotope Effects. Theoretical calculations were used to interpret the isotope effects in greater detail. As introduced above, the challenge in studying these reactions theoretically is the formation of ionic intermediates from a neutral η^2-Pd complex. In the gas phase, the ionization of a complex of **4** with $Pd(PMe_3)_2$ into separate acetate anion and η^3-Pd cation is uphill by

≈70 kcal/mol. The high-energy ionization is accordingly disdained in favor of processes affording neutral products, such as elimination of a molecule of acetic acid.

To circumvent this problem, three distinct approaches to calculationally modeling this reaction were explored. The first was to study the reaction of the amidinium ion **8**. With **8**, the neutral acetamidine is the leaving group and the 'ionization' process in the gas phase is not dominated by Coulombic effects. A drawback is that the energetics for ionization of **8** are unlikely to match those for ionization of **4** in solution, except by accident. However, this approach is straightforward, making practical the use of a relatively complete theoretical model including two $PHPh_2$ ligands. In the event, transition structure **10** and intermediates **9** and **11** were located in B3LYP/BS1[116] calculations (Figure 4-2).

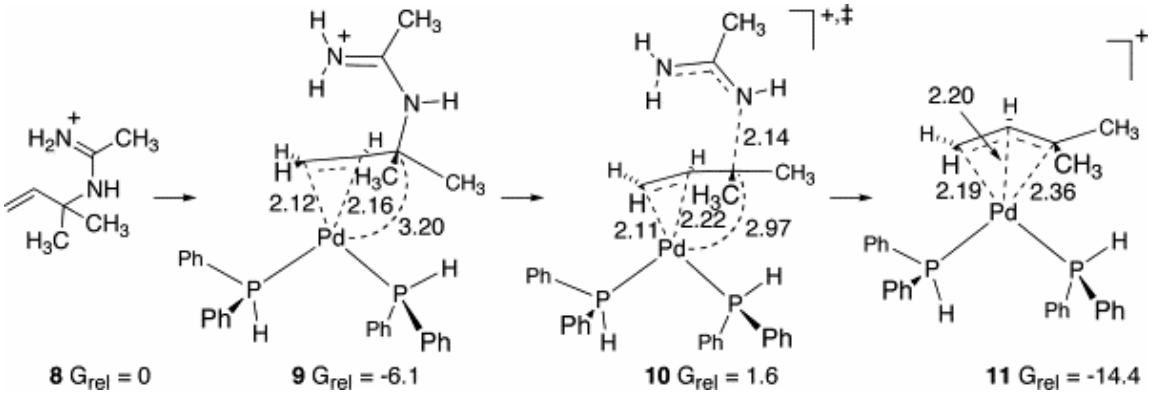


Figure 4-2. Calculated pathway (B3LYP/BS1[116]) for the ionization of **8** catalyzed by $Pd(PHPh_2)_2$. Free energies are relative to separate **8** and $Pd(PHPh_2)_2$ at standard state, based on unscaled harmonic frequencies at 25 °C, and are given in kcal/mol. Complete structures are given in the Appendix.

The second approach used an implicit solvent model. Transition structure **8** (Figure 4-3) for the ionization of **8** mediated by $Pd(PMe_3)_2$ was located using B3LYP/BS2[116] calculations and an Onsager solvent model for THF. (See the Appendix for calculational procedures.)

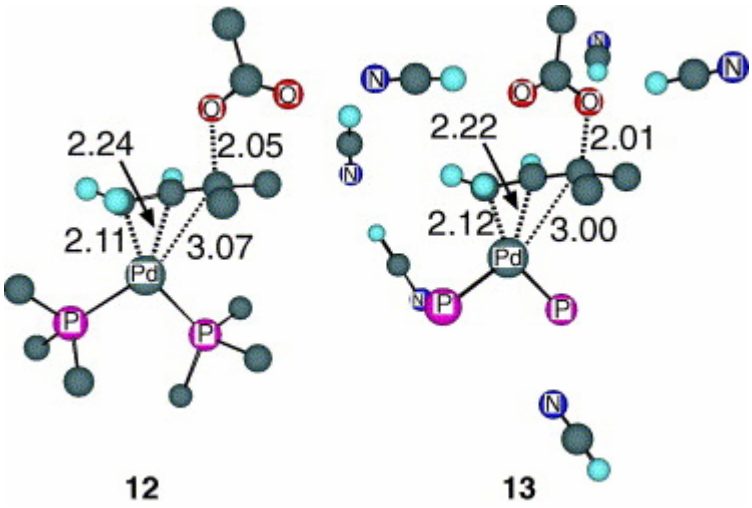


Figure 4-3. Transition structures for the ionization of **4** using solvent models. Structure **12** used an Onsager model for THF. Structure **13** used six HCN molecules. Most hydrogens have been removed for clarity.

The third theoretical model used explicit solvent molecules. It is normally difficult to use enough solvent molecules to sufficiently stabilize ion formation. Our strategy to attack this problem used 6 discrete HCN molecules. HCN was chosen because it is small, has a large dipole moment, and does not strongly interact with itself. As a result, a relatively small number of HCN molecules can greatly stabilize ionization. Transition structure **13** was located for the ionization of **4** mediated by $Pd(PH_3)_2$ in B3LYP/BS2[116] calculations. Many arrangements of the HCN molecules are possible and no effort was made to find the global-optimum arrangement. The goal was to model ionization as an

aid in the interpretation of the KIEs, and **13** may serve that purpose despite its limitations.

Theoretical KIEs were calculated based on each of the transition structures **10**, **12**, and **13**. The KIEs were predicted from the scaled theoretical vibrational frequencies[117] using conventional transition state theory by the method of Bigeleisen and Mayer.[10] Tunneling corrections were applied using an infinite parabolic barrier model.[11] The results are shown in Figure 4-1b.

Discussion

In many reactions, KIE predictions have proven highly accurate, often within the uncertainty of the experimental measurement.[2i] This is not true in the current case, and the difference between experiment and prediction may reflect the difficulty of modeling the ionization. The acetyl group carbons in particular exhibit experimental isotope effects near unity, but the predicted isotope effects are all in the 1.004–1.009 range. The predicted acetyl group KIEs in the three models are mainly the result of a mass effect on the moment of inertia,[118] not zero-point energy changes, and it is possible that this component of the isotope effect is not correctly predicted for an ionization in a solvent cage. Another issue is that the experimental KIEs assume that the dimethylallyl methyl carbons do not undergo isotopic fractionation—an error in this assumption would depress the KIEs, which are almost all smaller than predictions.

Within the dimethylallyl group, the experimental and predicted isotope effects are in qualitatively better accord. The predicted C3 KIEs fit perfectly with experiment. The calculations overestimate the olefinic carbon KIEs, though the scatter in the

experimental results is large and the pattern of KIEs predicted for **10** appears to fit reasonably. As structural models for the ionization, **10**, **12**, and **13** are qualitatively supported, though the low experimental olefinic KIEs suggest that these carbons may be undergoing less bonding change in the actual transition state than in the calculated transition structures.

In calculations of nucleophilic attack on (allyl)Pd(NH_3)$_2$, Norrby has previously noted that the transition structures are very product-like in character.[114a] This makes the transition structures resemble closely the corresponding η^2 complexes. Our KIEs and calculated structures support and amplify this idea. In **10**, **12**, and **13**, the Pd has not significantly begun to approach the ionizing carbon. The C2–C3 bond has shortened significantly at the transition structure (from 1.53 Å in **9** to 1.43 Å in **10**) and the Pd–C2–C3 angle bends downward (from 119.3° in **9** to 106.7° in **10**) as C3 becomes planar, and these changes have the effect of moving C3 toward the Pd atom, but the Pd coordination is still almost purely η^2. The Pd–C2 distance is greater at the transition structure than in the η^2 precursor, and the two phosphine ligands along with C1 and C2 are still nearly planar in their coordination of the Pd. In the ultimate η^3 structure **11**, the allyl moiety has twisted so that C1 and C3 are in the plane of the phosphines, but this process has not significantly commenced in the transition structures. There is no such twisting motion in the transition vectors associated with **10**, **12**, and **13**, and the slight approach of C3 and the Pd atom appears to be incidental. *The Pd atom is not carrying out an S_N2 displacement!*

How then is the Pd catalyzing the ionization? A clue comes from looking at the charge distribution in **11** versus **12**. In the process of forming **12**, the acetamidine moiety

transfers +0.28 *e* (Mulliken charges) to the remainder of the molecule. The dimethylallyl moiety gains +0.14 *e* between **11** and **12**, while the $Pd(PHPh_2)_2$ moiety gains +0.14 *e*. The $Pd(PHPh_2)_2$ moiety is thus serving to delocalize a large portion of the incipient positive charge. This stabilization does not require S_N2 character in the ionization; rather, the ionization seems best understood as S_N1 in character.

Conclusions

The results here have implications in understanding selectivity in palladium-catalyzed allylic alkylation reactions. Both the experimental isotope effects and the calculated structures suggest that the Pd center is not substantially migrating in the transition state. The transition state for ionization thus more closely resembles a η^2 complex than the ultimate η^3 intermediate. This idea may be useful in ligand design, for example, the effects of chiral ligands on the reactivity of enantiomeric allylic acetates should be reasonably understood from steric effects in the η^2 complex.

In many Pd-catalyzed allylations, the important selectivity issues arise at the stage of nucleophilic attack on the η^3 π-allyl complex rather than initial ionization. However, the transition state for nucleophilic attack on the η^3 π-allyl complex should be similar to that for ionization, and the Norrby observations[114a] are consistent with this idea. Nucleophilic attack on a η^3 intermediate should thus involve considerable reorganization of the allyl moiety toward a η^2 geometry. This would account for the often-observed attack of unhindered nucleophiles on the more substituted π-allyl carbon, as in the preferential formation of **6** from **5**. In considering enantioselective reactions, the twisting

of the PdL_2 moiety between the η^3 intermediate and the η^2-like transition state provides a mechanism by which chiral ligands can induce enantioselective attack on a prochiral η^3-allyl complex without directly interacting with the incoming nucleophile. A similar twisting has recently been invoked in Pd-catalyzed enantioselective hydroaminations.[118] All of these ideas suggest further investigations.

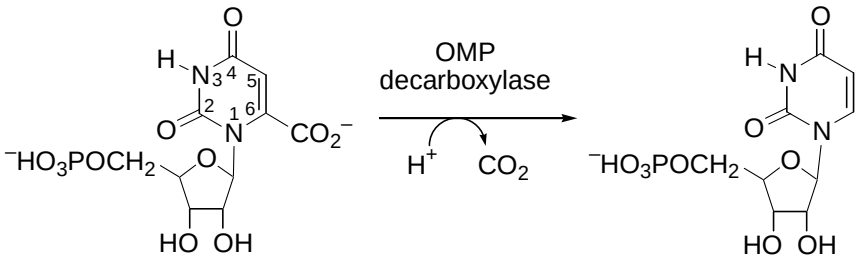
CHAPTER V

ISOTOPE EFFECTS AND THE NATURE OF DECARBOXYLATION / PROTON TRANSFER IN OROTIDINE DECARBOXYLASE

Introduction

Orotidine 5'-monophosphate decarboxylase (ODCase) catalyzes the decarboxylation of orotidine 5'-monophosphate (OMP, **1**) in the last step of the *de novo* biosynthesis of uridine 5'-monophosphate (UMP, **2)**, a nucleotide of RNA Scheme 5-1).[119]

Scheme 5-1



1 **2**

The chemical transformation is unique because the expected carbanion lacks stabilizing resonance; the carbanion generated is localized in an sp2 orbital perpendicular to the p- system of the pyrimidine.[120,121] In all other decarboxylases, the carbanion is either stabilized by delocalization into an adjacent carbonyl or covalently

bonded to a cofactor. This lack of stabilization results in an extremely slow uncatalyzed decarboxylation, taking 78 million years to be half complete. The enzyme is able to achieve remarkable catalytic efficiency, $k_{cat}/K_M/k_{non}$ of 2.0 x 10^{23} M^{-1}, with $k_{cat}/K_m \simeq 10^{17}$ (this corresponds to the reaction occurring about 39 times per second in the enzyme).[119] But how does nature's most proficient enzyme achieve such awe-inspiring catalytic efficiency?

Because of its unique efficiency, avid interest has developed in the mechanism of ODCase.[122,123,124,125,126,127,128,129,130,131] Several controversial hypotheses have been proposed to explain the mechanism and catalytic efficiency of ODCase. Debate over the mechanism of ODCase was piqued in 2000 when four research groups reported similar crystal structures for the enzyme complexed with uridine 5'-monophosphate (**2**) or with analogs of orotidine 5'-monophosphate (**1**).[132,133,134,135] The structures appear to exclude several proposed mechanisms in which the orotate ring undergoes an initial chemical conversion.[129,136,137] For example, in contrast to some expectations, the active site did not contain groups positioned to protonate the C-2 or C-4 carbonyls. Attention has therefore focused on a straightforward sequential decarboxylation / protonation process (Figure 5-1, eq 1). The active site places aspartate and lysine residues to interact with the carboxylate of **1** (Figure 5-2), but the nature of the exceptional catalytic acceleration provided by the enzyme is not obvious from the crystal structures. Based on QM/MM calculations, Gao and Pai proposed that the catalytic effect results from "electrostatic stress" in which the proximity of the orotate carboxylate to an aspartate induces strain that is relieved on decarboxylation.[133] This ground-state destabilization proposal has

been criticized in detail by Warshel.[138] Warshel applies a combination of *ab initio*-parameterized empirical valence bond and free-energy perturbation calculations to the problem, and attributes the catalysis to the enzyme stabilizing the increased dipole moment of the transition state for decarboxylation through its preorganization of complimentary charges. Gao has more recently criticized this analysis and emphasized the importance of transition-state relaxation of a distorted ODCase-substrate conformation in the catalytic effect of the enzyme.[139]

Two alternatives to the simple decarboxylation / protonation mechanism have been proposed to be consistent with the crystal structures. Ealick proposed an electrophilic substitution (S_E2) mechanism, in which the decarboxylation is aided by concerted protonation of C-6 (Figure 5-1, eq 5-2). This type of process has not yet been established for simpler chemical analogs, but was proposed to be favored by the ground-state destabilization by the proximal aspartate. An attractive feature of this mechanism is that it avoids the intermediacy of a high-energy localized vinylic anion. A more radical departure from the decarboxylation / protonation mechanism was suggested by Lee.[140] Based on quantum mechanical-free energy calculations and molecular dynamics simulations, Lee proposed that the orotate ring is initially protonated at C-5 (Figure 5-1, eq 5-3). Decarboxylation would then afford an ylide (or carbene-like) intermediate which could afford the product by either a direct 1,2-hydrogen shift or an indirect combination of protonation at C-6 and deprotonation at C-5.

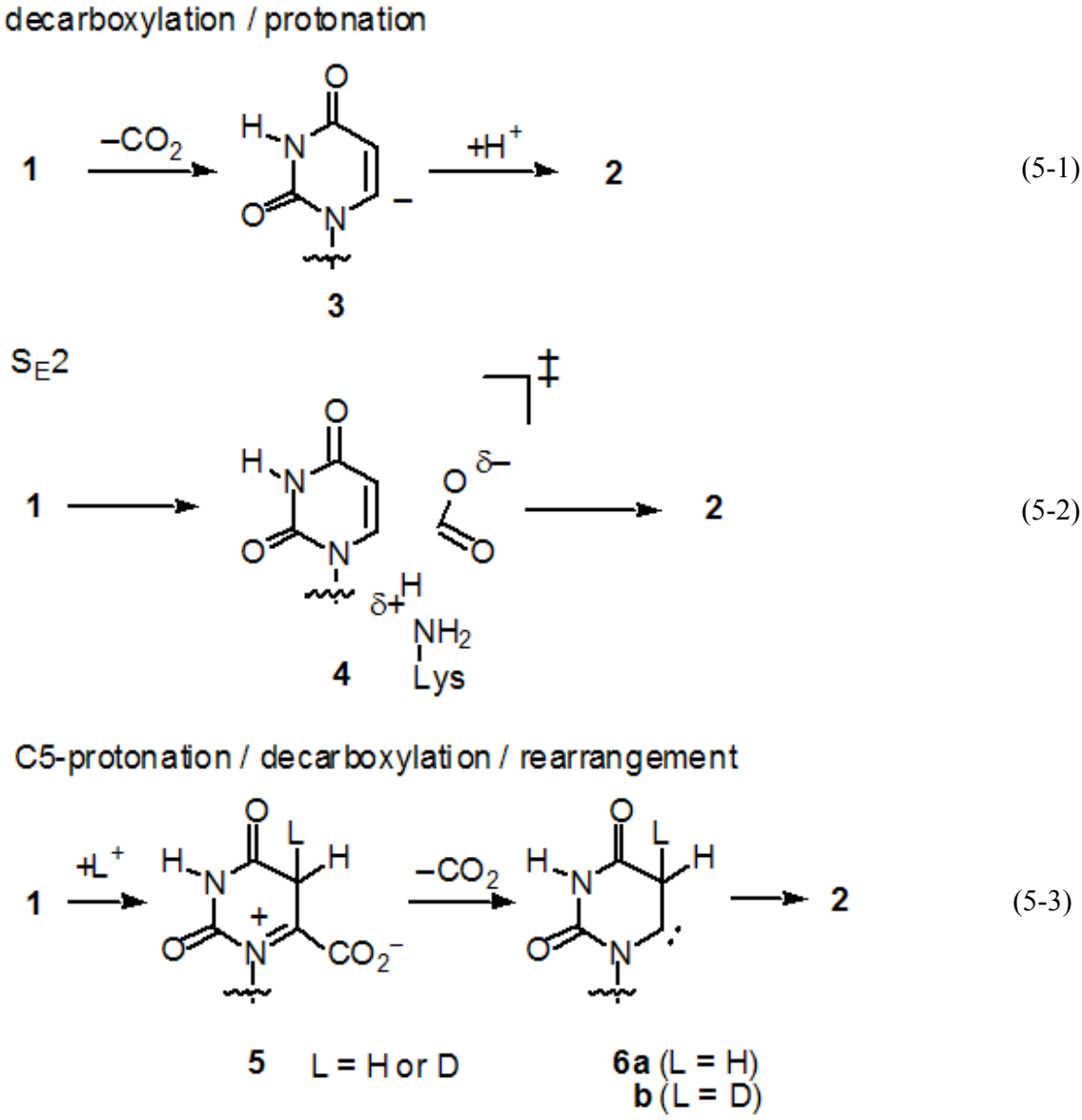


Figure 5-1. Recently postulated mechanisms for the decarboxylation of orotidine 5'-monophosphate **1**.

One might expect that the mechanisms of Figure 5-1 could be readily distinguished by a combination of isotope effects and labeling studies. Much of the data that would be expected to delineate the correct mechanism has in fact already been acquired. However, experimental observations can readily fail to allow a convincing qualitative

interpretation when the observations are in an intermediate range. For example, the observed deuterium solvent kinetic isotope effect (KIE) of 1.3 ± 0.2 is very difficult to interpret. The interpretation of this value is complicated by the uncertainty in the measurement, the potential impact of deuterated solvent on the enzyme's rate in ways that are unrelated to the mechanistic proton transfer,[141] and the possibility that proton transfer is occurring at a very late stage of the reaction coordinate with a resulting minimal effect on the rate.

The approach that is taken here is to first more explicitly define experimentally labeling observations and the solvent H/D KIE for this reaction, then apply DFT calculations to develop models for possible reaction mechanisms. By their nature, the simple calculational models explored cannot well address the question of the origin of the catalytic effect of ODCase. However, the calculational models can be used to interpret in detail the current and previous isotope effect observations in this reaction. The results serve to substantially resolve the basic ODCase mechanism and the nature of the proton transfer and decarboxylation processes.

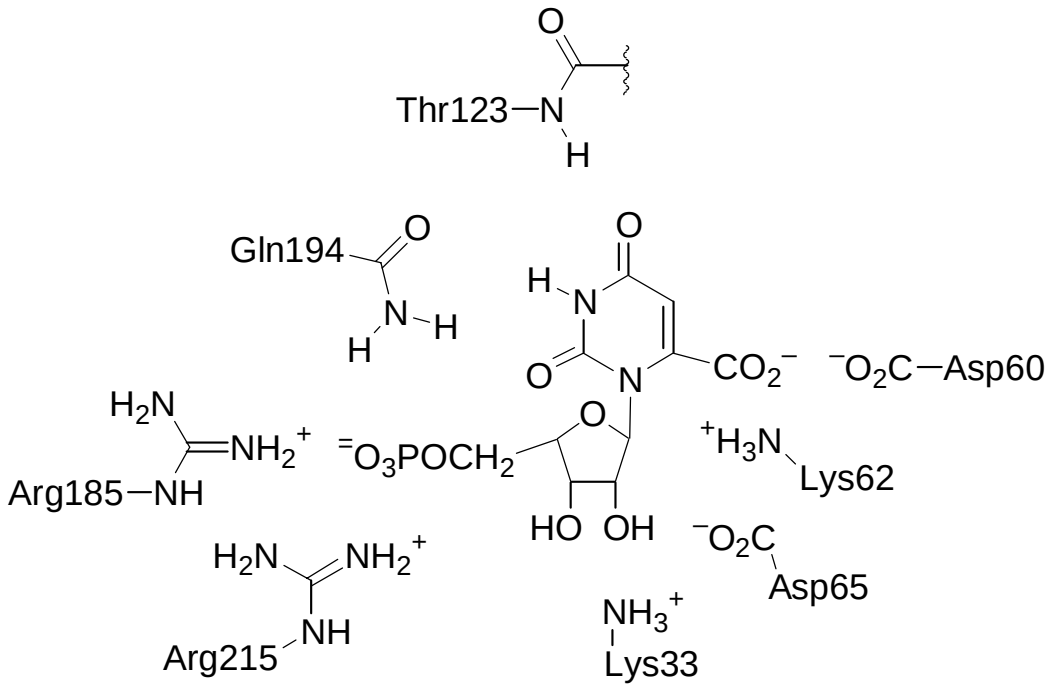


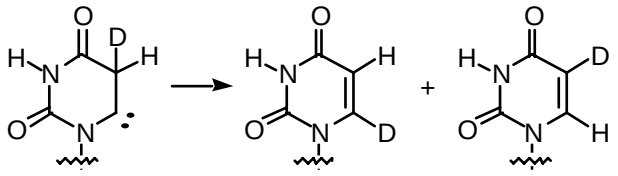
Figure 5-2. A schematic representative of the active site of ODCase. The numbering is *Bacillus subtilis* (see ref 134).

Results

Experimental

Experimental Decarboxylation in D_2O. The C5-protonation / decarboxylation mechanism of Lee led to an interesting prediction for reactions carried out in D_2O.[140] After C5-deuteration and decarboxylation, the intermediate **6b** can in principle afford **2** by a 1,2-migration. This is alternatively viewable as a carbene insertion into the adjacent C-H bond. Such processes are highly exothermic and usually fast, though the rearrangements can exhibit substantial orbital-alignment effects.[142] If this migration occurs directly, one might expect that both H and D would migrate, leading to the formation of both **7** and **8** (Scheme 5-2).

Scheme 5-2



6b **7** **8**

To check this issue, the decarboxylation of **1** with ODCase from *Saccharomyces cerevisiae* was carried out in D_2O (99.8% D initially, before equilibration with **1** and ODCase). The reaction mixture after completion was analyzed directly by ^1H NMR, and C6 was found to 99.3% deuterated. The residual proton signal at C6 was a doublet at δ 8.0 with a coupling constant of 8.1 Hz, just as is observed for the unlabeled **2**. Compound **8** would exhibit a singlet in this area, but this was not observed, and we estimate an upper bound for formation of **8** at 0.2%. The total hydroxylic ^1H content in the D_2O was analyzed after the reaction was complete and found to be 1.4% (by NMR using the ^1H signal of **2** as an internal standard). Thus the observed signal at δ 8.0 is consistent with residual ^1H in the solvent. It should be noted that this analysis does not exclude the presence of small amounts (<5%) of 5,6-dideuterio product, which can result from a very slow exchange of deuterium into the C5 position of **7**. However, the absence of **8** is the mechanistically significant observation – this excludes the uncatalyzed direct rearrangement of **6b**.

A related experiment using 5-deuterated **1** has been reported recently with essentially the same conclusion.[143] There are two advantages for the simple experiment

here. First, it is highly sensitive – since **8** would show up in a portion of the spectrum that has signal (due to the preponderance of **7**), very small amounts of **8** could be readily detected. Secondly, rearrangement here would be detected by transfer of H, not D, so that the possible operation of a large H/D isotope effect in the rearrangement would increase the detectability of 1,2-migration, rather than decrease detectability with 5-deuterated **1**.

Competition Isotope Effects in Mixed H_2O / D_2O. As introduced by O'Leary,[144] the use of a one-pot competition reaction employing mixed H_2O / D_2O solvent can avoid can avoid some of the general problems with solvent deuterium isotope effects, under the special condition that the proton transfer in a reaction is irreversible and occurs to a non-exchangeable site in the product. Such experiments effectively afford 'intramolecular' isotope effects and this leads to some complications in their interpretation,[144,145] but the O'Leary approach helps substantially in the example of the ODCase mechanism.

The decarboxylation of **1** with ODCase was carried out in 50:50 mixtures of H_2O and D_2O at 25 °C and buffered at pH 6 or pH 7. After the reaction was complete, the solvent was removed under vacuum and the product **2** was analyzed by NMR in d_6-DMSO. Some of the ribose ring protons were invariably obscured by residual H_2O but the uridine ring protons at C5 and C6 as well as the C1' anomeric proton on the ribose were readily observable at δ 5.6, 8.0, and 5.8, respectively. From the relative integrations of the signals at δ 8.0 versus δ 5.8 the incorporation of hydrogen versus deuterium at C6 was calculated. For comparison, the ^1H NMR of **2** derived from a

reaction in pure H_2O, but otherwise carried out identically, exhibited integrations for the signals at δ 5.6, 8.0, and 5.8 within 2% of 1:1:1. For four determinations at pH 6 the ratio of H to D at C6 was 0.98 with a standard deviation of 0.03.

Theoretical Calculations

C-5-Protonation / Decarboxylation / Rearrangement. The mechanistic pathway of eq 3 was previously explored calculationally by Lee using a combination of methods, and Lee discussed isotope effect expectations for N-1 and H-5 based on these calculations.[140] Our focus here is on the development of detailed transition structure models for the prediction of isotope effects. We also explore possible mechanisms for the effective 1,2-hydrogen migration in **6**. The decarboxylation of 1-methylorotate (**9**) was chosen as a computational model and its decarboxylation was studied in B3LYP calculations employing a 6-31+G(d,p) basis set.[146] In accord with the observations of Lee,[140] the gas-phase proton affinity of **9** at C5 (forming **10**) is predicted to be greater than the proton affinity at the C4 carbonyl oxygen, by 1 kcal/mol (290 versus 289 kcal/mol at B3LYP/6-31+G(d,p) + zpe). Also in agreement with Lee, the decarboxylation of **10** would be facile, with a gas-phase barrier of 8.9 kcal/mol for the transition structure **11**. The zwitterion / carbene **12** + CO_2 is predicted to be only 8.6 kcal/mol above **10**. Solvation and specific stabilization by the enzyme would have a substantial effect on these energetics,[140] but the calculations support the viability of decarboxylation of **5**, if it were formed. They cannot address realistically the plausibility of the formation of **5**.

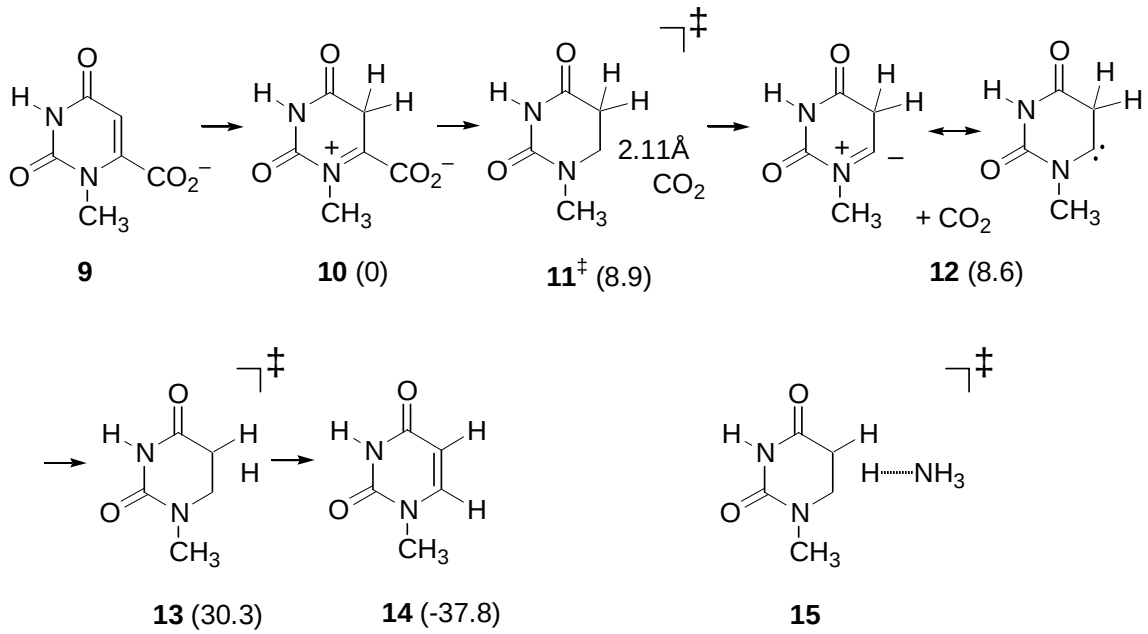


Figure 5-3. Calculated C5-protonation / decarboxylation / 1,2-rearrangement pathway for the decarboxylation of model **9**. Relative energies (B3LYP/6-31+G(d,p) + zpe, kcal/mol) are shown in parentheses.

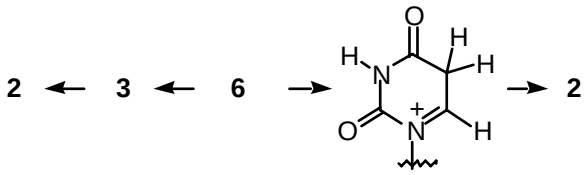
The last step in this mechanism is the conversion of zwitterion / carbene **6** to form uracil **2**. The direct rearrangement process has a high barrier in the gas phase (21.7 kcal/mol B3LYP/6-31+G(d,p) + zpe, 21.9 in MP2/6-31+G(d,p) single-point calculations). This is consistent with the experimental observations in D_2O above excluding an uncatalyzed direct rearrangement of **6b**. However, in transition structure **13** there is protonic character in the migrating hydrogen, raising the possibility that the proximity of a lysine residue could catalyze the concerted 1,2-migration. To explore this possibility, transition structure **15** was located for a migration mediated by a molecule of NH_3. This reduces the barrier to 16.0 kcal/mol in the gas phase. Since this catalyzed migration can be stereospecific and involve the same proton that was added to C-5 in the

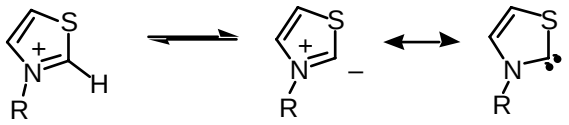
first place, it is consistent with the experimental absence of **8** in the product of D_2O reactions.

Two-step processes may be considered as an alternative to the direct rearrangement of **6** to **2**. One possibility is the deprotonation of **6** at C-5 to form the uridine anion **3** followed by protonation at C-6 to afford **2**. This would seem anti-intuitive from the standpoint that the mechanism would have arrived at **3** by a circuitous route when, alternatively, **3** can be formed directly from **1**. The barrier for direct decarboxylation of **1** would just be the endothermicity inherent in formation of the unstable anion **6**, since there is apparently no barrier for the reverse process,[2g] so it is not clear how the indirect route could be advantageous. A more attractive possibility is the protonation of **6** to form **21** followed by deprotonation to form **2**. To gauge crudely the basicity of **6** at C6, one may compare it with thiamine. Thiamine and related thiazolium ions (e.g., **22**) have pK_a's of 17-19,[147] but the high acidity of such structures is the result of a combination of stabilizing effects for the conjugate base (**23**). Stabilization by the ylide/carbene character of the structures would be expected to be similar for **2** versus **23**, but **6** lacks the stabilizing adjacent sulfur atom present in **23**. Addition of a phenylthio group to simple structures containing a single electron-withdrawing group decreases the pK_a by about 10,[148] so we would estimate the pK_a of the conjugate acid of **6** (**21**) at C6 to be 27-29. As an alternative approach to this issue, we calculated the energetics for protonation of **12** by Me_3NH^+, and this is predicted to be downhill by 14.2 kcal/mol. From either the qualitative argument above or the calculational results, protonation of **6** should be

extremely rapid if a proton donor is available. It should be noted, however, that the formation of **21** requires the overall donation of two protons from the enzyme.

Scheme 5-3



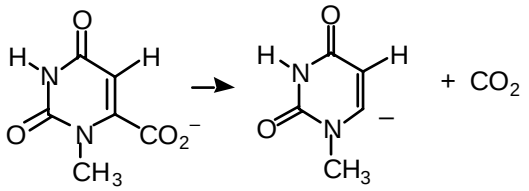


S_E2 Mechanism versus "Simple" Decarboxylation. For comparison with experimental observations, we required reasonable models in high-level calculations for both the electrophilic substitution of the S_E2 process and the direct decarboxylation mechanism. This modeling is fraught with both specific and general difficulties. In the process of dealing with the problems, it became apparent that the seemingly distinct S_E2 and direct decarboxylation mechanisms are better understood as the extremes of a mechanistic continuum. This idea will provide insight into both the uncatalyzed process in water and the enzymatic catalysis.

No potential energy saddle point could be located for the gas-phase decarboxylation of **9** to afford the N-methyluracil anion **24** + CO_2; the reverse reaction is apparently enthalpically barrierless. The variational transition state for decarboxylation,

at approximately the free-energy saddle point, would be extremely late, and its enthalpy should be reasonably approximated by separated **24** and CO_2. Formation of **24** + CO_2 is predicted to be uphill by 36.4 kcal/mol (B3LYP/6-31+G(d,p) + zpe). This is similar to results from other theoretical calculations.[129,133,149]

Scheme 5-4



9 **24**

It has been noted previously that the predicted barrier for decarboxylation corresponds closely to the experimental barrier for decarboxylation of **1** in water (38.5 kcal/mol[119]). This correspondence should not be misinterpreted; it certainly does not imply that solvation plays no role in the decarboxylation or that the gas-phase decarboxylation is a good model for the solution reaction. Rather, the correspondence implies that the solvation of the decarboxylation transition state is roughly similar in energetic magnitude to the solvation of the starting material. The starting carboxylate would be strongly solvated in water; an estimated enthalpy of solvation of **9**, based on the pK_a of its conjugate acid (0.4[150]) and values for other carboxylates in water, is 74 kcal/mol.[151] The transition state solvation must be approximately the same. However, the nature of the strong transition state solvation is unclear, particularly since the decarboxylation transition state is presumably very late with modest negative charge left on the CO_2.

Insight into the nature of solvation of the decarboxylation transition state was provided by a series of calculations aimed originally at examining the S_E2 mechanism. The transition structures **25-30** (Figure 5-4) were located for the decarboxylation of **9** assisted by single molecules of HF, formic acid, fluoromethanol, vinyl alcohol, methanol, and water. The proton donors in this series span a range of gas-phase acidity of about 50 kcal/mol. In each case the decarboxylation is highly advanced, and the H–O or H–F bond is only slightly elongated from its value in the isolated proton donor. However, all of the structures are substantially stabilized compared to separated proton donor / **24** / CO_2 (at a relative energy of 36.4 kcal/mol). (It should be understood clearly that this transition state stabilization would not engender *catalysis* for these simple reactions, as there would be equal or greater stabilization of the starting materials.)

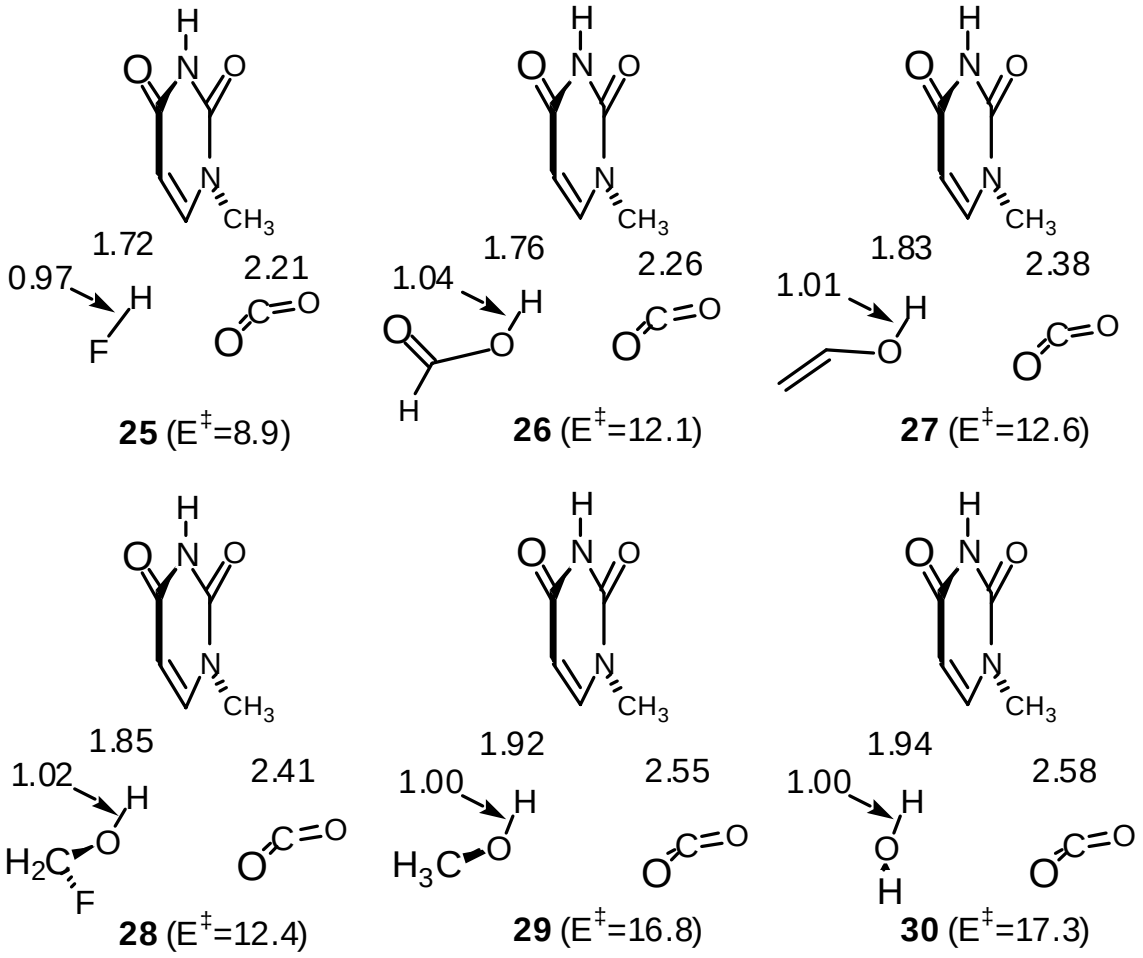


Figure 5-4. Transition structures for decarboxylation of **9** assisted by one molecule of a proton donor. Energies relative to separate **9** and proton donor are given in parentheses (B3LYP/6-31+G(d,p) + zpe, kcal/mol).

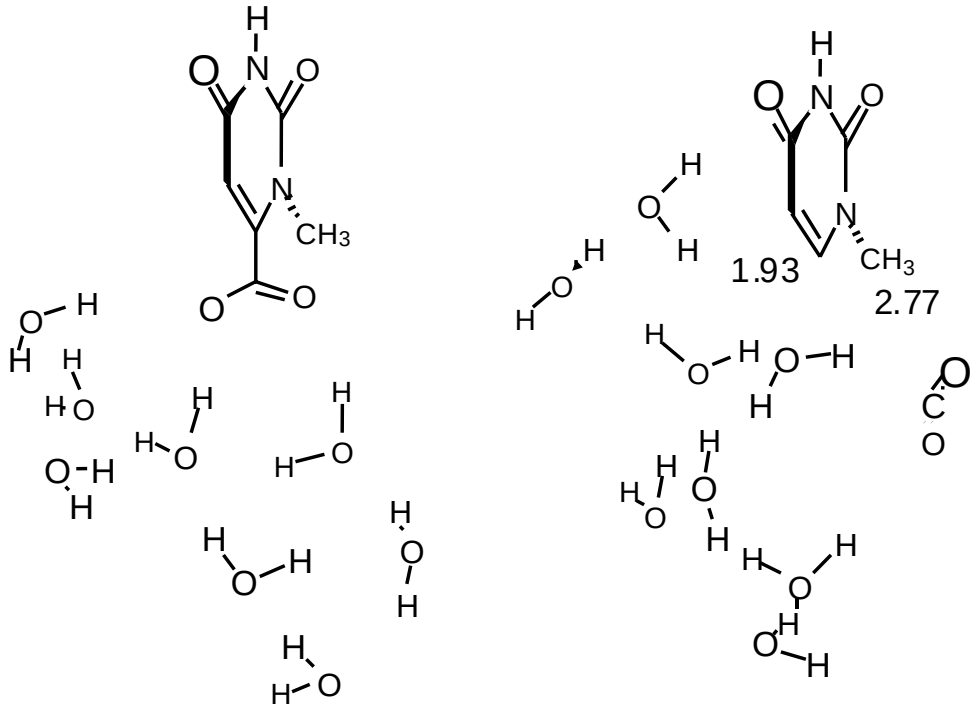
Looking at the detailed geometries, the series of structures are clearly a continuum. As the energetic assistance by the proton donor decreases, the C6--H distance increases and the decarboxylation transition state becomes later. The trends are highly consistent, despite the fact that ***29*** *and* ***30*** *are not transition structures for an* S_E2 *mechanism.* While **25**-**28** ultimately undergo proton transfer to afford the uracil **14**, **29** and **30** lead to a solvated uracil anion, never consummating the proton transfer. This is not surprising;

the gas phase proton affinity of **24** (364 kcal/mol) is less than that of hydroxide or methoxide (388 and 378 kcal/mol, respectively, predicted at B3LYP/6-31+G(d,p) + zpe). The structures **25-30** appear to be best understood as "solvated decarboxylations" rather than "electrophilic substitutions." This is most obvious for **29** and **30**, but even with **25-28**, the proton transfer is an "afterthought," proceeding long after the transition state.[152] The stronger acids solvate the transition state to a greater extent, aiding in the decarboxylation, but the range of activation barriers is much smaller than the range of acidities in the solvating acids.

To explore the decarboxylation in water further, the decarboxylation transition state and the starting **9** were each optimized in a cluster of 8 water molecules. The best ground-state and transition-state structures located were **31** and **32**; some others are given in the Appendix. The structures studied were chosen to model minimal expectations for solvation in bulk water, including a network of water molecules supporting the transition state solvation and the hydrogen bonding to the carboxylate oxygens in **9**. Otherwise, the structures are not meant to be realistic. No effort was made to identify the best of the many possible cluster structures, and even if the best were found, it would be questionably representative of bulk water. The solvated transition structure **32** is 30.1 kcal/mol above the solvated **9**. Considering the complications, this is in very reasonable agreement with the experimental barrier in water. The breaking of the C6---CO_2 bond has proceeded to a somewhat greater extent in **32** than in **30**, but otherwise the structures are similar. However, **32** is now formally

an S_E2 transition state – the extra water molecules stabilize the formation of a hydroxide anion allowing protonation of the uracil at C6 (Scheme 5-5).

Scheme 5-5



31 (E_{rel}=0) **32** ($E_{rel}^{\ddagger}$=30.1)

Overall, these calculations support the idea that the decarboxylation transition state in water is in fact tremendously stabilized by solvation. In order to achieve catalysis, the enzyme must "solvate" (bind to) the transition state to an even greater extent than water.

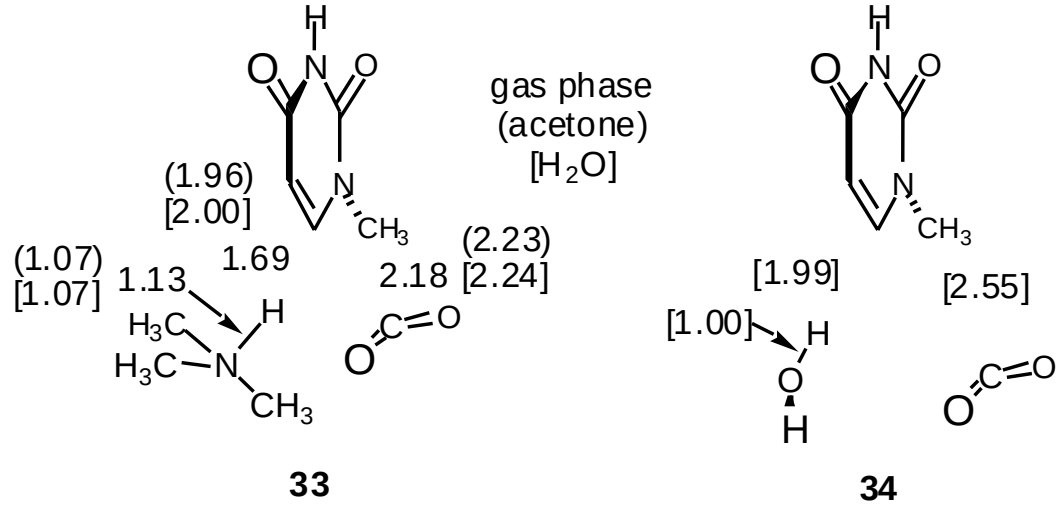
In the enzyme, a lysine residue (Lys62 in *Bacillus subtilis* numbering[134] – see Figure 5-2) would likely play the key role in solvating the decarboxylation transition state and donating a proton in the formal S_E2 process. To model this process, the transition structure **33** was located for the decarboxylation of **9** stabilized by a

trimethylammonium cation.[153] Because of its positive charge, a trimethylammonium ion is much more acidic in the gas phase than any of the neutral proton donors used in structures **25-30**. The gas phase structure then has the appearance of being the extreme of the continuum, with shorter C6--H and C6--CO_2 distances than **25**. This is misleading relative to the solution chemistry, and the transition structure was also optimized using a polarizable continuum (PCM) solvent model for acetone ($\varepsilon = 20.7$) or water ($\varepsilon = 78.39$).[154] The resulting structures have much less S_E2 character, with the C6--H distance increasing to 1.96 – 2.00 Å. For comparison, structure **34** results when **30** is reoptimized using a PCM solvent model in water – the change in C6--H is small with water as the proton donor. Based on the large C6--H distance in **33** in solvent, it seems unlikely that a lysinium-mediated decarboxylation in the enzyme would have much more S_E2 character than the uncatalyzed reaction in water (Scheme 5-6).

The S_E2 character for **33** in solvent is low, but this does not address the basic energetic question of how much the presence of the ammonium stabilizes the decarboxylation transition state. Because of the large charge-charge interaction effects, there is no simple adequate way to calculate the stabilization energy in high-level calculations – the fundamental problem is that there is no "fair" starting material with which to compare **33** to calculate a barrier. At one extreme, **33** is 65 kcal/mol below separate 1-methylorotate and trimethylammonium ion in the gas phase. At the other extreme, it may be recognized that ammonium ions do not catalyze the decarboxylation at all in free solution – solvation of the starting carboxylate would be expected to exceed solvation of the transition structure. In an attempt to mimic the starting state in the

enzyme, a geometry-optimized trimethylammonium ion was placed directly above C_6 of a geometry-optimized **9** with a C_6--H separation of 2.3 Å. The energy was then calculated without further geometry optimization (which would ultimately lead to proton transfer to the carboxylate). From this structure, the barrier to formation of **33** was 13.9 kcal/mol. The inadequacy of this calculation is plain, but it does serve to show that preorganization of ammonium ion near an orotate can plausibly decrease the barrier for the decarboxylation.

Scheme 5-6



33 **34**

Warshel concludes that these types of electrostatic interactions in the protein account for the enzyme's ability to promote decarboxylation.[138] These electrostatic effects are due to repulsions between the carboxylates of two aspartate residues (Asp-60 & Asp-65, Figure 5-2) rather than protein carboxylate repelling the substrate carboxylate. This carboxylate electrostatic repulsion stabilizes the lysinium residue at the transition state. In the enzyme the carboxylates are preorganized to repel each other

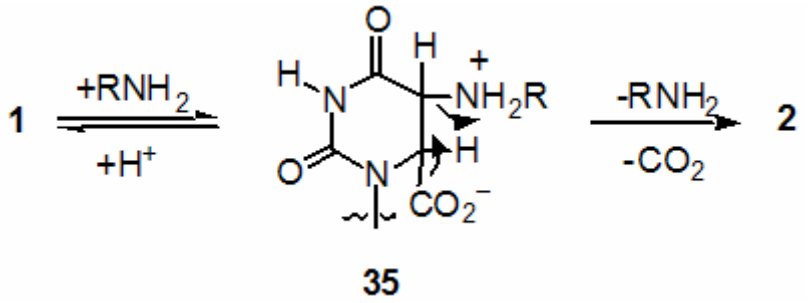
in the ground state so that their repulsion is not part of the reaction barrier.[152] Alternatively, when the same reaction is considered in water, the water molecules that stabilize the proton donor in the transition state also repel each other. This water-water repulsion is part of the activation barrier. The net effect is a very large transition-state stabilization in the enzyme relative to water.

Another clue suggesting some transition state stabilization by the presence of a proximal ammonium cation is the surprisingly short C6--CO_2 distances in **33**. If the ammonium cation were providing no more stabilization to the transition state than a water molecule as in **34**, then one would expect the loss of CO_2 to be similarly late. The much shorter C6--CO_2 distance of 2.24Å, signaling an earlier decarboxylation transition state, is similar to the corresponding distances in **25** and **26**. This supports the idea that an ammonium cation can provide greater transition state stabilization than water.

Decarboxylative Elimination. In 1982, Silverman and Groziak proposed a mechanism for ODCase in which an initial Michael addition to C_5 of OMP is followed by a decarboxylative elimination to afford UMP.[137] Within the context of the crystal structures, this mechanism is conceivable if a neutral Lys62 residue acts as the nucleophile, as in Scheme 5-7. To account for the observation of a substantial ^{13}C KIE in the carboxylate carbon, the formation of intermediate **35** would have to be rapidly reversible. A key test of this mechanism was the measurement by Wolfenden and coworkers of a near unity H/D KIE (1.00 ±0.06 on k_{cat}/k_M) at C_5 of OMP.[122] Because an inverse H/D KIE would be expected if an sp^3-hybridized C_5 (as in **35**) were involved, the Silverman mechanism has been largely dismissed in the literature. This dismissal

seems hasty, since the uncertainty on the C_5 H/D KIE is large (particularly after consideration of commitment, *vide infra*) and a late elimination transition state could conceivably exhibit a low H/D KIE. For this reason, we briefly investigated the mechanism theoretically with the goal of providing a basis for the quantitative comparison of predicted and experimental KIEs.

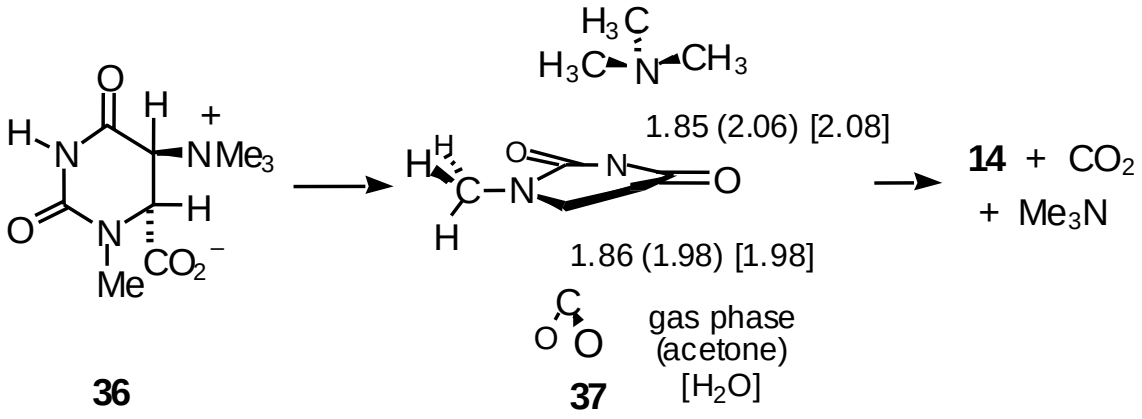
Scheme 5-7



35

As a model for the decarboxylative elimination, transition structure **37** was located in B3LYP/6-31+G** calculations in the gas phase and including acetone and water PCM solvent models. This reaction involves the concerted formation of three neutral products from a zwitterion, and the gas-phase reaction would be highly exothermic (47.2 kcal/mol). The gas-phase transition structure is accordingly very early with a barrier of only 1.3 kcal/mol. The transition structures obtained in solvent models are later, with barriers of 12.5 and 13.6 kcal/mol for acetone and water, respectively (Scheme 5-8). These barriers suggest that the decarboxylative elimination step can be energetically viable if the formation of the intermediate zwitterion is sufficiently facile. The latter point is tricky to theoretically evaluate and no attempt was made to do so – transition structure **37** was sufficient for our purpose of experimentally accessing the mechanism using isotope effects.

Scheme 5-8



Predicted Isotope Effects. The qualitative interpretation of kinetic isotope effects has long been a standard mechanistic tool, but this approach is often limited in its ability to distinguish between similar mechanisms. This is true for ODCase. For example, the observation of a large ^{13}C KIE of 1.049[123] at the carboxylate carbon of OMP does not qualitatively distinguish between any of the mechanisms involving rate-limiting cleavage of the C_6--CO_2 bond. In recent years, a considerable advance in the interpretation of isotope effects has been the comparison of experimental KIEs with predicted KIEs based on high-level theoretical calculations. Predictions of heavy-atom KIEs in particular have proven highly accurate, so long as the underlying calculation accurately depicts the mechanism and transition state geometry.[155,156] Thus, comparison of experimental isotope effects with those predicted for a choice of mechanisms can be used to distinguish between the possibilities.

Appropriate ^{13}C, ^{2}H, and ^{15}N KIEs for the various mechanisms were predicted from the scaled theoretical vibrational frequencies[157] using conventional transition state theory by the method of Bigeleisen and Mayer.[158] Tunneling corrections were applied

using the one-dimensional infinite parabolic barrier model.[159] The results are summarized in Table 1, along with the experimental KIEs for comparison.

The experimental KIEs require comment. The value of 1.049 for the carboxylate carbon was the maximum obtained at pH 4. Smaller values were obtained at higher pH's, indicative of a commitment to catalysis, and it is unclear whether this commitment is fully relieved at pH 4. The full intrinsic isotope effect may thus be higher than 1.049. The H/D KIE at C_5 was measured at pH 6 and presumably some commitment to catalysis is involved in this measurement, as the ^{13}C KIE for the carboxylate carbon is only 1.0272 at ph 6. This has the effect of increasing the uncertainty of the measurement to 1.00 ± 0.11 for the intrinsic isotope effect. The experimentally observed ^{15}N KIE at N_1 of 1.0036 was at pH 6.5, and extrapolation of this value based of the commitment observed in the ^{13}C KIE at pH 6.5 leads to an intrinsic ^{15}N KIE of 1.0068.[131] However, there are two problems with this extrapolation. The first is that there is a relatively high uncertainty in the effect of commitment.[131] The second is that with such a small KIE, any small isotope effect for binding of substrate[160] will lead to a relatively large error in the extrapolation. For example, if the binding isotope effect were 1.003, the correct extrapolated intrinsic ^{15}N KIE would be 1.0041. A significant uncertainty in the ^{15}N KIE should therefore be recognized.

Many comments on the KIE predictions are in order. The carboxylate CO_2, C_5 H/D, and N_1 isotope effects for the S_E2, C_5-protonation / decarboxylation, and decarboxylative elimination mechanisms are all based on the decarboxylation transition structures, assuming that this step is fully rate limiting. Calculation of isotope effects for

the direct decarboxylation is complicated by the lack of a potential-energy saddle point for loss of CO_2. The approach of Lee and Phillips was to base the KIE on the equilibrium isotope effect for orotate versus uridine anion.[149] The rationalization for such an "equilibrium model" would be that the endothermic loss of CO_2 would have a very late transition state. Their resulting N_1 KIE was strikingly close to the extrapolated experimental value. However, if this model is applied to the carboxylate carbon, the predicted isotope effect would be 0.997, obviously far from experiment. The alternative approach here is to assume that the enzymatic transition state is earlier to an unknown degree, calculate isotope effects for a series of C_6--CO_2 separations,[161] and pick the best match with the experimental carboxylate isotope effect. Applying this procedure, the predicted ^{13}C KIE reaches a maximum plateau of 1.039 centered on a C_6--CO_2 distance of 2.2 Å. This distance is intuitively short, but an accurate calculation is difficult because of the formation of an anion at the transition state. There is not accurate method to address this difficulty, without employing intrinsic solvent molecules that would stabilize the incipient charge. Unfortunately, this would not accurately depict a direct decarboxylation.

The most complicated KIE predictions are those for H/D transfer to C_6. The reference state used for predicting H/D KIEs from the S_E2 and decarboxylative elimination transition structures (**33** and **37**, respectively) was liquid HOD. A reduced isotopic partition ratio for liquid HOD that is applicable for comparison with B3LYP/6-31+G** calculations was calculated by correcting the gas-phase theoretical result for HOD by the experimental vapor pressure isotope effect for HOD.[162] The use of liquid

water as a reference state in these two mechanisms, as opposed to a lysinium ion that is presumably effecting the actual proton transfer to C_6, assumes that H/D equilibration of the lysinium ion (Lys62) with solvent is faster than the decarboxylation itself. This seems reasonable since the catalyzed reaction still has a substantial barrier and the Lys62 is near the surface of the enzyme.

The H/D isotope effect at C_6 for the C_5-protonation / decarboxylation mechanism depends on whether C_6 is protonated by the same proton that was initially added to C_5 (as in the conversion of **12** to **14**) or by an external proton (as in the conversion of **6** to **21**). In the former case, the isotope effect would be determined by transition structure **11**. (It is necessary to assume that H-transfer from C_5 to C_6 is stereospecific to account for the ultimate absence of deuterium at C_5.) The isotope effect if an external proton is transferred to C_6 was based on a transition structure for transfer of a proton from trimethylammonium cation to **6** (see Appendix). For this primary H/D isotope effect, no tunneling correction was applied, and the calculated KIE is likely a lower limit.

In the sequential decarboxylation/protonation mechanism, the transfer of a proton to C_6 of the uracil anion would presumably have a very low barrier. The observed isotope effect will reflect the concentration of H/D in a position or positions capable of transferring the proton to C_6 (K_{fract}), along with a competition isotope effect if more than one position can transfer the proton ($k_{H/D,compet}$). From the crystal structures and previous studies of the sequential decarboxylation/protonation mechanism, we assume that a lysine residue (Lys62) is transferring the proton. If this transfer is so fast that rotation about the C-N bond of the lysinium ion doesn't have time to occur, the observed

isotope effect would be K_{fract}. Little appears to be known about H/D fractionation factors for lysinium ion within enzymes, but the fractionation factor for a primary alkylammonium ion in water is ≈1.08.[163] This fractionation factor is decreased by hydrogen bonding in water – the predicted fractionation factor for gas-phase $MeNH_3^+$ versus liquid HOD (B3LYP/6-31+G**) is 1.23. In previous modeling of the proton transfer step for this mechanism, the lysinium proton undergoing transfer to C_6 starts with no apparent hydrogen bonding, and the fractionation factor for this position would be expected to be ≥1.08. Based on this, the expected H/D isotope effect at C_6 for the sequential decarboxylation/protonation mechanism would be ≤0.92.

Alternatively, if the proton transfer from the lysinium ion to C_6 of the uracil anion has a barrier of a few kcal/mol, the observed isotope effect would in part reflect a competition between protium and deuterium in the $R\text{-}NH_nD_{3-n}$ groups. Lysinium ions containing either 3 deuterium or 3 protium (≈1/4 of the total) would not contribute to the isotope effect, excepts as reflected in K_{fract}. The remaining lysinium ions, consisting of either NH_2D or NHD_2 groups, would contribute to the observed isotope effect in a way that depends on an intrinsic rate difference for transfer of H versus D corrected by a statistical factor. If the intrinsic rate difference is assumed to be 2.0 and K_{fract} is 0.92, the overall predicted isotope effect would be 1.46.

Table 5-1. Experimental versus predicted kinetic isotope effects (k_{12C}/k_{13C}, k_H,k_D, k_{14N},k_{15N}) for orotate decarboxylation by various mechanisms.

	$\underline{C}O_2$	H/D on C_5	N_1	H/D transferred to C_6
		Experimental		
	1.049[a]	1.00 ± 0.06[b]	1.0036 [1.0068][c]	0.98 ± 0.03
Mechanism		Predicted		
Decarboxylation / protonation (equilibrium model)[d]	0.997	1.02	1.0056	0.92[e] 1.46[e]
Decarboxylation / protonation (C_6---CO_2 = 2.2 Å)[f]	1.039	1.00	1.0041	0.92[e] 1.46[e]
S_E2[g]	1.052	1.00	1.0039	0.97
C_5-Protonation / decarboxylation[h]	1.038	1.03[i]	1.0036	1.23[j] 3.78[k]
Decarboxylative elimination[l]	1.049[m] 1.050[n]	0.838[m] 0.851[n]	0.9969[m] 0.9969[n]	1.08[m] 1.09[n]

[a]See ref 123. [b]See ref 122. [c]See ref 131. The first value is experimental. The value in brackets is extrapolated based on an expected commitment to catalysis. [d]Assumes a very late decarboxylation transition state, modeled as **24** + CO_2 versus starting material **9**. [e]See text. [f]KIEs predicted based on a transition structure in which the C_6---CO_2 distance in **9** is elongated to 2.2 Å. This distance was chosen to best fit the experimental ^{13}C KIE. [g]KIEs based on transition structure **33** (in acetone PCM solvent model) versus starting materials **9** / liquid HOD. [h]KIEs based on transition structure **11** versus starting materials **9** / liquid HOD. [i]Ref 140 had predicted 1.012, but that calculation was debatably based on the intermediate prior to the decarboxylation transition state. [j]KIE if rate-limiting decarboxylation is followed by a stereospecific hydrogen shift from C_5 to C_6. [k]KIE based on a transition structure for transfer of a proton from Me_3NH^+ to **6**. (See Supporting Information.) This KIE does not include a tunneling correction. [l]KIE based on transition structure **37** versus starting materials **9** / liquid HOD. [m]Acetone PCM solvent model. [n]Water PCM solvent model.

Discussion

In considering the mechanistic implications of the experimental isotope effects, the most critical observation would appear to be the very large ^{13}C KIE for the carboxylate carbon. The ^{13}C KIEs for decarboxylations have been extensively studied and it is worthwhile to consider known structural effects on the isotope effects observed.[164] (See Appendix for a series of examples.) Simple decarboxylations of carboxylate anions typically exhibit ^{13}C KIEs in a range from 1.01 to 1.04. Such reactions generally afford less stable anions, making the reactions uphill processes enthalpically. The magnitude of the KIE in these cases is limited by the late transition state, since the *equilibrium* isotope effect for decarboxylations is invariably near unity or slightly inverse, and limited by the absence of an enthalpic barrier through which tunneling can occur. Many examples of decarboxylation KIEs > 1.04 are known, but these invariably involve formation of either a highly stabilized anion or a neutral product. Such large decarboxylation KIEs thus suggest an exothermic decarboxylation process with a discrete barrier.

These ideas are mirrored in the predicted ^{13}C KIEs in Table 5-1. In both the decarboxylation / protonation and C_5-protonation / decarboxylation mechanisms, the decarboxylation step itself is an uphill process and the predicted ^{13}C KIE is, at its maximum, 1.039. We do not believe that a simple uphill decarboxylation to form a uracil anion can account for the experimental intrinsic KIE of 1.049 (or greater). On the other hand, the downhill S_E2 and decarboxylative elimination mechanisms lead to predicted ^{13}C KIE that fit well with experiment.

The H/D KIE on C_5 does not fit with the decarboxylative elimination mechanism. This is in agreement with the original interpretation of Wolfenden and coworkers,[122] though we believe the isotope effect calculation strengthens their conclusion. The remaining mechanisms are consistent with an H/D KIE near unity.

The best ^{15}N KIE prediction, 1.0056, arises from an "equilibrium model" for simple decarboxylation that is untenable due to its poor ^{13}C KIE prediction. The ^{15}N KIE does rule out the decarboxylative elimination mechanism, but considering the uncertainties in the extrapolation of the observed KIE, it is arguably consistent with any of the other mechanistic models.

Traditionally, the k_H/k_D of 0.98 for transfer of H/D to C_6 might be interpreted as ruling out the S_E2 mechanism. After all, the S_E2 mechanism formally involves the transfer of H/D in the rate-limiting step, and a primary H/D isotope effect, typically > 2, would be expected. This qualitative interpretation would be overly simplistic for two reasons. The first is that the S_E2 transition states, as described above, are best understood as solvated decarboxylations rather than electrophilic substitutions. The degree of proton transfer in transition structure **33** is quite small, and the H/D being transferred is in an only modestly looser position at the transition state than it was in the starting ammonium ion. The second reason is that the appropriate reference state for the H/D transfer is bulk water rather than ammonium ion, and due to hydrogen bonding the water reference state is itself a looser position than ammonium ion. The predicted S_E2 KIE of 0.97 may thus be viewed as resulting from the combination of a normal KIE for the S_E2 process and an inverse isotope effect for formation of a lysinium ion. Overall,

the H/D KIE predicted for the S_E2 mechanism ends up in striking agreement with experiment.

It is difficult to see how either the C_5-protonation / decarboxylation mechanism or the decarboxylative elimination mechanism could account for the H/D KIE at C_6, but the sequential decarboxylation / protonation mechanism requires further consideration. At one mechanistic extreme, in which protonation of the uracil anion is too fast to allow an isotopic selection, the expected isotope effect would be more inverse than observed. However, if, for unknown reasons, the highly exothermic transfer of a proton from a lysinium ion to a uracil anion faces a significant barrier, it would probably be possible to rationalize a wide range of experimental results H/D KIEs, including that observed. Overall, the strongest evidence against the decarboxylation / protonation mechanism is not the C_6 H/D KIE but its difficulty in rationalizing the carboxylate ^{13}C KIE.

Conclusions

The combination of theoretical calculations, isotope effects, and a cumulative interpretation of all the experimental results available supports a very simple S_E2 mechanism for the ODCase catalyzed decarboxylation. A protonated lysinium ion stabilizes the transition state for decarboxylation. A high energy vinyl carbanion is avoided by a proton transfer at a stage where negative charge develops during decarboxylation. When C-6 becomes sufficiently basic proton transfer occurs rapidly.

CHAPTER VI

ISOTOPE EFFECTS AND THE MECHANISM OF EPOXIDATION OF CYCLOHEXENONE WITH TERT-BUTYLHYDROPEROXIDE

Introduction

The epoxidation of α,β-unsaturated carbonyls with hydroperoxides under basic conditions, the Weitz-Scheffer reaction, is valuable transformation in organic synthesis.[165],[166] The mildness of the reaction conditions and the high selectivity for the oxidation of electron-poor alkenes has allowed the application of these reactions to diverse complex structures.[167] The oldest and simplest reaction conditions utilize alkaline hydrogen peroxide, but reactions using alkyl hydroperoxides have advantages in many circumstances.[168],[169] Diverse approaches to enantioselective epoxidations have been developed,[170] including catalysis by polyamino acids (the Juliá-Colonna epoxidation)[171] and chiral phase-transfer catalysts,[172] reactions employing chiral alkyl hydroperoxides,[173] and reactions using zinc reagents and O_2 in the presence of a chiral alcohol.[174]

The accepted two-step mechanism of these reactions (Scheme 6-1), first proposed by Bunton and Minkoff,[166a] involves the conjugate addition of a hydroperoxy or alkylperoxy anion **2** to afford a peroxyenolate **3** followed by ring-closing intramolecular nucleophilic substitution of C_2 of the enolate on the O-O bond to afford the epoxide **4**.

Strong evidence for an intermediate in these reactions includes their non-stereospecificity; unlike epoxidations of electron-rich alkenes with peracids, the stereochemistry of the starting alkene is not necessarily retained in the epoxide. For example, the epoxidations of *E*- and *Z*-3-methyl-3-penten-2-one with basic H_2O_2 in methanol both afford predominantly the *E* epoxide product.[175]

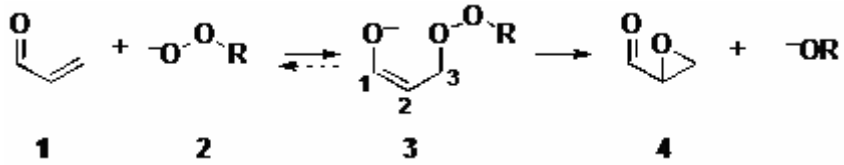


Figure 6-1. General mechanism for the addition of peroxide to α,β-unsaturated carbonyl.

While the overall mechanism is well-established, a consistent picture of the rate-limiting step has been elusive. In the reaction of *Z*-3-methyl-3-penten-2-one (**5**) with alkaline hydrogen peroxide, House found that *Z*-*E* isomerization occurred at rates comparable to epoxidation (Scheme 6-2).[175] This suggests significant reversibility of the initial addition under these conditions. On the other hand, substituent effect studies of the epoxidation of 4-aryl-3-buten-2-ones under similar conditions have been interpreted as favoring a rate-limiting addition step.[176] In a careful study of the epoxidation of β-deuterium labeled phenyl vinyl ketone with hydrogen peroxide, Kelly and Roberts found that *Z*-*E* isomerization was much faster than epoxidation under Juliá-Colonna conditions using polyleucine as catalyst.[177] This strongly supports rate-limiting ring closure. In contrast, isomerization and epoxidation were comparable in the absence

of the polyleucine. This suggests that the rate-limiting step may vary depending on the detailed reaction conditions.

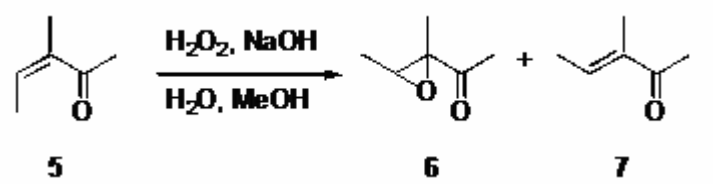


Figure 6-2. House found that *Z*-*E* isomerization occurred at rates comparable to epoxidation in the reaction of *Z*-3-methyl-3-penten-2-one with alkaline hydrogen peroxide.

This uncertainty in the rate-limiting step and a lack of knowledge of the structural characteristics of the transition state thwarts a detailed understanding of diastereoselectivity or enantioselectivity in these reactions. This is particularly true for epoxidations with alkyl hydroperoxides under typical synthetic conditions and for epoxidations of cyclic enones, where little mechanistic information is available. We describe here a study of the epoxidation of cyclohexenone with *tert*-butyl hydroperoxide (*t*-BuOOH) / DBU (Figure 6-3) using a combination of experimental kinetic isotope effects (KIEs) and theoretical calculations. The results provide insight into the stereoselectivity of these reactions and should aid the further development of stereocontrolled epoxidations.

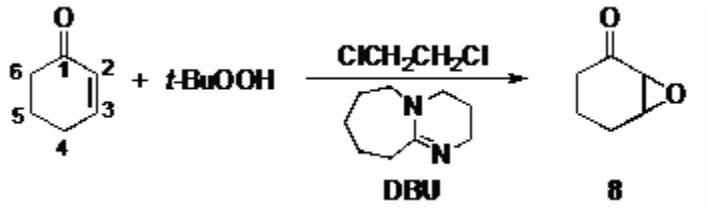


Figure 6-3. The expoxidation of cyclohexenone with *tert*-butyl hydroperoxide with DBU.

Results

Experimental

Experimental Isotope Effects. The epoxidation of an enone using a combination of an alkyl hydroperoxide and DBU in an aprotic solvent was first reported by Schlessinger and Poss.[167b] Yadav demonstrated the utility of these conditions with a range of α,β-unsaturated carbonyls,[169] and they have been commonly applied in enantioselective reactions using chiral alkyl hydroperoxides.[173] Under the prototypical epoxidation conditions employed here (stoichiometric DBU and *t*-BuOOH in dichloroethane at 22 °C), cyclohexenone is converted to **8** cleanly and essentially quantitatively.

The ^{13}C KIEs for the epoxidation of cyclohexenone were determined combinatorially by NMR methodology at natural abundance.[5] Two reactions of cyclohexenone were taken 83.4% and 89.1% conversion, and the unreacted cyclohexenone was recovered by an extractive workup followed by flash chromatography and fractional distillation. The samples of recovered cyclohexenone were analyzed by ^{13}C NMR, along with standard samples that had not been subjected to the reaction conditions. The change in isotopic composition in each position was

determined relative to the α-methylene carbon in cyclohexenone,[178] with the assumption that isotopic fractionation in this position was negligible. From the percentage conversions and the changes in isotopic composition, the KIEs were calculated as previously described.

Table 6-1 shows the results of two separate KIE determinations (each based on six sets of spectra) for each of the two reactions. The independent sets of ^{13}C KIEs agree within the standard deviation of the measurements, though the KIEs here are more variable than in previous KIE determinations on cyclohexenone due to the presence of an interfering trace impurity in the samples. Despite the variability, the qualitative features of the KIEs are apparent. Only the C_2 and C_3 KIEs differ significantly from unity, with a relatively large C_3 isotope effect and a smaller KIE at C_2. The qualitative interpretation of the C_3 KIE is that the rate-limiting step involves a substantial bonding change at C_3, as would be expected for a rate-limiting addition of *t*-BuOO$^-$ to cyclohexenone. The medium-sized C_2 KIE is less readily interpreted. A more detailed interpretation of these KIEs will be possible with the aid of theoretical calculations.

Table 6-1. Experimental and predicted ^{13}C kinetic isotope effects (k_{12C}/k_{13C}) for the epoxidation of cyclohexenone with *t*-BuOOH / DBU.

	C_1	C_2	C_3	C_4	C_5
Experimental KIEs					
	0.998	1.010	1.033	1.005	0.996
	1.003	1.009	1.027	1.002	0.999
	[b]	1.010	1.037	1.002	0.995
	[b]	1.010	1.029	1.008	1.003
average	1.001	1.010	1.032	1.004	0.998
std dev		0.000	0.004	0.003	0.004
Predicted KIEs					
axial addition **(10)**	1.004	1.008	1.027	0.997	0.999
equatorial addition **(13)**	1.004	1.007	1.031	1.001	1.001
axial ring closure **(12)**	1.006	1.012	0.997	0.996	0.999
equatorial ring closure **(15)**	1.005	1.012	1.000	0.999	1.001

[a]Experimental isotope effects are for 22 °C. Predicted isotope effects are for 25 °C. [b]The NMR data was collected with a time between pulses inadequate for relaxation of the carbonyl carbon, precluding an accurate integration.

Theoretical Calculations

Theoretical Mechanisms. The epoxidation of cyclohexenone with *t*-BuOOH mediated by the simplified DBU model **9** was studied in B3LYP calculations using 6-31G* and 6-31+G** basis sets and using a PCM solvent model with full geometry optimization in all cases. The involvement of charged species limits the reliability of a calculational mechanistic study of this reaction by itself, but consideration of the experimental isotope effects allows assessment of the calculational predictions. In turn, the prediction of isotope effects from the theoretical models facilitates a detailed interpretation of the experimental isotope effects.

A series of conformationally varying pathways for the epoxidation were explored. The diastereotopic faces of a half-chair cyclohexenone may undergo addition of the *tert*-butylperoxy anion in either an "axial" or an "equatorial" orientation. (The discussion here will consistently use the axial / equatorial notation to denote epoxidation pathways and products, always basing the description on the orientation of the initial addition.) The pathways explored allowed for axial versus equatorial attack on the cyclohexenone, allowed for two possible orientations of **9**, and allowed for an *anti* (O–O--C=C of approximately 180°) versus *gauche* (O–O--C=C of approximately 75°) orientation of the attacking oxygen atoms versus the carbon-carbon double bond. Only the lowest-energy axial and equatorial pathways from the B3LYP/6-31+G**/PCM calculations are presented here (Figure 6-4); structures and energies associated with the full set of pathways as well as gas-phase and 6-31G* calculations are given in the Appendix.

The lowest-energy calculated pathway involves an axial addition of the peroxide with oxygens oriented *anti* versus the carbon-carbon double bond, as in transition structure **10**. This transition structure leads by a minimum-energy path to the zwitterionic enolate/iminium intermediate **11**. As a side process, **11** could readily undergo proton transfer to afford neutrals **9** and 4-*t*-butylperoxycyclohexanone. However, 4-*t*-butylperoxycyclohexanone is predicted to be 9.6 kcal/mol uphill in free energy (B3LYP/6-31+G**/PCM + zpe + harmonic entropy and enthalpy estimates at 25 °C) from separate starting materials. From this, 4-*t*-butylperoxycyclohexanone should not build up under the reaction conditions and its formation must be reversible.

There is predicted to be a low barrier for **11** to complete the epoxidation by ring-closure via transition structure **12**. The alternative equatorial process via **13**, **14**, and **15**

is similar but 2-3 kcal/mol higher in energy. The calculations are predicting that the addition step for the axial attack should be rate limiting, since **10** is 0.7 kcal/mol higher in energy than **12**. In notable contrast, the equatorial pathway would have the ring-closure step as mainly rate limiting. In either case, these relative energies should not be taken too seriously due to the limitations of the calculational model, the solvent model, and the calculational method itself. A more reasonable conclusion from the calculational results is that the addition and ring-closure steps should be crudely comparable in barrier, which supports the idea that the rate-limiting step may depend on the detailed reaction conditions.

The formation of termolecular transition structures such as **10** from separate reactants should involve a substantial entropic penalty. Including an entropy estimate based on the harmonic frequencies at 25 °C, the free-energy barrier (at standard state) for reaction via **10** would be 37.1 kcal/mol. This is too high by about 12-15 kcal/mol for a reaction that proceeds in less than at day at 25 °C. However, the consideration of two issues may ameliorate this problem. The first issue is that the gas phase entropy of compounds is decreased on dissolution in organic solvents, typically by 15 e.u.[179] From this, the entropy loss for forming a termolecular transition state might be expected to be decreased compared to a gas-phase calculation by roughly 30 e.u., decreasing the free-energy barrier by 9 kcal/mol. The second issue is that *t*-BuOOH may form a complex with DBU. The formation of a complex between *t*-BuOOH and **9** is predicted to be downhill by 4.2 kcal/mol in dichloroethane (B3LYP/6-31+G**/PCM + zpe) but is predicted to be endergonic by 5.6 kcal/mol after inclusion of the gas-phase entropy estimate. However, as evidence for a significant amount of complex formation, addition

of 1 M DBU to a 1 M solution of *t*-BuOOH in dichloroethane leads to a temperature rise of 4 °C. Estimating the heat capacity of the solution as that of dichloroethane (129 J mol^{-1} K^{-1}),[180] this translates into a heat of mixing at 1 M of 1.5 kcal/mol, suggesting that a substantial portion of the *t*-BuOOH / DBU mixture forms a complex. The predicted free-energy barrier for reaction of a *t*-BuOOH / **9** complex with cyclohexenone is only 31.5 kcal/mol. Considering these issues along with the limitations of the calculational and solvent models, the calculated barrier is reasonably consistent with the facility of the experimental reaction.

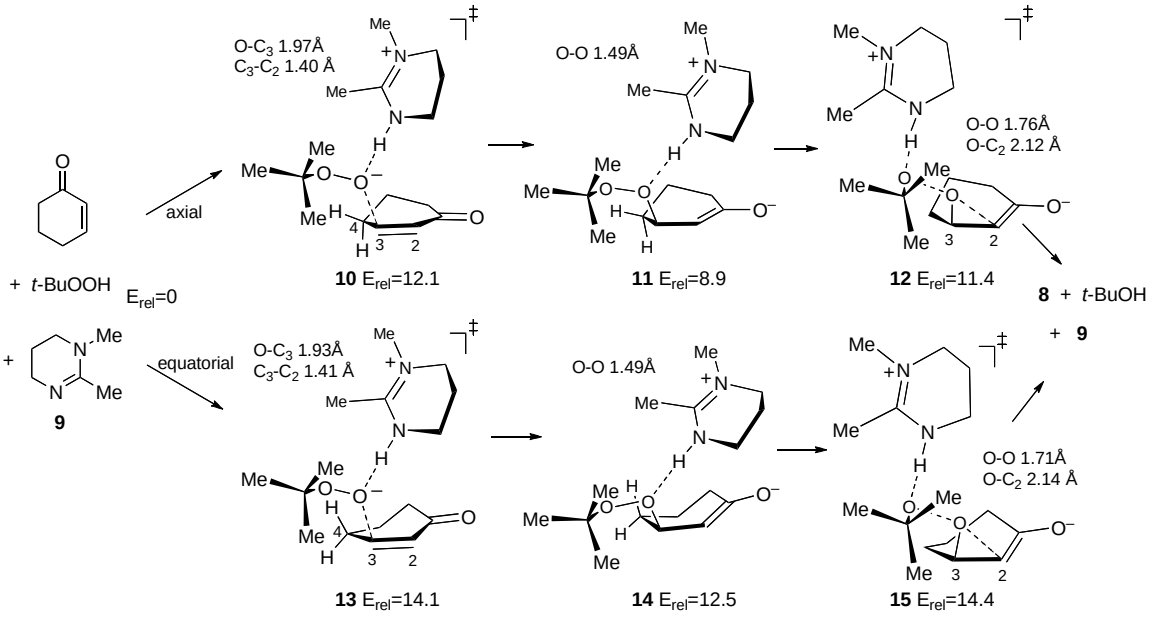


Figure 6-4. Lowest energy axial (top) and equatorial (bottom) pathways for the epoxidation of cyclohexenone with *t*-BuOOH mediated by DBU model **9** in B3LYP/6-31+G**/PCM calculations. Energies (B3LYP/6-31+G**/PCM + zpe) are in kcal/mol relative to separate starting materials.

Predicted Isotope Effects. The ^{13}C KIEs associated with the transition structures in Figure 1 were predicted from the scaled theoretical vibrational frequencies[181] using conventional transition state theory by the method of Bigeleisen and Mayer.[182] Tunneling corrections were applied using the one-dimensional infinite parabolic barrier model.[183] Such KIE predictions have proven highly accurate in reactions not involving hydrogen transfer, so long as the calculation accurately depicts the mechanism and transition state geometry.[184]

The results are summarized in Table 6-1. The addition transition structures **10** and **13** lead to predicted KIEs of about 1.03 at C_3 and 1.008 at C_2, with small isotope effects predicted for the remaining carbons. In contrast, ring-closure transition structures **12** and **15** lead to predicted KIEs at C_3 near unity and 1.012 at C_2. These predictions fit well with conventional expectations. In the addition step, C_3 is undergoing a major σ-bonding change and is expected to exhibit a substantial normal isotope effect, while the bonding change at C_2 is more minor and the predicted KIE, while still significantly greater that unity, is low. In the ring-closure step, little change is occurring at C_3 so the predicted isotope effect is near unity. The predicted isotope effect for C_2 at 1.012 is near the low end of *primary* carbon KIEs (KIEs associated with a σ-bonding change in the rate-limiting step) but is in keeping with the relatively low KIEs observed in other epoxidation reactions.[184d,185]

Discussion

The natural-abundance ^{13}C KIE determination did not work as well as normal for the current reaction. Aside from the relatively high run-to-run variability in the ^{13}C KIE,

particularly at C_3 where the standard deviation is 0.004, it is bothersome that the C_4 and C_5 KIEs were not consistently close to their expected values near unity. Nonetheless, the overall pattern in the KIEs was sufficiently reproducible for the purpose at hand of distinguishing the rate-limiting step in the epoxidation reaction.

Some care must be taken in the qualitative interpretation of these isotope effects. The observed C_3 KIE fits well with conventional expectations and with the β ^{13}C KIEs observed in other additions to α,β-unsaturated carbonyl compounds (Figure 6-5). [186,187] However, we have previously reported that the presence of weak bonds in reactive intermediates can result in *secondary* ^{13}C KIEs (^{13}C KIEs that are not the result of a σ–bonding change in the rate-limiting step) that are so large as to mimic *primary* ^{13}C KIEs.[188] Because the C_3–O bond in intermediates resembling **3** should be weak, the KIE to be expected at C_3 if ring closure were the rate-limiting step was not clear. In addition, the observed C_2 KIE of 1.010 is ambiguously diagnostic. As noted above, epoxidation reactions tend to exhibit small primary ^{13}C KIEs, in part because the equilibrium isotope effect for an epoxidation is significantly inverse.[184d] Because of this, the 1.010 is qualitatively consistent with rate-limiting ring closure. However, the α carbon in other additions to α,β-unsaturated carbonyl compound can exhibit a significantly normal ^{13}C KIEs (Figure 6-5), such as 1.007 in free-radical polymerization.

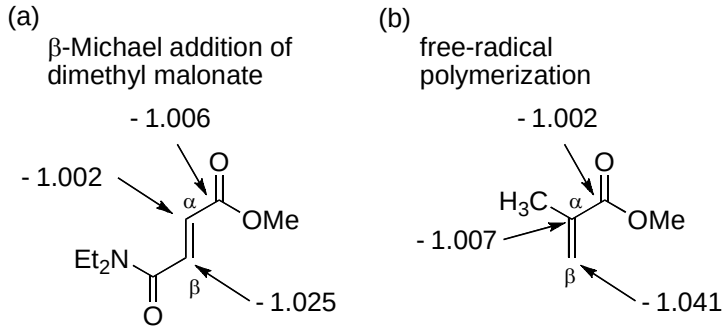


Figure 6-5. ^{13}C KIEs for other additions to α,β-unsaturated carbonyl compounds. (a) Base-catalyzed β-addition of dimethyl malonate in methanol at 64 °C. See ref 186. (b) Free-radical polymerization at 60 °C. See ref 187.

The theoretically predicted isotope effects serve to pin down the rate-limiting step. Despite the concerns expressed above, the predicted C_3 ^{13}C KIEs based on **12** and **15** for rate-limiting ring closure are near unity. The large observed ^{13}C KIE of approximately 1.030 is thus inconsistent with rate-limiting closure of the epoxide ring. In comparing the experimental KIEs with the predicted KIEs based on **10** and **13** for rate-limiting addition, the match-up is not as good as typically observed in other examples.[184] However, considering the difficulty of accurately modeling this reaction due to the involvement of charged intermediates, along with the spread of the experimental KIEs, the correspondence of experimental and predicted KIEs is quite reasonable, particularly for the key C_3 and C_2 positions. Overall, the KIEs very strongly support rate-limiting addition to the enone.

The choice of rate-limiting step and the factors affecting this choice may be best understood by considering the relative facility of forward versus backward reactions for the enolate intermediates such as **11** or **14**. The ring closure of **11** faces a very low barrier because of the weakness of the O–O bond and because its geometry is well

positioned for the S_N2 displacement by C_2. A slight repositioning of the **9**•H^+ counterion to hydrogen bond with the *tert*-butoxy oxygen appears to aid in catalyzing the displacement. On the other hand, the cleavage of **11** back to starting materials is also understandably facile. From the isotope effect analysis above, we know that the barrier for the backward cleavage of the enolate in reality is higher than that for ring closure. If the ring-closure step were 20% rate-limiting, as would be expected from the calculated relative energies of **10** and **12**, the predicted KIE for C_3 would be 1.022, at the limit of consistency with experiment. From this, it appears that the difference in energy between addition and ring-closure transition states in reality is at least as high as the calculated difference between **10** and **12**.

The higher energy of **14** along the equatorial pathway versus **11** on the axial pathway may be ascribed to a near eclipsing interaction of C_3 and C_4 in **14** versus the nearly perfectly staggered **11**. The barrier for backward cleavage of **14** via **13** is slightly lower than ring closure via **15**, so that ring closure in this case would be predicted to be mainly rate limiting. The difference in predicted rate limiting steps for the axial and equatorial pathways may be thought of as resulting from the ease of backward cleavage of **14** via **13**, since this loses the strain of the eclipsing interaction.

With the knowledge that the addition step is rate limiting, consideration of the calculated transition structures provides insight into the stereochemistry of these epoxidations with substituted cyclohexenones. For 5-substituted cyclohexenones, there is a substantial preference for both hydrogen peroxide- and alkyl hydroperoxide-mediated reactions to afford axial epoxidation.[189,190] This is illustrated by the widely-

used epoxidation of carvone (**16**) to afford **17**.[169,190] 6-Substituted cyclohexenones also tend to epoxidized axially,[191] though there has been one report of an exception.[192] The observation of axial epoxidation in these cases is in agreement with the calculated preference for axial transition structure **10** over **13** and **15** in the equatorial pathway. However, the epoxidation of other substituted cyclohexenones has been stereochemically more enigmatic. With 4-monosubstituted cyclohexenones as in **18** and **20**, there is a tendency for epoxidation to occur on the face opposite the 4-substituent, as in **19** and **21**.[193] This would be considered equatorial epoxidation if the 4-substituent is equatorial during the reaction. However, when the 4-substituent is held rigidly equatorial, as in **23**, axial epoxidation predominates.[194] This observation suggests that the epoxidations of **18** and **20** may be occurring through conformers in which the 4-substituent has flipped to axial. Consideration of analogs of **10** and **13** with an added group at C_4 supports this idea. If the equatorial hydrogen at C_4 of **10** is replaced by a methyl group, there is a substantial steric interaction with the *tert*-butoxy oxygen with an unrelaxed O---H distance of about 1.6 Å. This hindered conformation would lead to the minor product **22** from **20**. The major product **21** could in principle be formed in two ways, either by placing the methyl group axial in an axial transition state analogous to **10** or by placing the methyl group equatorial in an equatorial pathway analogous to **13** / **15**. The former should be favored because the energy cost of putting a methyl group axial should only be about 1 kcal/mol,[195] while the predicted cost of the equatorial pathway is 2.3 kcal/mol.

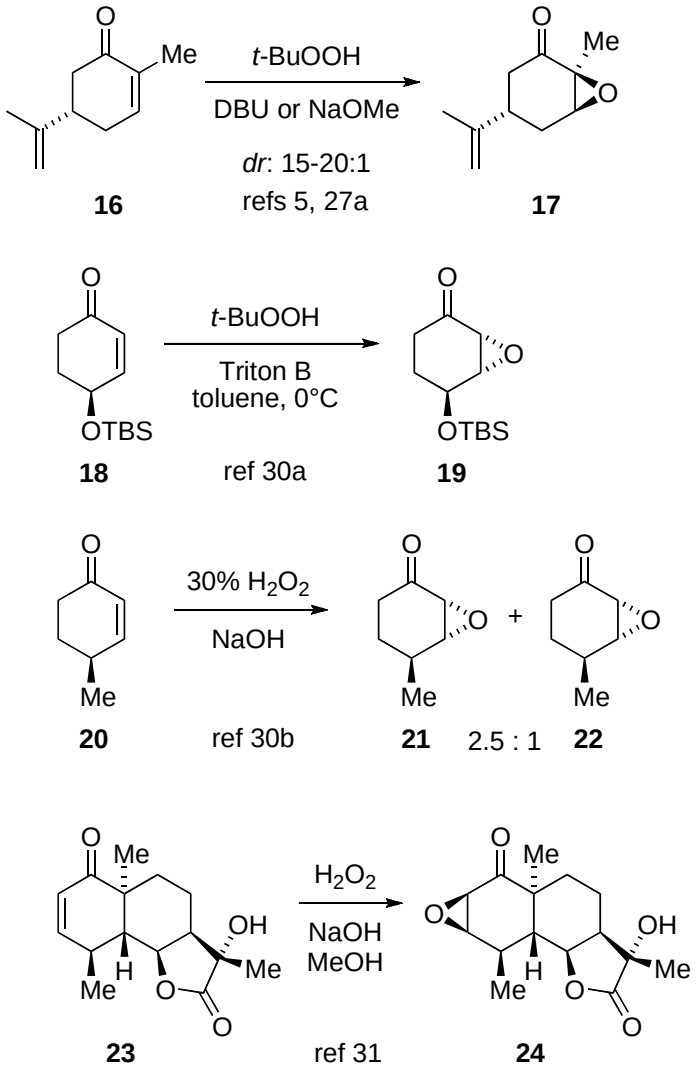


Figure 6-6. Examples of stereoselective epoxidations.

Conclusions

In epoxidations of electron-deficient alkenes mediated by hydroperoxides under basic conditions, reactivity and stereoselectivity will be controlled by the energy of the transition state for the rate-limiting step. Either the addition step or the ring-closure step may in principle be rate limiting, with no obvious qualitative reason to favor one over

the other. In the work of Kelly and Roberts on the epoxidation of phenyl vinyl ketone under Juliá-Colonna conditions, it appears clear that the ring-closure step is rate limiting.[177] Here, in the first detailed mechanistic study with a cyclic enone, the experimental kinetic isotope effects supplemented by theoretically predicted isotope effects strongly support the addition step as being rate limiting.

While the theoretical calculations here correctly predict that the addition step should be rate-limiting, it seems best to emphasize that the addition and ring-closure steps are fairly similar in barrier. Because of this, it is reasonable to suppose that the rate-limiting step may change depending of the detailed reaction conditions and substrate structure. Indeed, the rate-limiting step for the equatorial epoxidation pathway is predicted to be ring closure instead of addition. This overall mechanistic uncertainty complicated the understanding and control of diastereoselectivity or enantioselectivity in these reactions, as it may be uncertain what combination of transition states along major and minor pathways is deciding the selectivity. However, it appears that kinetic isotope effects are a readily applicable tool for determining the rate-limiting step is systems of interest.

CHAPTER VII

EXPERIMENTAL

Experimental

Borylation of 1,3-Dibromobenzene & m-xylene

Example Procedure. All reagents were purified and prepared for airless conditions. A mixture of 8.02 g (33 mmol) of 1,3-dibromobenzene, 6.53 g (51 mmol) of pinacolborane, 282.6 mg (0.68 mmol) of (Ind)Ir(Cod), and 270.9 mg (0.68 mmol) of *bis*-(diphenylphosphino)ethane in 4.36 g (34 mmol) of nonane was heated to 150 °C for 12.5 h. At this time, NMR analysis of an aliquot indicated a percentage conversion of the 1,3-dibromobenzene of 74.9%, based on the ratio unreacted starting material versus the nonane methyl groups, and corroborated by the ratio of starting material to product. The reaction mixture was cooled to room temperature and passed through a silica gel plug to remove iridium metal complexes, then diluted with 25 mL of nonane and rinsed with three 100-mL portions of water. The organic layer was dried (Na_2SO_4) and fractionally distilled through a 15 cm Vigreaux column under reduced pressure (0.05 mm Hg) to afford 270 mg of 1,3-dibromobenzene contaminated by 6.6% nonane.

In a second analogous reaction, 8.10 g of 1,3-dibromobenzene was reacted for 12.5 h at 150 °C to achieve 73.5% conversion, and 269 mg of 1,3-dibromobenzene was recovered. In another similar procedure using 11.63 g (68 mmol) of dodecane in place of nonane, 7.25 g of *m*-xylene, 549 mg (1.32 mmol) of (Ind)Ir(Cod), and 198 mg (1.32

mmol) of *bis*-(dimethylphosphino)ethane was reacted for 16 h at 150 °C to achieve 72.7% conversion, and 364 mg of *m*-xylene was recovered.

Preparation of *m*-Xylene-5-d. To a stirred mixture of 15 g (0.62 mol) of Mg turnings in 100 mL of dry ether was added dropwise over 4 h a solution of 52.5 g (0.284 mol) of 5-bromo-*m*-xylene in 400 mL of ether. Stirring was continued until no further reaction of the Mg could be discerned, then 50 mL of D_2O (99.9% D) was added dropwise. The ether layer was decanted, dried (Na_2SO_4), and fractionally distilled to afford 17.41 g (58%) of *m*-xylene-5d. The deuterium incorporation in this material was calculated as 79.8%, based on the ^1H NMR integration at 500 Mhz for the 5 position versus the integration for the methyl groups, corrected for the analogous ratio observed with unlabeled **3**.

Borylation of *m*-Xylene-5-d Example Procedure. A mixture of 1.07 g (10 mmol) of *m*-xylene-5d, 1.92 g (15 mmol) of pinacolborane, 83 mg (0.2 mmol) of (Ind)Ir(Cod), and 30 mg (0.2 mmol) of *bis*-(dimethylphosphino)ethane in 5 mL g (3.75 g, 22 mmol) of dodecane was heated to 150 °C for 8 h. At this time, NMR analysis of an aliquot indicated a overall percentage conversion of 42.5%, based on the integration for the multiplet at δ 7.0 (H's in the 2, 4, and 6 positions) versus the dodecane methyl groups, corrected for the ratio from a time=0 aliquot.

NMR Measurements. For 1,3-dibromobenzene, NMR samples were prepared using 270 mg in 1.21 g of $CDCl_3$ in a 5-mm NMR tube. For *m*-xylene, NMR samples were prepared using 364 mg in 1.34 g of $CDCl_3$ in a 5-mm NMR tube. The ^{13}C spectra were recorded at 125.701 MHz using inverse gated decoupling, 85 s delays between

calibrated π/2 pulses, and a 6 s acquisition time to collect 300,000 points. Integrations were determined numerically using a constant integration region for each peak. A zeroth-order baseline correction is generally applied, but in no case was a first-order (tilt) correction applied. Twelve spectra were obtained for each 1,3-dibromobenzene sample along with six spectra for the corresponding 1,3-dibromobenzene standards. Six spectra were obtained for each of the *m*-xylene samples and standards. The resulting ^{13}C integrations for these spectra are given in Supporting Information. From the ^{13}C integrations, the KIEs and uncertainties were calculated as previously described.[5]

^{13}C Results. For the ^{13}C spectra of 1,3 dibromobenzene the integrations of the ortho carbon (C1) were set at 1000. For the ^{13}C spectra of *m*-xylene the integrations of the ortho carbon (C2) were set at 1000.The average integrations and standard deviations (in parentheses) for the other carbons are shown in Table 7-1 along with the number of spectra recorded for each sample (n). The values for R/R_O, calculated as the ratio of average integrations in Table 1 relative to standard, are shown in Table 7-2. The ^{13}C KIEs for 1,3 Dibromobenzene and *m*-xylene were then calculated (Table 7-3).

Table 7-1. Average ^{13}C integrations for 1,3 dibromobenzene and *m*-xylene, with standard deviations (in parentheses).

% conversion	C_1	C_2	C_3	C_4	N
1,3 Dibromobenzene					
Standard	1000	1002.4 (3.4)	2008.2 (5.9)	1985.6 (6.5)	6
MSU 27 – 1 74.9 ± 1%	1000	1018.7 (5.4)	2009.7 (9.3)	1986.8 (6.4)	6
MSU 27 - 2 74.9 ± 1%	1000	1018.1 (6.6)	2011.2 (5.7)	1979.9 (4.2)	6
MSU 29 – 1 73.5 ± 1%	1000	1017.3 (5.6)	2011.1 (13.6)	1986.0 (11.3)	6
Standard	1000	1002.8 (5.5)	1988.4 (7.6)	1962.2 (5.5)	6
MSU 28 – 1 78.9 ± 1%	1000	1023.5 (3.9)	1975.6 (4.9)	1972.5 (6.1)	6
Standard	1000	999.1 (3.6)	1975.7 (5.0)	1972.6 (5.2)	6
MSU 29 – 2 73.5 ± 1%	1000	1015.9 (3.1)	1976.3 (8.8)	1974.0 (8.6)	6

% conversion	C_1	C_2	C_3	C_4	C_5	N
m-xylene						
Standard	1982.7 (3.8)	1000	1002.0 (1.0)	2002.1 (4.2)	1891.7 (2.0)	6
MSU 23 – 1 72.7 ± 1%	1980.8 (2.2)	1000	1017.3 (1.5)	2004.7 (2.4)	1886.7 (2.6)	6

Table 7-2. R/R_O for ^{13}C for 1,3 dibromobenzene and *m*-xylene.

	C_2	C_3	C_4
1,3 Dibromobenzene			
MSU 27-1 74.9% R/R_O	1.016	1.001	1.001
Stand dev	0.006	0.006	0.005
MSU 27-2 74.9% R/R_O	1.016	1.001	0.997
Stand dev	0.007	0.004	0.004
MSU 29-1 73.5 % R/R_O	1.015	1.001	1.000
Stand dev	0.007	0.007	0.007
MSU 28-1 78.9% R/R_O	1.020	0.994	1.005
Stand dev	0.007	0.005	0.004
MSU 29-2 73.5% R/R_O	1.017	1.000	1.001
Stand dev	0.005	0.005	0.005

	C_1	C_3	C_4	C_5
m-xylene				
MSU 23-1 72.7% R/R_O	0.999	1.015	1.001	0.997
Stand dev	0.002	0.002	0.002	0.002

Table 7-3. ^{13}C KIEs for 1,3 dibromobenzene and *m*-xylene, with standard deviations (in parentheses)**.**

	C_2	C_3	C_4
1,3 Dibromobenzene			
MSU 27-1 74.9 $\pm$ 1 %	1.012(5)	1.001(4)	1.000(3)
MSU 27-2 74.9 $\pm$ 1 %	1.011(5)	1.001(3)	0.998(3)
MSU 29-1 73.5 $\pm$ 1 %	1.011(5)	1.001(6)	1.000(5)
MSU 28-1 78.9 $\pm$ 1 %	1.013(4)	0.996(3)	1.003(3)
MSU 29-2 73.5 $\pm$ 1 %	1.013(4)	1.000(4)	1.001(4)

	C_1	C_3	C_4	C_5
m-xylene				
MSU 23-1 72.7 $\pm$ 1 %	0.999(2)	1.012(1)	1.001(2)	0.998(1)

C^2-C^6 Enyne Allene Cyclization

NMR Kinetic Studies. The unlabelled allenol acetate **9a**[88] (10 mg, 0.028 mmol) was dissolved in toluene-d_8 (0.075 mL) and transferred to an NMR tube and immediately placed into the probe of a Varian Inova 300 MHz NMR spectrometer to minimize spontaneous cyclization of **9a** (Scheme 3-4). Prior to the experiment, the variable temperature thermostat of the NMR was calibrated using an ethylene glycol standard by measuring its chemical shift at 50 ^{o}C. The heights of selected aromatic protons of **9a** and the cyclization product **10a** were monitored by ^{1}H NMR at 50 °C over 6 h until no further change in the heights of the aromatic protons was observed. Data were collected every 30 min and normalized to the height of the residual methyl signal of toluene-d_8. The same procedure was carried out for the deuterated allenol acetate **9b,** and both experiments were repeated. In each case no side products were observable and the formation of product appeared essentially quantitative. Kinetic isotope effect values were computed by plotting the selected ^{1}H-NMR peak heights against time and fitting the data to a first-order simulation to obtain rate constants for the cyclization of both **9a** and **9b**. The two replications were used to obtain averaged values and standard deviations for the observed kinetic isotope effects.

Palladium Catalyzed Allylic Alkylation

Allylic Alkylation of 1,1 Dimethyallyl Acetate with Dimethylmalonate. As an example procedure, to a dry 500 mL three neck round bottom flaske equipped with a magnetic stir bar containing 200 mL of purified THF (distilled from Na/benzophenone)

was added 57.4 mg (0.125 mmol) of $Pd_2(dba)_3$ (Strem), 80.34 mg (0.375 mmol) of triphenylphosphine, 32.0 g (250 mol) of 1,1-dimethylallyl acetate, 24.77 g (187.5 mol) of dimethylmalonate, 20.34 g (100 mol) N,O,-bis(trimethylsilyl)acetamide, and 8.64 g (62.5 mol) 1,4-dimethoxybenzene asn internal standard. The reaction mixture was stirred at 25 ^oC. After 2 h and 4 h, an additional 100 mg (109 mmol) of $Pd_2(dba)_3$ and 150 mg (703 mmol) triphenylphosphine were added to the reaction. After 5 h the conversion was determined to be 75 ± 3% conversion by NMR analysis of an aliquot (comparing the integrations of the dimethyl and the internal and terminal vinylic peaks of unreacted 1,1-dimethylallyl acetate versus the methoxy peak of 1,4-dimethoxybenzene). The reaction mixture was passed through a silica gel column (5 inch height, 2 inch diameter), to remove the Pd. The reaction mixture was then washed with water, NaHSO4 (aq), $NaHCO_3$ (aq), and dried over anhydrous Na_2SO_4. Impure 1,1-Dimethylallyl acetate was then collected by fractional distillation with a 20 cm Vigreaux column in the second and third fraction (GC analysis). 1,1-Dimethylallyl acetate was further purified by fractional distillation. 367 mg of 1,1-dimethylallyl acetate was collected with a 24 % siloxane impurity.

An analogous reaction (Exp. 2) using 32.0 g of styrene each were taken to 71 ± 3%. For experiment 2, 292 mg with a 21 % siloxane impurity, of 1,1-dimethylallyl acetate was recovered.

NMR Measurements. NMR measurements were taken on 367:539 (mg:mg) 1,1-dimethyallyl acetate:$CDCl_3$ at 75 ± 3% conversion and on 292:522 (mg:mg) 1,1-dimethyallyl acetate:$CDCl_3$ at 71 ± 3% conversion. Samples of 1,1-dimethylallyl acetate

in $CDCl_3$ in 5-mm NMR tubes filled to a constant height of 5 cm. A T1 determination by the inversion-recovery method was carried out for each NMR sample, and the T1 for each NMR signal remained constant within experimental error from sample to sample.

The ^{13}C spectra were recorded at 125.69 MHz with inverse gated decoupling, using 185 s delays between calibrated 45^o pulses and an acquisition time of 6.000 s collecting 300000 points. Integrations were determined numerically using a constant region for each peak and using only a zeroth order baseline correction.

Results for All Reactions. The relative integrations, R/Ro's, and KIEs (standard deviations are in parentheses) for the palladium-catalyzed allylic alkylation of 1,1-dimethylallyl acetate are shown in Table 7-4, 7-5, and 7-6, respectively. For the ^{13}C spectra of 1,1-dimethylallyl acetate the integrations of the 2 methyl carbons were set at 2000.

Table 7-4. Average ^{13}C integrations for 1,1-dimethylallyl acetate, with standard deviations (in parentheses).

% conversion	C=O	C-quat	-CH=CH_2	-CH=CH_2	2 Me	O=C-CH_3	n
1,1-Dimethylallyl acetate							
Standard 1 run a,b	959.69 (3.7)	1081.28 (2.2)	1046.09 (3.2)	1086.19 (1.9)	2000	981.69 (2.3)	6
Exp. 1 run a (75 ± 3%)	953.21 (3.6)	1137.52 (4.5)	1047.63 (3.3)	1091.34 (4.9)	2000	974.96 (2.2)	6
Exp. 1 run b (75 ± 3%)	959.72 (4.9)	1139.11 (3.9)	1050.47 (3.8)	1097.45 (5.8)	2000	981.83 (3.3)	6
Standard 1 run c	958.18 (3.1)	1083.25 (2.2)	1043.15 (2.3)	1086.58 (1.9)	2000	983.14 (3.0)	6
Exp. 1 run c (75 ± 3%)	960.19 (3.4)	1142.23 (4.0)	1055.22 (2.8)	1094.00 (5.6)	2000	984.98 (5.8)	6
Standard 2 run a	966.29 (2.7)	1075.58 (3.9)	1050.76 (2.1)	1085.40 (3.9)	2000	978.37 (3.8)	6
Exp. 2 run a (71 ± 3%)	966.81 (3.4)	1123.00 (3.1)	1053.97 (3.0)	1091.97 (4.9)	2000	978.15 (3.2)	6
Standard 2 run b	954.48 (4.1)	1078.35 (4.0)	1050.76 (2.1)	1089.78 (4.1)	2000	979.42 (4.4)	6
Exp. 2 run b (71 ± 3%)	952.01 (3.1)	1122.87 (2.1)	1048.46 (4.3)	1092.21 (3.9)	2000	980.94 (2.7)	6
Standard 2 run c	952.23 (4.7)	1076.48 (3.1)	1050.76 (2.1)	1089.73 (4.2)	2000	978.37 (3.7)	6
Exp. 2 run c (71 ± 3%)	951.84 (2.6)	1125.44 (2.7)	1054.34 (3.0)	1101.28 (6.0)	2000	977.01 (3.5)	6

Table 7-5. R/R_O for ^{13}C for 1,1-dimethylallyl acetate.

	C=O	C-quat	-CH=CH_2	-CH=CH_2	2 Me	O=C-CH_3
1,1-Dimethylallyl Acetate					assumed	
Exp. 1a R/R_0	0.993	1.052	1.001	1.005	1.000	0.993
Standard dev	0.004	0.004	0.003	0.004	0	0.002
Exp. 1b R/R_0	1.000	1.053	1.004	1.010	1.000	1.000
Standard dev	0.005	0.003	0.003	0.004	0	0.003
Exp. 1c R/R_0	1.002	1.054	1.011	1.007	1.000	1.002
Standard dev	0.003	0.004	0.003	0.004	0	0.005
Exp. 2a R/R_0	1.005	1.044	1.003	1.006	1.000	1.000
Standard dev	0.004	0.004	0.003	0.004	0	0.004
Exp. 2b R/R_0	0.997	1.041	0.997	1.002	1.000	1.001
Standard dev	0.004	0.004	0.004	0.004	0	0.004
Exp. 2c R/R_0	1.000	1.045	1.003	1.010	1.000	0.999
Standard dev	0.004	0.003	0.003	0.005	0	0.004

Table 7-6. ^{13}C KIEs for 1,1-dimethylallyl acetate, with standard deviations (in parentheses).

	C=O	C-quat	-CH=CH_2	-CH=CH_2	2 Me	O=C-CH_3
1,1-Dimethylallyl acetate					assumed	
Exp. 1a (75 ± 3%)	0.995 (4)	1.038 (4)	1.001 (3)	1.003 (4)	1.000	0.995 (2)
Exp. 1b (75 ± 3%)	1.000 (5)	1.039 (3)	1.003 (3)	1.007 (4)	1.000	1.000 (3)
Exp. 1c (75 ± 3%)	1.002 (3)	1.040 (4)	1.008 (3)	1.005 (4)	1.000	1.001 (5)
Exp. 2a (71 ± 3%)	1.000 (4)	1.035 (4)	1.002 (3)	1.005 (5)	1.000	1.000 (4)
Exp. 2b (71 ± 3%)	0.998 (4)	1.033 (4)	0.998 (4)	1.002 (4)	1.000	1.001 (4)
Exp. 2c (71 ± 3%)	1.000 (4)	1.036 (3)	1.003 (3)	1.008 (5)	1.000	0.999 (4)

Decarboxylation of Orotodine

Decarboxylations in Mixed H_2O / D_2O. A stock solution of 50 units of ODCase (Sigma) in 100 mL of 1:1 H_2O:D_2O was prepared and allowed to equilibrate for 12 h. A solution of 3.5 mg (7.8 μmol) of orotidine 5'-monophosphate trisodium salt in 240 μL of 50 mM phosphate buffer at pH 6.0 or pH 7.0 in 1:1 H_2O:D_2O was prepared, and 10 μL

of the ODCase solution was added. After mixing, the resulting mixture was allowed to stand at 25 °C. After 10 h the starting material could no longer be observed by NMR analysis of the reaction mixture. The solvent was removed from the reaction mixture under vacuum at 25 °C. To minimized residual protons, the residue was thrice dissolved in D_2O and the volatiles removed under vacuum. The residue was then dissolved in d_6-DMSO for NMR analysis.

Epoxidation of 2-Cyclohexenone

Epoxidation of 2-Cyclohexenone with *tert*-Butylhydroperoxide and DBU. A mixture of 19.2 g (0.20 mol) of 2-cyclohexenone, 3.4 g of dodecane (internal standard). 27.6 g (0.16 mol) of DBU, and 50 mL (0.21 mol) of 4.1 M tert-BuOOH in dichloroethane was prepared at 0 °C and allowed to warm slowly to 22 °C. Aliquots were periodically removed and the conversion was checked by GC. After 18 h at room temperature, the conversion was determined to be 83.4%. The reaction mixture was diluted with 300 mL of chloroform and 300 mL of water and stirred for 30 min. The organic layer separated and washed with H_2O, dried (anhydrous $MgSO_4$), and concentrated under vacuum below 30 °C. The residue was then chromatographed on a 5 cm x 45 cm flash silica gel column using 10% ethyl acetate / 30-60° petroleum ether as eluent to afford 9.5 g of a mixture of 2-cyclohexenone and 2,3-epoxy-2-cyclohexenone in the approximate ratio of 17: 83. Vacuum transfer of the volatiles from this mixture on a water aspirator followed by fractional distillation using a 10-cm Vigreux column afforded a 5.2 g fraction (bp 90-95 °C) of an approximately 45: 55 mixture of 2-

cyclohexenone and 2,3-epoxy-2-cyclohexenone. This fraction was chromatographed on a 4 cm x 30 cm. flash silica gel column using 1:1 chloroform / hexanes as eluent to afford 0.5 g of 2-cyclohexenone (>99% purity by GC) along with mixtures of 2-cyclohexenone and 2,3-epoxy-2-cyclohexenone in various ratios. A second reaction performed by an analogous procedure proceeded to 89.1% conversion.

NMR Measurements. NMR samples were prepared using 200 mg of cyclohexenone in a 5-mm NMR tube filled to a 5-cm sample height with $CDCl_3$. The ^{13}C spectra were recorded at 100.5 MHz using inverse gated decoupling, 60 s delays, and a 5.0 s acquisition time to collect 400,000 points. Integrations were determined numerically using a constant equal integration region for peaks compared. A zeroth-order baseline correction is generally applied, but in no case was a first-order (tilt) correction applied. Six spectra were obtained for each of two independent samples of cyclohexenone.

Results for All Reactions. The relative integrations, R/Ro's, and KIEs (standard deviations are in parentheses) for the epoxidation of cyclohexenone are shown in Table 7-7, 7-8, and 7-9, respectively. For the ^{13}C spectra of cyclohexenone the integrations of the methylene carbons were set at 2000.

Table 7-7. Average ^{13}C integrations for cyclohexenone, with standard deviations (in parentheses).

% conversion	C=O	CH=CH	CH=CH	O=C-CH_2	-CH_2-CH_2	=CH-CH_2	n
Cyclohexenone							
Standard 1 400 MHz	866.35 (8.0)	972.25 (8.2)	945.51 (5.2)	1000	1005.63 (5.1)	1009.24 (3.5)	6
Exp. 1A (89.1 ± 3%)	861.90 (13.4)	1044.11 (5.9)	965.74 (8.8)	1000	996.30 (5.2)	1020.08 (2.7)	6
Exp. 2A (83.4 ± 3%)	871.24 (9.9)	1019.89 (4.9)	960.82 (5.1)	1000	1004.63 (2.9)	1011.98 (5.5)	6
Standard 2 500 MHz	765.22 (1.1)	1031.66 (4.4)	1022.46 (3.2)	1000	990.08 (2.3)	988.54 (2.9)	5
Exp. 1B (89.1 ± 3%)	802.77 (3.1)	1097.52 (2.9)	1044.80 (3.1)	1000	997.53 (4.1)	1006.67 (2.1)	5
Exp. 2B (83.4 ± 3%)	790.19 (4.1)	1100.65 (5.7)	1041.03 (7.2)	1000	981.61 (5.1)	992.29 (4.9)	5

Table 7-8. R/R_O for ^{13}C for cyclohexenone.

	C=O	-CH=CH-	-CH=CH-	O=C-CH_2	-CH_2-CH_2	=CH-CH_2
Cyclohexenone				assumed		
Exp. 1A R/R_0	0.995	1.074	1.021	1.000	0.991	1.011
Standard dev	0.008	0.007	0.005	0	0.003	0.002
Exp. 1B R/R_0	1.006	1.049	1.016	1.000	0.999	1.003
Standard dev	0.008	0.007	0.004	0	0.003	0.003
Exp. 2A R/R_0	1.049	1.064	1.021	1.000	1.008	1.018
Standard dev	0.003	0.004	0.002	0	0.002	0.002
Exp. 2B R/R_0	1.032	1.067	1.018	1.000	0.991	1.004
Standard dev	0.004	0.006	0.005	0	0.003	0.003

Table 7-9. ^{13}C KIEs for cyclohexenone, with standard deviations (in parentheses)**.**

	C=O	-CH=CH-	-CH=CH-	O=C-CH$_2$	CH$_2$-CH$_2$	=CH-CH$_2$
Cyclohexenone				assumed		
Exp. 1A (89.1 ± 3%)	0.998 (8)	1.033 (7)	1.010 (5)	1.000	0.996 (3)	1.004 (2)
Exp. 1B (83.4 ± 3%)	1.003 (8)	1.027 (7)	1.010 (4)	1.000	0.999 (3)	1.002 (3)
Exp. 2A (89.1 ± 3%)*	1.022 (3)	1.028 (4)	1.010 (2)	1.000	1.003 (2)	1.008 (2)
Exp. 2B (83.4 ± 3%)*	1.018 (4)	1.037 (6)	1.010 (5)	1.000	0.995 (3)	1.002 (3)

* Due to time constraints, the recycle time was only 30 s. This did not allow for adequate relaxation of the carbonyl center, but was adequate for all other positions.

CHAPTER VIII

CONCLUSIONS

The Singleton group has developed a methodology for predicting the combinatorial kinetic isotope effects (KIEs) at every atomic position, typically carbon or hydrogen, at natural abundance. KIEs alone provide knowledge about the transition state structure and geometry may not provide the complete reaction path. A combination of experimental isotope effects and density functional theory (DFT) calculations has greatly aided our ability to predict and understand the geometry of the transition state at the rate-limiting step. Additionally, it has improved our ability to completely describe a reaction's mechanism. This dissertation has highlighted several examples where the determination of the kinetic isotope effects alone did not lead to the complete determination of a reaction's mechanism and understanding of selectivity.

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152. Warshel concludes that electrostatic effects due to protein-protein interactions between two carboxylate residues stabilize the positive charge on the lysinium at the transition state. This transition state stabilization results in the large rate enhancement for the decarboxylation versus water.

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APPENDIX

GEOMETRIES AND ENERGIES OF CALCULATED STRUCTURES

All structures and energies were obtained using standard procedures in Gaussian98[3] and Gaussian03.[4]

Iridium-Catalyzed Arene C-H Borylation

B3LYP//SDD on Ir, 6-31G on all other atoms unless otherwise noted**

H2
E(RB+HF-LYP) = -1.17853931815

Zero-point correction= 0.010168 (Hartree/Particle)
Thermal correction to Energy= 0.012529
Thermal correction to Enthalpy= 0.013473
Thermal correction to Gibbs Free Energy= -0.001320
Sum of electronic and zero-point Energies= -1.168371
Sum of electronic and thermal Energies= -1.166011
Sum of electronic and thermal Enthalpies= -1.165066
Sum of electronic and thermal Free Energies= -1.179859

	E (Thermal)	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	7.862	4.968	31.133

H,0,0.,0.,0.371478
H,0,0.,0.,-0.371478

Benzene
E(RB+HF-LYP) = -232.253117949

Zero-point correction= 0.100633 (Hartree/Particle)
Thermal correction to Energy= 0.105022
Thermal correction to Enthalpy= 0.105966

Thermal correction to Gibbs Free Energy= 0.073170
Sum of electronic and zero-point Energies= -232.152485
Sum of electronic and thermal Energies= -232.148096
Sum of electronic and thermal Enthalpies= -232.147152
Sum of electronic and thermal Free Energies= -232.179948

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	65.902	17.142	69.024

C,0,-0.0143582981,0.,-1.3965983824
C,0,-1.2165519591,0.,-0.686043202
C,0,-1.2023086577,0.,0.7107489284
C,0,0.0141062514,0.,1.3965985425
C,0,1.2166514282,0.,0.6858656666
C,0,1.2024406046,0.,-0.7105315203
H,0,-2.1378694919,0.,1.2632171425
H,0,-0.0249643079,0.,-2.4830394272
H,0,0.0253400902,0.,2.4830366452
H,0,2.1630303804,0.,1.2195695726
H,0,2.1376713665,0.,-1.2635492108
H,0,-2.163084253,0.,-1.2194749193

HBPin
E(RB+HF-LYP) = -254.602039032

Zero-point correction= 0.079157 (Hartree/Particle)
Thermal correction to Energy= 0.083724
Thermal correction to Enthalpy= 0.084668
Thermal correction to Gibbs Free Energy= 0.051107
Sum of electronic and zero-point Energies= -254.522882
Sum of electronic and thermal Energies= -254.518315
Sum of electronic and thermal Enthalpies= -254.517371
Sum of electronic and thermal Free Energies= -254.550933

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	52.538	14.888	70.637

C,0,-0.9440490034,0.,-0.724884269
C,0,-0.8580456639,0.,0.8249130945
O,0,0.4229804405,0.,-1.1735108352
H,0,-1.4469561594,-0.8886229556,-1.1200123719
H,0,-1.4469561594,0.8886229556,-1.1200123719

H,0,-1.3138930432,0.8886820776,1.2734382017
H,0,-1.3138930432,-0.8886820776,1.2734382017
O,0,0.550251005,0.,1.1193554365
B,0,1.2273330661,0.,-0.0680880401
H,0,2.4117495143,0.,-0.1333412223

PhBPin
E(RB+HF-LYP) = -485.674761514

Zero-point correction= 0.161425 (Hartree/Particle)
Thermal correction to Energy= 0.169788
Thermal correction to Enthalpy= 0.170732
Thermal correction to Gibbs Free Energy= 0.126860
Sum of electronic and zero-point Energies= -485.513337
Sum of electronic and thermal Energies= -485.504974
Sum of electronic and thermal Enthalpies= -485.504029
Sum of electronic and thermal Free Energies= -485.547902

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	106.544	32.062	92.337

C,0,-3.1523829832,0.,-0.6014847062
O,0,-1.7903190037,0.,-1.0500204825
B,0,-0.9705585604,0.,0.0543040123
O,0,-1.6620611743,0.,1.2431473073
C,0,-3.0656505317,0.,0.9492917089
H,0,-3.6601859152,-0.8877313295,-0.9936020545
H,0,-3.6601859152,0.8877313295,-0.9936020545
H,0,-3.5265569278,0.8877317954,1.3955909204
H,0,-3.5265569278,-0.8877317954,1.3955909204
C,0,0.5784182589,0.,-0.0323456537
C,0,1.3667661174,0.,1.1324718871
C,0,2.7591787163,0.,1.057527824
C,0,3.3891200335,0.,-0.1895879201
C,0,2.6240065894,0.,-1.3586587438
C,0,1.2319237812,0.,-1.2778278163
H,0,0.8777540989,0.,2.1027864373
H,0,3.3538296665,0.,1.9669480001
H,0,4.474210188,0.,-0.2502930354
H,0,3.1135118905,0.,-2.3287306437
H,0,0.6377341774,0.,-2.1875426289

Ir(dmpe)(BPin)$_3$
E(RB+HF-LYP) = -1787.53406933

Zero-point correction= 0.422265 (Hartree/Particle)
Thermal correction to Energy= 0.452674
Thermal correction to Enthalpy= 0.453618
Thermal correction to Gibbs Free Energy= 0.358714
Sum of electronic and zero-point Energies= -1787.111805
Sum of electronic and thermal Energies= -1787.081396
Sum of electronic and thermal Enthalpies= -1787.080451
Sum of electronic and thermal Free Energies= -1787.175355

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	284.057	107.871	199.742

C,0,-0.0998131177,3.2568065064,-1.1552701002
C,0,-1.53510628,3.1758412935,-0.6082769419
P,0,-1.7485392914,1.6962272453,0.5346572546
Ir,0,-0.2754951103,-0.0662230201,-0.2156894707
B,0,-1.0755465087,-1.5239398737,1.0484418065
O,0,-0.5839766411,-2.1808422998,2.1700741798
C,0,-1.5817699311,-3.0809984012,2.6641008626
C,0,-2.6302920835,-3.154014752,1.5381042893
O,0,-2.367316897,-1.9907671463,0.7418762704
P,0,0.4736036486,1.5923924697,-1.7936993464
B,0,0.9400309886,-1.5958866449,-0.968973738
O,0,2.2844852697,-1.4788362592,-1.3532793715
C,0,2.7765585758,-2.7735430525,-1.7219486515
C,0,1.50588777,-3.6156850644,-1.9375677668
O,0,0.4758978209,-2.8812307237,-1.265874026
B,0,1.2320940715,0.3337536033,1.0443468917
O,0,1.6275225251,1.6592903401,1.3417142442
C,0,2.6258908048,1.6099369763,2.3715706276
C,0,3.0842310265,0.1384932015,2.3833864848
O,0,2.0324245486,-0.5677467169,1.7263975732
C,0,2.2715409997,1.8610427246,-2.1014058035
C,0,-0.2111595926,1.5393848358,-3.5177571117
H,0,-0.0140308356,4.0293683758,-1.9290731359
H,0,0.5956993026,3.5068778012,-0.3468481106
C,0,-1.5040128154,2.4169878822,2.2185331801
C,0,-3.5782536981,1.4229436078,0.4933314916
H,0,-1.8154924832,4.1036590793,-0.0959002577
H,0,-2.2468426843,3.0397804773,-1.4324692408

H,0,-3.6612726232,-3.1259977852,1.9070436487
H,0,-2.5075725048,-4.0522133236,0.9194475068
H,0,-2.0046701925,-2.6804337317,3.5959039472
H,0,-1.1253471235,-4.0513280443,2.8854031672
H,0,1.5810985793,-4.6207370518,-1.5099032033
H,0,1.2493634305,-3.7128679146,-3.0013258492
H,0,3.3983946246,-3.168895203,-0.9083818245
H,0,3.3957994676,-2.69353832,-2.6219543291
H,0,3.2211567115,-0.2568616815,3.3949771746
H,0,4.0197590543,-0.0032257885,1.826003086
H,0,2.1730819854,1.9059851991,3.3273378541
H,0,3.4335706585,2.312132087,2.1402564159
H,0,2.4531376452,2.6749743011,-2.8109826595
H,0,2.7489630116,2.0899345681,-1.1462137224
H,0,2.6986286922,0.9281862065,-2.4760307203
H,0,0.0927100535,2.4119639534,-4.105965506
H,0,0.1482361305,0.6332850918,-4.0136237471
H,0,-1.3035550198,1.4928816315,-3.487511442
H,0,-4.1375945339,2.3230439508,0.7695239
H,0,-3.8767789712,1.1061538315,-0.5098568302
H,0,-3.8249025403,0.609818897,1.1804060133
H,0,-2.146742446,3.2876280983,2.3861495683
H,0,-1.7307528906,1.6511895897,2.9655268481
H,0,-0.4542820861,2.6973650053,2.3246329488

Ir(dmpe)(BPin)$_3$(^{2}-PhH)
E(RB+HF-LYP) = -2019.79555903

Zero-point correction= 0.523859 (Hartree/Particle)
Thermal correction to Energy= 0.560872
Thermal correction to Enthalpy= 0.561816
Thermal correction to Gibbs Free Energy= 0.449088
Sum of electronic and zero-point Energies= -2019.271700
Sum of electronic and thermal Energies= -2019.234687
Sum of electronic and thermal Enthalpies= -2019.233743
Sum of electronic and thermal Free Energies= -2019.346471

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	351.952	130.644	237.255

C,0,-2.2916822971,1.5759029348,1.6622833517
C,0,-2.7741112471,0.5550243263,2.4887691367
C,0,-4.1158303591,0.1684724725,2.4183904767

C,0,-4.9798742715,0.8027545169,1.5218878869
C,0,-4.5024739349,1.8260163218,0.6970093003
C,0,-3.1610208746,2.2101410135,0.7671995676
Ir,0,0.1802273989,-0.1082158897,-0.0458592637
B,0,0.5867050299,1.9060302909,-0.4825691087
O,0,0.6116994925,2.4505172295,-1.7764759802
C,0,0.8350518697,3.8629218705,-1.7077366293
C,0,1.1166245715,4.144990506,-0.215265736
O,0,0.7984685195,2.9207344787,0.4543239648
P,0,-0.3434414243,-2.4413616558,0.3242255597
C,0,-0.9244988879,-3.1417068582,-1.3136744736
C,0,-1.8424660438,-2.1472196606,-2.0423539574
P,0,-1.0825103243,-0.4317014703,-2.0900660165
C,0,-0.0904695112,-0.4437864937,-3.6486851782
C,0,0.9563669436,-3.6438464887,0.8431395383
C,0,-1.7348668485,-2.8750046669,1.4710430607
C,0,-2.5183065164,0.6244226795,-2.5794924383
B,0,1.2287213893,0.1388999664,1.7445476872
O,0,2.5741402083,-0.115478236,2.0199427914
C,0,2.8796904567,0.3306549328,3.3450416474
C,0,1.5047744432,0.5540413378,4.007097625
O,0,0.577172491,0.5589332677,2.9154474477
B,0,1.9673626693,-0.460211098,-0.8897642096
H,0,-1.4217833487,-4.1088222334,-1.1706196506
H,0,-0.0153118977,-3.3169080409,-1.8990897964
H,0,-2.0796018348,-2.4956895743,-3.0547572863
H,0,-2.7940023277,-2.0487249954,-1.5049079169
H,0,3.4838280537,-0.4237936507,3.8606946538
H,0,3.4632372414,1.2584901491,3.2881947688
H,0,1.2441725387,-0.255315859,4.7029233415
H,0,1.4425424723,1.5035699988,4.5489658976
H,0,1.6757904906,4.1358189797,-2.3548856528
H,0,-0.0579802871,4.3900915992,-2.069192234
H,0,2.1701644434,4.3898787197,-0.0331119851
H,0,0.5017312837,4.9575520543,0.1874661671
H,0,1.2828051311,-3.3978770873,1.8572202558
H,0,0.5910990963,-4.6760270225,0.8202443505
H,0,1.8087365538,-3.5310861872,0.1710301614
H,0,-1.4488221621,-2.5999086751,2.4899313327
H,0,-2.6285444338,-2.3014993054,1.2131941699
H,0,-1.9659961489,-3.9452658966,1.4399607029
H,0,-2.1480321004,1.6375739173,-2.7558784936
H,0,-3.0039858135,0.2543205521,-3.4888211478
H,0,-3.2453415182,0.6624304698,-1.7647728303

H,0,0.3375373895,0.5536964066,-3.7766772785
H,0,0.7277382714,-1.1599994151,-3.5461108695
H,0,-0.7016812065,-0.7016413749,-4.5201008121
H,0,-2.0906840044,0.0808443539,3.1855964699
H,0,-4.4910288556,-0.618815586,3.0672680743
H,0,-6.0247355389,0.5077245783,1.4718053402
H,0,-5.1777457626,2.3266546887,0.0079284272
H,0,-2.7887473231,3.0075428456,0.1302136607
H,0,-1.2534916568,1.8831239582,1.7377226492
O,0,3.0199060004,0.4358791341,-1.0346351262
O,0,2.311746835,-1.704699504,-1.4584748535
C,0,4.1693253639,-0.2649999087,-1.5097252468
C,0,3.607781915,-1.5898456969,-2.06259774
H,0,4.6805400121,0.331746132,-2.2721810794
H,0,4.8612852299,-0.4306828565,-0.6740201438
H,0,3.495956256,-1.5661079542,-3.1550936682
H,0,4.2190158268,-2.4586088779,-1.797448366

dmpeBpin3n2PhH2nd
E(RB+HF-LYP) = -2019.79458162

Zero-point correction= 0.524007 (Hartree/Particle)
Thermal correction to Energy= 0.560930
Thermal correction to Enthalpy= 0.561874
Thermal correction to Gibbs Free Energy= 0.448007
Sum of electronic and zero-point Energies= -2019.270575
Sum of electronic and thermal Energies= -2019.233652
Sum of electronic and thermal Enthalpies= -2019.232708
Sum of electronic and thermal Free Energies= -2019.346575

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	351.989	130.544	239.653

C,0,-3.089996002,1.9896355956,0.8749470094
C,0,-2.1805983876,1.5092291397,1.8248088884
C,0,-2.6129057599,0.5954809253,2.7925720448
C,0,-3.9414812816,0.1629156935,2.8108776055
C,0,-4.8447558417,0.6423164791,1.8578434105
C,0,-4.4191076929,1.5573437093,0.8904038184
Ir,0,0.1499834675,-0.0428335071,-0.0919024786
B,0,1.9630684022,-0.5341314303,-0.8088743835
O,0,2.1716517432,-1.6246183893,-1.6804290854
C,0,3.5427526946,-1.6163371685,-2.1023707323

C,0,4.240029459,-0.6700422207,-1.1061859278
O,0,3.1759725049,0.0856041186,-0.5279065192
B,0,0.6067792152,1.9360152739,-0.615536944
O,0,0.0682001111,3.0549001224,0.0304316997
C,0,0.6181349731,4.2491114876,-0.535562343
C,0,1.3257762677,3.7789931688,-1.8242719985
O,0,1.3615116554,2.351831818,-1.7203699844
P,0,-0.4478240364,-2.3523483211,0.3071598566
C,0,-1.8557720904,-2.7949852496,1.4297526359
P,0,-1.0805961777,-0.3566957828,-2.1523692115
C,0,-2.5105372814,0.7178322091,-2.6302654467
B,0,1.2123662422,0.1547299152,1.7065978716
O,0,2.0182929953,-0.8358840302,2.2952967367
C,0,2.6616432194,-0.2901785717,3.4528948842
C,0,1.85329746,0.9803604099,3.7701632942
O,0,1.1489483845,1.2632280294,2.5563074569
C,0,-0.9935370907,-3.0564145241,-1.342164006
C,0,-1.8694345996,-2.0594133209,-2.1156749327
C,0,0.8454302973,-3.5574055293,0.8343123932
C,0,-0.0885031536,-0.3592463416,-3.709670706
H,0,-1.5108473443,-4.0136288695,-1.2041232507
H,0,-0.068931147,-3.2512404206,-1.8961370058
H,0,-2.0716697733,-2.413897187,-3.133539884
H,0,-2.8399694603,-1.9411037164,-1.6174338676
H,0,2.4837525145,1.8341615791,4.0385872389
H,0,1.131158656,0.8186764922,4.5823857002
H,0,3.7078418192,-0.0610296428,3.211494325
H,0,2.6479843928,-1.0229459369,4.2669433316
H,0,2.3454073586,4.1689552123,-1.9136869642
H,0,0.7722764656,4.0640137776,-2.7294017351
H,0,1.3180055586,4.6974040557,0.1807406021
H,0,-0.1829341006,4.9714951013,-0.7280235002
H,0,1.2405797363,-3.2405623946,1.8014863337
H,0,0.4520176991,-4.5773964116,0.8977212702
H,0,1.6603285601,-3.519382945,0.1084314918
H,0,-1.5790052859,-2.5484632368,2.4583986259
H,0,-2.7408721228,-2.2060318638,1.177426362
H,0,-2.0968573211,-3.8619186274,1.3713870658
H,0,-2.1425111149,1.728492135,-2.8282788926
H,0,-3.0183733877,0.3427980973,-3.525219569
H,0,-3.221249352,0.7716901481,-1.8022264126
H,0,0.3702774853,0.626865651,-3.8217294387
H,0,0.7124164997,-1.0943758144,-3.6136769769
H,0,-0.7076238089,-0.5839148427,-4.5845391868

H,0,-1.9086374432,0.2320908327,3.5358359593
H,0,-4.2759636077,-0.5403626755,3.5690979949
H,0,-5.8799052997,0.3114576429,1.8755407753
H,0,-5.1264667772,1.9410621237,0.1594332271
H,0,-2.7484127645,2.7101819571,0.1386094949
H,0,-1.1564349036,1.8684161155,1.8251115379
H,0,4.9546615467,0.0041657352,-1.5891955201
H,0,4.7634677662,-1.2227867122,-0.3147649938
H,0,3.6004531858,-1.2426242333,-3.1331616982
H,0,3.9433123905,-2.6351570178,-2.0808957707

dmpeBpin3n2PhHGood
E(RB+HF-LYP) = -2019.79555903

Zero-point correction= 0.523859 (Hartree/Particle)
Thermal correction to Energy= 0.560872
Thermal correction to Enthalpy= 0.561816
Thermal correction to Gibbs Free Energy= 0.449088
Sum of electronic and zero-point Energies= -2019.271700
Sum of electronic and thermal Energies= -2019.234687
Sum of electronic and thermal Enthalpies= -2019.233743
Sum of electronic and thermal Free Energies= -2019.346471

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	351.952	130.644	237.255

C,0,-2.2916822971,1.5759029348,1.6622833517
C,0,-2.7741112471,0.5550243263,2.4887691367
C,0,-4.1158303591,0.1684724725,2.4183904767
C,0,-4.9798742715,0.8027545169,1.5218878869
C,0,-4.5024739349,1.8260163218,0.6970093003
C,0,-3.1610208746,2.2101410135,0.7671995676
Ir,0,0.1802273989,-0.1082158897,-0.0458592637
B,0,0.5867050299,1.9060302909,-0.4825691087
O,0,0.6116994925,2.4505172295,-1.7764759802
C,0,0.8350518697,3.8629218705,-1.7077366293
C,0,1.1166245715,4.144990506,-0.215265736
O,0,0.7984685195,2.9207344787,0.4543239648
P,0,-0.3434414243,-2.4413616558,0.3242255597
C,0,-0.9244988879,-3.1417068582,-1.3136744736
C,0,-1.8424660438,-2.1472196606,-2.0423539574
P,0,-1.0825103243,-0.4317014703,-2.0900660165
C,0,-0.0904695112,-0.4437864937,-3.6486851782

C,0,0.9563669436,-3.6438464887,0.8431395383
C,0,-1.7348668485,-2.8750046669,1.4710430607
C,0,-2.5183065164,0.6244226795,-2.5794924383
B,0,1.2287213893,0.1388999664,1.7445476872
O,0,2.5741402083,-0.115478236,2.0199427914
C,0,2.8796904567,0.3306549328,3.3450416474
C,0,1.5047744432,0.5540413378,4.007097625
O,0,0.577172491,0.5589332677,2.9154474477
B,0,1.9673626693,-0.460211098,-0.8897642096
H,0,-1.4217833487,-4.1088222334,-1.1706196506
H,0,-0.0153118977,-3.3169080409,-1.8990897964
H,0,-2.0796018348,-2.4956895743,-3.0547572863
H,0,-2.7940023277,-2.0487249954,-1.5049079169
H,0,3.4838280537,-0.4237936507,3.8606946538
H,0,3.4632372414,1.2584901491,3.2881947688
H,0,1.2441725387,-0.255315859,4.7029233415
H,0,1.4425424723,1.5035699988,4.5489658976
H,0,1.6757904906,4.1358189797,-2.3548856528
H,0,-0.0579802871,4.3900915992,-2.069192234
H,0,2.1701644434,4.3898787197,-0.0331119851
H,0,0.5017312837,4.9575520543,0.1874661671
H,0,1.2828051311,-3.3978770873,1.8572202558
H,0,0.5910990963,-4.6760270225,0.8202443505
H,0,1.8087365538,-3.5310861872,0.1710301614
H,0,-1.4488221621,-2.5999086751,2.4899313327
H,0,-2.6285444338,-2.3014993054,1.2131941699
H,0,-1.9659961489,-3.9452658966,1.4399607029
H,0,-2.1480321004,1.6375739173,-2.7558784936
H,0,-3.0039858135,0.2543205521,-3.4888211478
H,0,-3.2453415182,0.6624304698,-1.7647728303
H,0,0.3375373895,0.5536964066,-3.7766772785
H,0,0.7277382714,-1.1599994151,-3.5461108695
H,0,-0.7016812065,-0.7016413749,-4.5201008121
H,0,-2.0906840044,0.0808443539,3.1855964699
H,0,-4.4910288556,-0.618815586,3.0672680743
H,0,-6.0247355389,0.5077245783,1.4718053402
H,0,-5.1777457626,2.3266546887,0.0079284272
H,0,-2.7887473231,3.0075428456,0.1302136607
H,0,-1.2534916568,1.8831239582,1.7377226492
O,0,3.0199060004,0.4358791341,-1.0346351262
O,0,2.311746835,-1.704699504,-1.4584748535
C,0,4.1693253639,-0.2649999087,-1.5097252468
C,0,3.607781915,-1.5898456969,-2.06259774
H,0,4.6805400121,0.331746132,-2.2721810794

H,0,4.8612852299,-0.4306828565,-0.6740201438
H,0,3.495956256,-1.5661079542,-3.1550936682
H,0,4.2190158268,-2.4586088779,-1.797448366

dmpeBpin2HPhHCHactTS
E(RB+HF-LYP) = -1766.33817527

Zero-point correction= 0.457975 (Hartree/Particle)
Thermal correction to Energy= 0.488483
Thermal correction to Enthalpy= 0.489428
Thermal correction to Gibbs Free Energy= 0.395496
Sum of electronic and zero-point Energies= -1765.880200
Sum of electronic and thermal Energies= -1765.849692
Sum of electronic and thermal Enthalpies= -1765.848748
Sum of electronic and thermal Free Energies= -1765.942680

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	306.528	112.423	197.696

C,0,-1.4113980182,-2.889770394,2.498108917
C,0,-0.6256955146,-2.0728633679,1.6806707522
C,0,-0.9966191976,-0.7462931242,1.38022892
C,0,-2.1716883774,-0.2699010063,1.9913608474
C,0,-2.9638508671,-1.0819680628,2.8107040135
C,0,-2.590511238,-2.4015517273,3.0642999339
Ir,0,0.172773075,0.3731371944,-0.1925135085
B,0,1.9434496339,1.0511850985,0.7526180279
O,0,2.9461346287,0.2403412752,1.2550779552
C,0,4.0486148403,1.0607843688,1.6516576836
C,0,3.4603271293,2.4841726252,1.7250611391
O,0,2.2375735309,2.4018787221,0.9765468128
B,0,1.4363550976,0.9282784024,-1.8163954427
O,0,2.7990395953,0.6617132673,-1.9164243117
C,0,3.2861552086,1.0498714455,-3.2042762261
C,0,2.1432623344,1.8810905772,-3.8162702464
O,0,1.007945333,1.5867415697,-2.9874699354
P,0,-0.8941034704,2.5277713368,-0.1308819528
C,0,-0.0492302547,3.9261404971,-0.9927541655
P,0,-1.511951661,-0.1523513376,-1.8220853018
C,0,-1.0779503513,-0.8945237382,-3.4540659372
C,0,-1.3808941374,3.3780137371,1.440487942
C,0,-2.5103192407,2.3746796492,-1.0686288147
C,0,-2.3482513282,1.4542805104,-2.2911608508

C,0,-2.9163728286,-1.2319614385,-1.2982444564
H,0,-3.6694417324,-1.3035901999,-2.0897692366
H,0,-2.5328884347,-2.2297876963,-1.0701672324
H,0,-3.3701570425,-0.8423045361,-0.3854532532
H,0,-0.6582892031,-1.8904105565,-3.2873278935
H,0,-0.3239457633,-0.2690084706,-3.9331404604
H,0,-1.9579576614,-0.9793672473,-4.0997893067
H,0,-1.7002220171,1.9254417138,-3.0377715374
H,0,-3.3161258702,1.2547973863,-2.766228071
H,0,-2.8773871547,3.3635604558,-1.367853285
H,0,-3.2442875831,1.9523611149,-0.3718067023
H,0,0.1735050137,3.6315701968,-2.0194828497
H,0,-0.6636623135,4.8326164233,-0.9827601418
H,0,0.8945179652,4.1113671702,-0.4745584616
H,0,-1.9451751455,4.2953550023,1.2425331494
H,0,-0.4618607704,3.6340093214,1.9749685578
H,0,-1.9729588897,2.721574272,2.0802442747
H,0,0.9423519523,-1.0256869064,-0.3954434394
H,0,3.2318088314,2.7852552485,2.7557202576
H,0,4.1143067698,3.2414147473,1.2809061593
H,0,4.4428463716,0.7106407683,2.6108999404
H,0,4.8429419921,0.9826456919,0.8988128996
H,0,0.2945453695,-2.4693563759,1.2641454671
H,0,-1.0948955402,-3.9111934559,2.6964936505
H,0,-3.2011483201,-3.0349046455,3.7020570622
H,0,-3.8721286447,-0.6771736858,3.2519107519
H,0,-2.4990757838,0.7503652373,1.8192092555
H,0,4.214088865,1.6199274556,-3.0923286254
H,0,3.5053120948,0.1496989209,-3.7923927898
H,0,2.3460898941,2.9590259832,-3.7764389464
H,0,1.9234940202,1.6111379407,-4.8543801252
H,0,0.373324809,0.2341306459,1.4159871372

Ir(dmpe)(BPin)$_3$(Ph-H) C-H Activation TS
E(RB+HF-LYP) = -2019.75161969

Zero-point correction= 0.520550 (Hartree/Particle)
Thermal correction to Energy= 0.556183
Thermal correction to Enthalpy= 0.557127
Thermal correction to Gibbs Free Energy= 0.451442
Sum of electronic and zero-point Energies= -2019.231069
Sum of electronic and thermal Energies= -2019.195437
Sum of electronic and thermal Enthalpies= -2019.194492
Sum of electronic and thermal Free Energies= -2019.300177

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	349.010	129.835	222.433

C,0,-0.3450394906,-3.4871937447,0.010675699
C,0,0.7905237207,-3.2170102301,1.0096381213
P,0,0.684876834,-1.4778419057,1.6941851808
Ir,0,0.0394794169,-0.0267468695,-0.1161052507
B,0,0.2551081677,1.6240939733,1.1708030244
O,0,0.5196450645,2.9464197731,0.8446960715
C,0,0.4678483561,3.7594111319,2.0187107259
C,0,0.4822466329,2.7538863821,3.1864400256
O,0,0.1776663165,1.4945913603,2.5736984024
P,0,-0.4986714744,-2.1309492135,-1.2751363649
B,0,-0.9639222067,1.1925575946,-1.5581248928
O,0,-1.8230221053,0.6543740557,-2.5243121702
C,0,-2.4185350877,1.7237346908,-3.2714705689
C,0,-1.6471038071,2.9864774862,-2.8259716627
O,0,-0.856330524,2.5602251015,-1.7148046269
B,0,-1.9564277613,0.043902379,0.6254265364
O,0,-2.6950968716,-1.0740328881,1.0593085259
C,0,-3.9411740647,-0.6374440891,1.6228778123
C,0,-4.0571021133,0.8377314613,1.1951064754
O,0,-2.7397175723,1.1897103396,0.7606156449
C,0,-2.2120597946,-2.4256495053,-1.9009704332
C,0,0.464556149,-2.7761951472,-2.7273832361
H,0,-0.2249601235,-4.4640984761,-0.4722892802
H,0,-1.3056621644,-3.4939363563,0.5367618731
C,0,-0.398167317,-1.6691815918,3.1747734526
C,0,2.3317076436,-1.2213618103,2.4805858299
H,0,0.7745839957,-3.9438824146,1.8307028068
H,0,1.7664156721,-3.3088902778,0.5189888401
H,0,-0.2632121865,2.9814232156,3.9557254198
H,0,1.4671831265,2.6937384051,3.6686448803
H,0,-0.4517638224,4.35770288,2.0002055396
H,0,1.3234115501,4.4429425135,2.0337760087
H,0,-2.3115577055,3.798193183,-2.512093596
H,0,-0.9844161659,3.3693402054,-3.6117949568
H,0,-3.486348771,1.7814837078,-3.0273706493
H,0,-2.3214871789,1.5199060285,-4.3432377239
H,0,-4.3631936015,1.4962127078,2.0141276846
H,0,-4.7600168238,0.9727092594,0.3631118031
H,0,-3.900740294,-0.7498861223,2.714023811

H,0,-4.757080909,-1.2605980068,1.2426117266
H,0,-2.3296570468,-3.4539339593,-2.2592006271
H,0,-2.91476286,-2.2309837843,-1.0897497649
H,0,-2.4105682646,-1.7189267182,-2.7079547502
H,0,0.0932092875,-3.75760254,-3.040946322
H,0,0.3471881489,-2.0720111719,-3.556326208
H,0,1.5295023643,-2.8509715677,-2.504076596
H,0,2.5611930301,-2.0272806153,3.1850979118
H,0,3.1061364724,-1.1653909119,1.7139728319
H,0,2.2995390988,-0.2694242897,3.0153146309
H,0,0.0199353663,-2.4033511546,3.8711143394
H,0,-0.4664919355,-0.6929252622,3.6592771421
H,0,-1.3955613698,-1.9741294086,2.8563008387
H,0,0.7711373351,0.6055100575,-1.4218688747
C,0,2.2409970682,0.2018068572,-0.7102976822
C,0,3.0511548132,-0.9105596868,-1.0110444122
C,0,4.4306039491,-0.7944719181,-1.2139191348
C,0,5.0478519574,0.4547446913,-1.1505092988
C,0,4.2641658295,1.5780542421,-0.8853409516
C,0,2.887253683,1.4538826766,-0.6745455463
H,0,2.6154088646,-1.9016696346,-1.06748327
H,0,5.0189302634,-1.6850449002,-1.4246182028
H,0,6.1178310278,0.5510813871,-1.3139851137
H,0,4.7224056515,2.5637075948,-0.846343622
H,0,2.3031602448,2.3453191212,-0.4743158764

dmpeBpin3PhHCHactTSSptSptBack11
E(RB+HF-LYP) = -2019.75362566

Zero-point correction= 0.520806 (Hartree/Particle)
Thermal correction to Energy= 0.556124
Thermal correction to Enthalpy= 0.557069
Thermal correction to Gibbs Free Energy= 0.453517
Sum of electronic and zero-point Energies= -2019.232820
Sum of electronic and thermal Energies= -2019.197501
Sum of electronic and thermal Enthalpies= -2019.196557
Sum of electronic and thermal Free Energies= -2019.300108

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	348.973	129.740	217.942

C,0,3.0590310152,-1.1722052726,0.7278761158
C,0,2.2224844971,-0.046916182,0.865985636

C,0,2.8164881658,1.1042022645,1.4204950026
C,0,4.1714772967,1.1427353768,1.7649149776
C,0,4.9839638341,0.0235016275,1.5844389562
C,0,4.4159438976,-1.1403282781,1.0664428275
Ir,0,0.0677090561,-0.0340407579,0.0608750295
P,0,0.8459503376,-0.2146060172,-2.2173248726
C,0,0.5159163445,-1.9672143978,-2.7864256439
C,0,0.7208602502,-3.0030501218,-1.6692385575
P,0,-0.1743204978,-2.4719549637,-0.1117248334
B,0,-1.8904136592,0.2870915673,-0.7107434801
O,0,-2.3927714439,-0.2949912123,-1.8910013748
C,0,-3.6877340946,0.250777151,-2.1836220329
C,0,-4.0939437931,0.9806332961,-0.8900629651
O,0,-2.877587168,1.094881794,-0.1453586736
B,0,-1.1389420278,-0.0137202848,1.8166720049
O,0,-1.8210076815,-1.1612347589,2.2526155861
C,0,-2.4622954756,-0.8653476993,3.5025622907
C,0,-2.3893702518,0.6696928142,3.6066740872
O,0,-1.367479787,1.0400095305,2.6785279372
B,0,0.0892517052,2.0687648063,-0.0102979827
O,0,0.25534787,2.9381384697,1.0624430334
C,0,0.3250989932,4.286988793,0.5952465976
C,0,-0.1181959351,4.2075391453,-0.878134726
O,0,-0.0381067875,2.8127378529,-1.1978905529
H,0,-3.6055116167,0.9360867799,-3.0370411439
H,0,-4.3752470338,-0.5567884166,-2.4555039425
H,0,-4.5081746086,1.9768512417,-1.0744987341
H,0,-4.8237961183,0.4070282943,-0.3043436724
H,0,-3.4879301341,-1.2480012498,3.4915648676
H,0,-1.9151553448,-1.3621362148,4.3144496838
H,0,-3.332526872,1.1462683685,3.310661759
H,0,-2.1214972097,1.0197149632,4.6084340666
H,0,-1.1517494489,4.5499430693,-1.0167020068
H,0,0.5280244079,4.7800739602,-1.5521226916
H,0,-0.3276671195,4.9209395323,1.2037803298
H,0,1.3551317778,4.6545847628,0.6980421404
H,0,0.69777474,-0.071555093,1.5624813343
H,0,2.665333049,-2.0983126218,0.3252363608
H,0,5.0255518851,-2.0302551044,0.9248971784
H,0,2.2031572325,1.9802416449,1.5980872602
H,0,4.5884146372,2.0548245412,2.1860843923
H,0,6.0365009872,0.0527503393,1.8530459516
C,0,0.1208038977,0.7675981578,-3.5978535306
C,0,2.6522130673,0.029537755,-2.5165306839

C,0,-1.8740970339,-3.1468961188,-0.3790812596
C,0,0.4307235667,-3.6516146831,1.1812206091
H,0,0.3768320202,-3.9937649983,-1.9898204617
H,0,1.7852363618,-3.0956097486,-1.4251663189
H,0,-0.5312014016,-1.9686063456,-3.1071807588
H,0,1.1322953909,-2.2010603739,-3.6625558446
H,0,2.9104885073,-0.1983666961,-3.5557798338
H,0,2.8998535303,1.0731843814,-2.3046529101
H,0,3.24078341,-0.5922515559,-1.8408536294
H,0,0.5840939043,0.4942942982,-4.5513944467
H,0,-0.9514313521,0.5729107682,-3.6343938835
H,0,0.2764131436,1.8263912234,-3.3874261751
H,0,0.3416690941,-4.6921846005,0.8516987214
H,0,1.4665880306,-3.4428953936,1.4531206043
H,0,-0.1912655768,-3.5017500172,2.0675180759
H,0,-1.8509323249,-4.2292124971,-0.5449480405
H,0,-2.4600838641,-2.9215101958,0.5147220427
H,0,-2.3361442424,-2.6444956997,-1.2300217964

dmpeBpin3PhHCHactTSParSptBack
E(RB+HF-LYP) = -2019.75310567

Zero-point correction= 0.520791 (Hartree/Particle)
Thermal correction to Energy= 0.556120
Thermal correction to Enthalpy= 0.557065
Thermal correction to Gibbs Free Energy= 0.453312
Sum of electronic and zero-point Energies= -2019.232315
Sum of electronic and thermal Energies= -2019.196985
Sum of electronic and thermal Enthalpies= -2019.196041
Sum of electronic and thermal Free Energies= -2019.299794

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	348.971	129.731	218.366

C,0,2.891351283,1.1939365057,-0.2357381002
C,0,2.1588766654,0.1853664459,0.395665178
C,0,2.7851053326,-0.8391692412,1.1323166771
C,0,4.1827825832,-0.7450497441,1.2641701756
C,0,4.9250363614,0.2640730164,0.6401607978
C,0,4.2826703908,1.2348161196,-0.1269990806
Ir,0,1.5709680628,-2.5960432904,1.9360026943
B,0,-0.1930323796,-1.4645937586,1.954050739
O,0,-1.432243962,-1.89864642,1.4555939839

C,0,-2.4356731769,-0.9311920454,1.7924616027
C,0,-1.638133946,0.3128104328,2.2347990187
O,0,-0.3072905333,-0.1677085991,2.4374487869
H,0,4.8523455333,2.0220506514,-0.6134330793
P,0,1.1971208618,-3.4222835756,-0.3057594867
C,0,1.8795643351,-2.4272927722,-1.7062405151
P,0,3.3959147319,-4.2800169512,1.9084901327
C,0,5.185400071,-4.0211728764,2.3221010264
B,0,0.2091293834,-4.083873952,2.6323975726
O,0,-0.1129267668,-5.2682196919,1.9391550535
C,0,-1.1926207322,-5.9361528884,2.6086716338
C,0,-1.2583544505,-5.2586313042,3.9890768096
O,0,-0.5010789948,-4.0552125072,3.8330329901
B,0,1.7350024811,-2.402420129,4.0473870107
O,0,0.9878649463,-1.588603983,4.8770327293
C,0,1.270047178,-1.9293274913,6.2359533431
C,0,2.5821884467,-2.7338224109,6.1637861747
O,0,2.6724397733,-3.1349237466,4.7877219007
C,0,2.1201113113,-5.0334518799,-0.4878874084
C,0,3.508643087,-4.9464800278,0.1620235804
C,0,-0.4866051164,-3.8374048416,-0.9252689339
C,0,3.0708743637,-5.8106089901,2.8953476817
H,0,-0.802183331,-5.8752398413,4.7745817978
H,0,-2.2804920401,-5.0137282536,4.294631266
H,0,-0.9843899052,-7.0096259929,2.664611476
H,0,-2.1161975855,-5.7913487055,2.0340941912
H,0,2.5788988222,-3.6196844795,6.8069806298
H,0,3.4581714678,-2.1232905502,6.418133745
H,0,0.442456232,-2.5299519111,6.6341218895
H,0,1.3591121931,-1.0169292078,6.8338322397
H,0,-3.06029953,-1.3292659137,2.6019497772
H,0,-3.0757731132,-0.7441721103,0.9234785875
H,0,-2.0157265414,0.7518262706,3.1637814411
H,0,-1.6285223017,1.0959290559,1.464694287
H,0,2.201241262,-1.2903949853,2.6657156462
H,0,1.0775969618,0.2064890539,0.3195496195
H,0,2.3682930908,1.9577040336,-0.8070515843
H,0,4.7082178814,-1.4575692122,1.888937221
H,0,6.0048897642,0.2947461268,0.7681064911
H,0,4.0067839947,-5.9233060383,0.1569203853
H,0,4.1484995977,-4.2556357552,-0.4000909284
H,0,1.5078679552,-5.7881843006,0.014733627
H,0,2.1947375505,-5.3066723924,-1.5472142686
H,0,1.7483395198,-2.9612157952,-2.6532339788

H,0,1.3695387556,-1.4638495276,-1.7613300925
H,0,2.9397513118,-2.2256316042,-1.5405994867
H,0,-0.440818366,-4.2352697101,-1.9441136069
H,0,-0.9257508133,-4.573940385,-0.2523733713
H,0,-1.1066641221,-2.9397365518,-0.8982868226
H,0,5.7363118604,-4.9657012956,2.2631139543
H,0,5.642312612,-3.3041896432,1.6375096736
H,0,5.2556996484,-3.6309994951,3.3406400611
H,0,3.8491039973,-6.5634376827,2.7319962767
H,0,3.0454047115,-5.52786452,3.9496678054
H,0,2.0968423348,-6.2177067341,2.6186813622

dmpeBpin3PhHCHactTSParWrdBack
E(RB+HF-LYP) = -2019.75100331

Zero-point correction= 0.521093 (Hartree/Particle)
Thermal correction to Energy= 0.556395
Thermal correction to Enthalpy= 0.557339
Thermal correction to Gibbs Free Energy= 0.452880
Sum of electronic and zero-point Energies= -2019.229911
Sum of electronic and thermal Energies= -2019.194608
Sum of electronic and thermal Enthalpies= -2019.193664
Sum of electronic and thermal Free Energies= -2019.298124

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	349.143	129.407	219.854

C,0,-2.6600629804,1.207915644,-0.4011663438
C,0,-1.9444945855,-0.0027490882,-0.5062878704
C,0,-2.6839839291,-1.1351072444,-0.8961299082
C,0,-4.0678791094,-1.0846228657,-1.097596278
C,0,-4.7591346902,0.1151053042,-0.9347018808
C,0,-4.0428674917,1.2644174345,-0.594620048
Ir,0,0.2802631172,-0.0234575698,0.030578203
P,0,-0.0000058687,0.8216853644,2.2703082969
C,0,0.4872488067,-0.5445733975,3.4442821479
C,0,-0.1159275156,-1.8846007672,3.0046606567
P,0,0.1984871758,-2.2177818991,1.1855465691
B,0,2.3537635321,0.3151925144,0.4015178123
O,0,3.0693998163,1.4135838304,-0.0677741608
C,0,4.4573220763,1.256489386,0.2340755266
C,0,4.4925490239,0.1347623739,1.289860475
O,0,3.1965186041,-0.4757958905,1.201716189

B,0,1.2101919549,-1.0012699938,-1.6064945413
O,0,0.8425028948,-2.2978666089,-1.9981052237
C,0,1.7374646734,-2.7441294769,-3.0278243175
C,0,2.477800256,-1.4655736027,-3.463934019
O,0,2.2527173447,-0.5409097326,-2.3941432827
B,0,0.4275007691,1.8773137161,-0.8434145262
O,0,0.4878145079,2.116328103,-2.210702442
C,0,0.404906396,3.522262634,-2.4572896472
C,0,0.5767092536,4.168267459,-1.0685799333
O,0,0.3494842988,3.0927164506,-0.1476466949
H,0,4.9952409132,0.9791950631,-0.6811385518
H,0,4.8668068328,2.2028290219,0.6024032622
H,0,5.2669081596,-0.6140901248,1.094877003
H,0,4.6399962508,0.5233232553,2.3064264742
H,0,2.4204781271,-3.4967162422,-2.6117049395
H,0,1.1647114469,-3.2072783185,-3.8370379372
H,0,3.5531131586,-1.6176120241,-3.6000879832
H,0,2.0661300795,-1.0461944134,-4.3902894817
H,0,1.5912192273,4.5589004758,-0.9194600368
H,0,-0.1386146905,4.9753943742,-0.878243966
H,0,1.1867221823,3.8207464295,-3.1631564082
H,0,-0.5711130049,3.7535702561,-2.9035867639
H,0,-0.5480487945,-0.2238652499,-1.3491973059
H,0,-2.1325987943,2.1258047078,-0.1604203435
H,0,-4.5601091335,2.2152599049,-0.4857972517
H,0,-2.1693576384,-2.0720701998,-1.0779726256
H,0,-4.5996884042,-1.9846941505,-1.3979628275
H,0,-5.8335504439,0.1600540059,-1.0911190647
C,0,1.0101656908,2.2440018826,2.864021341
C,0,-1.6887924315,1.2881216465,2.8617243832
C,0,1.727708229,-3.25800216,1.2070489722
C,0,-1.0607587417,-3.538064276,0.8631640883
H,0,0.2705641903,-2.7104575919,3.6130622142
H,0,-1.2044642965,-1.8707690839,3.1381143958
H,0,1.580713988,-0.5951196973,3.4096381485
H,0,0.1919469834,-0.2891038689,4.4691327601
H,0,-1.6760536993,1.5083513507,3.9341813902
H,0,-2.0347277018,2.1697250272,2.3183734627
H,0,-2.3921268119,0.4777876571,2.6594099495
H,0,0.7925883014,2.4755890771,3.9115711194
H,0,2.0706194627,2.0052635757,2.7573443087
H,0,0.7920467506,3.102187114,2.2262626982
H,0,-0.9335602483,-4.3677281401,1.5666870691
H,0,-2.0712986345,-3.1366038973,0.9577981635

H,0,-0.9273803612,-3.9121804539,-0.1549983008
H,0,1.6098960269,-4.1200606947,1.872166635
H,0,1.9094348541,-3.6121521967,0.1889668226
H,0,2.5758686445,-2.6464101188,1.5149943678

dmpeBpin3PhHCHactTSSptParBack
E(RB+HF-LYP) = -2019.75119685

Zero-point correction= 0.520306 (Hartree/Particle)
Thermal correction to Energy= 0.555888
Thermal correction to Enthalpy= 0.556832
Thermal correction to Gibbs Free Energy= 0.452440
Sum of electronic and zero-point Energies= -2019.230891
Sum of electronic and thermal Energies= -2019.195309
Sum of electronic and thermal Enthalpies= -2019.194365
Sum of electronic and thermal Free Energies= -2019.298757

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	348.825	129.864	219.712

C,0,-2.9679686767,-1.3176188993,-0.6004005485
C,0,-2.0930665967,-0.2725223462,-0.955803379
C,0,-2.6145730063,0.7064440687,-1.8257081452
C,0,-3.9383639691,0.6683241174,-2.2731866144
C,0,-4.7910839054,-0.3628760953,-1.8789421279
C,0,-4.2950654495,-1.3604955511,-1.0395688897
Ir,0,-0.0064117173,-0.0774396752,-0.0178992983
P,0,-0.8584822208,0.0511522216,2.2255733243
C,0,-0.5415948128,-1.6009257374,3.0558816852
C,0,-0.6763555679,-2.7873885353,2.0882660609
P,0,0.2696442277,-2.4662205796,0.5000284875
B,0,1.8968429124,0.5300713091,0.7331327522
O,0,2.1840171823,1.8052482052,1.2242769739
C,0,3.5947387524,1.9384414271,1.4266626881
C,0,4.1308189048,0.4951966747,1.3559253086
O,0,3.0526774143,-0.26008951,0.7887186403
B,0,1.3759963507,-0.2510967816,-1.626230436
O,0,1.6798297635,-1.4858302155,-2.2162726641
C,0,2.7740216109,-1.3061761558,-3.1256389989
C,0,2.8677929108,0.2213019288,-3.3071296457
O,0,2.1198992308,0.7591090735,-2.2116089181
B,0,-0.2644465269,1.9905349593,-0.2681056554
O,0,-0.0307720713,2.7337202863,-1.4206213887

C,0,-0.5014388261,4.0714229018,-1.2335325872
C,0,-0.7720033695,4.1780914409,0.2792785267
O,0,-0.8167858481,2.8174346824,0.724341897
H,0,4.0115014477,2.5727792568,0.6349214229
H,0,3.786210904,2.4198804871,2.3915931144
H,0,5.0191208984,0.4008200434,0.7229422366
H,0,4.373673885,0.0913912903,2.3478163684
H,0,3.6853964997,-1.7254543755,-2.6801397358
H,0,2.5675991298,-1.8386031148,-4.0594934734
H,0,3.896566707,0.5933362511,-3.268824932
H,0,2.414280549,0.5554925087,-4.2488102822
H,0,0.0354297535,4.7040942414,0.8051117502
H,0,-1.7196125339,4.6757892255,0.5110382369
H,0,0.2543746656,4.7816191427,-1.5839177469
H,0,-1.414408535,4.2197397825,-1.8263715841
H,0,-0.5557046257,-0.4182410347,-1.5135168975
H,0,-2.6255888038,-2.1102467542,0.0548925324
H,0,-4.9387888149,-2.178541621,-0.7234985925
H,0,-1.9673775447,1.5075383413,-2.1680246779
H,0,-4.2987748993,1.4468859577,-2.941550282
H,0,-5.8197437727,-0.395176564,-2.227333602
C,0,-0.1515392188,1.2335201778,3.449437165
C,0,-2.6649842108,0.3531670624,2.4495664256
C,0,1.945078122,-3.1361773663,0.9006745741
C,0,-0.3331578146,-3.7882079376,-0.6456372038
H,0,-0.3295279476,-3.7155188092,2.5582497912
H,0,-1.7285113834,-2.9386760197,1.8215249179
H,0,0.4841230525,-1.5484243908,3.4406956283
H,0,-1.2025753605,-1.7190006412,3.9227906291
H,0,-2.9500076371,0.2851169741,3.5043768936
H,0,-2.8728545865,1.3590179278,2.0761413588
H,0,-3.2498160817,-0.3522440693,1.8576930553
H,0,-0.6022244886,1.0896656762,4.4368450636
H,0,0.9300736568,1.1052492366,3.5107898963
H,0,-0.3510934501,2.2419145355,3.0843605829
H,0,-0.2600475655,-4.7822026115,-0.1917845265
H,0,-1.3645407567,-3.5995233908,-0.94816147
H,0,0.2949022424,-3.748138381,-1.5391339894
H,0,1.8845701688,-4.1854462115,1.2092342564
H,0,2.5671996508,-3.0481540641,0.0077630231
H,0,2.4134081549,-2.5369910652,1.6819189921

Ir(dmpe)(BPin)$_2$(η^2-BPinH)(Ph)
E(RB+HF-LYP) = -2019.76522987

Zero-point correction= 0.524049 (Hartree/Particle)
Thermal correction to Energy= 0.559197
Thermal correction to Enthalpy= 0.560142
Thermal correction to Gibbs Free Energy= 0.456709
Sum of electronic and zero-point Energies= -2019.241181
Sum of electronic and thermal Energies= -2019.206032
Sum of electronic and thermal Enthalpies= -2019.205088
Sum of electronic and thermal Free Energies= -2019.308521

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	350.902	129.474	217.693

C,0,-3.2669007519,0.5502560795,-0.1985304741
C,0,-2.2305549621,-0.3297706726,-0.5741570041
C,0,-2.6184846537,-1.3667303948,-1.452089677
C,0,-3.9366474852,-1.5408555036,-1.886696065
C,0,-4.9398195865,-0.6684426682,-1.4636152366
C,0,-4.5913331082,0.3865301821,-0.621140956
Ir,0,-0.0930588267,-0.0489670331,-0.0760815658
P,0,-0.4654747645,0.2754135432,2.2319387089
C,0,0.0920060863,-1.2529957299,3.1408004948
C,0,-0.365312609,-2.5134202447,2.3969697851
P,0,0.1959013068,-2.4428413328,0.6155021261
B,0,1.9047732148,0.626314487,0.4068995346
O,0,2.2989371955,1.9586563175,0.347051849
C,0,3.6941943691,2.0642819458,0.6423081728
C,0,4.0553078383,0.7042326785,1.2710534227
O,0,2.9492570686,-0.1481856529,0.9345113349
B,0,1.2787199413,-0.4232325442,-1.7165731946
O,0,1.5769723612,-1.7330401453,-2.1188824881
C,0,2.73772895,-1.6895728338,-2.9586331195
C,0,2.842038619,-0.2111574715,-3.3756707638
O,0,2.0802645124,0.490508986,-2.3882534873
B,0,-0.4670085079,1.9580164366,-0.5066387862
O,0,-0.3759377839,2.5338488392,-1.7629386201
C,0,-0.6373998808,3.9359354011,-1.6620096697
C,0,-1.2329209056,4.1209029881,-0.2503006771
O,0,-0.9312955884,2.8937000289,0.4298775047
H,0,4.2446116915,2.249026349,-0.288506127
H,0,3.8673837366,2.9076211678,1.3188090321
H,0,4.9822966962,0.2788504288,0.8736764953
H,0,4.1462955609,0.761244876,2.3639166983

H,0,3.6134338939,-2.017187026,-2.3826659017
H,0,2.6037000748,-2.3688130879,-3.8059298433
H,0,3.870920503,0.1617680465,-3.3831013178
H,0,2.3996732125,-0.0296565694,-4.3634530234
H,0,-0.7884760153,4.9615378305,0.2928056483
H,0,-2.3213113,4.2598870226,-0.2750550675
H,0,0.3026618998,4.4876128952,-1.7875432556
H,0,-1.3271414404,4.2391895711,-2.456190559
H,0,-0.103016567,-0.1637373864,-1.7414110117
H,0,-3.037886236,1.4104543392,0.4221989823
H,0,-5.3492021011,1.0975141759,-0.2972910673
H,0,-1.8681551085,-2.0537625713,-1.8323349659
H,0,-4.1748061827,-2.3566665157,-2.566590265
H,0,-5.9661313048,-0.7981681326,-1.7972198107
C,0,0.4292240131,1.6303819781,3.1015745693
C,0,-2.1777829293,0.5176337065,2.8790391144
C,0,1.8940060796,-3.1677607012,0.7262351
C,0,-0.7348519211,-3.8642393068,-0.1163371132
H,0,0.0147361918,-3.419883664,2.8822874497
H,0,-1.4598161745,-2.5796516943,2.3923251761
H,0,1.1861764728,-1.2133355758,3.180778203
H,0,-0.2809959193,-1.2301077121,4.171274161
H,0,0.1173108357,1.6873840631,4.1490354937
H,0,1.5059072888,1.4594621173,3.0536479103
H,0,0.2009715215,2.5645242245,2.5861162356
H,0,-2.1696625143,0.4450135954,3.9714104292
H,0,-2.5323403478,1.5084605302,2.5898012964
H,0,-2.8576934197,-0.2250701682,2.4596154903
H,0,1.8813277731,-4.1264986244,1.255640329
H,0,2.2685928057,-3.3143471469,-0.2882591542
H,0,2.5552936123,-2.4590905783,1.226673482
H,0,-0.54439246,-4.783169542,0.4480120532
H,0,-1.8051890432,-3.6506475612,-0.1182461092
H,0,-0.408934453,-4.0085347605,-1.1497249755

Ir(dmpe)(BPin)$_2$(H)(Ph-Bpin) Reductive Elimination TS
E(RB+HF-LYP) = -2019.77073889

Zero-point correction= 0.522052 (Hartree/Particle)
Thermal correction to Energy= 0.557082
Thermal correction to Enthalpy= 0.558026
Thermal correction to Gibbs Free Energy= 0.454334
Sum of electronic and zero-point Energies= -2019.248686
Sum of electronic and thermal Energies= -2019.213657

Sum of electronic and thermal Enthalpies= -2019.212713
Sum of electronic and thermal Free Energies= -2019.316405

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	349.574	128.390	218.239

C,0,-4.0737126198,-1.0096046351,1.2465683863
C,0,-3.0166203928,-0.9771064391,0.3335901212
C,0,-2.253488567,0.1868384355,0.1160322364
C,0,-2.6376497066,1.3407690414,0.8277125824
C,0,-3.6933214968,1.3205978718,1.7416686883
C,0,-4.4090183608,0.1415750634,1.9629506802
Ir,0,0.1917157006,-0.0608539667,-0.097847614
B,0,0.5520315799,1.9810152113,0.246027211
O,0,0.2742220955,2.6683074585,1.4372649147
C,0,0.7956949122,4.0026605574,1.3459744839
C,0,1.1386774296,4.1767284663,-0.1459011483
O,0,1.1548344163,2.8435478576,-0.6658881975
B,0,2.1788652761,0.0879360528,-0.6429371725
O,0,3.2954432909,0.1996433536,0.1991537996
C,0,4.4884307112,0.2316018987,-0.5975357559
C,0,3.9794718675,0.408876559,-2.0423162455
O,0,2.5891263406,0.0816827096,-1.9742933122
P,0,0.2836220789,-2.486376251,-0.4452135765
C,0,-0.9711750986,-3.5634717595,-1.2837278248
P,0,0.6651560375,-0.5956585478,2.133538417
C,0,-0.7636715169,-0.5584981069,3.2991711952
B,0,-1.4838074337,0.3958446844,-1.6084706241
O,0,-1.7706465974,1.6786902125,-2.1353552754
C,0,-2.6865537602,1.5006619221,-3.2098528577
C,0,-2.4604294211,0.046900551,-3.6599696403
O,0,-1.9773913547,-0.6103989835,-2.4890882837
C,0,0.4277534764,-3.2656055318,1.2534971183
C,0,1.2461770374,-2.3730507512,2.2004566014
C,0,1.8308957701,-3.0713154856,-1.2790121994
C,0,1.9576514081,0.3051345581,3.0817386848
H,0,-0.0278391494,0.3278116749,-1.696929013
H,0,1.2077572776,-2.7478971043,3.2300519444
H,0,2.29941149,-2.3602123262,1.8967623598
H,0,0.8618220642,-4.270197611,1.1848319517
H,0,-0.5948103898,-3.3804788593,1.6328628461
H,0,-1.7070039869,-0.0106765242,-4.4595584093
H,0,-3.3764669044,-0.4413673093,-4.0115017166

H,0,-2.481412052,2.2315317617,-3.9994948979
H,0,-3.7178613395,1.6517474171,-2.8557622358
H,0,2.112842386,4.6495115799,-0.3075835384
H,0,0.3778405779,4.7595990271,-0.6797411907
H,0,1.6827529874,4.0871585183,1.9875868731
H,0,0.0453071854,4.716652426,1.7004524188
H,0,4.4823908031,-0.2528045877,-2.7554884385
H,0,4.0881927062,1.4425727379,-2.3925769774
H,0,5.037781586,-0.7095974742,-0.4626550191
H,0,5.1304511874,1.0536838964,-0.2657550541
H,0,-2.1058048264,2.2696114574,0.66219259
H,0,-3.9630892154,2.2283425323,2.2760106433
H,0,-5.2335606507,0.1255077986,2.6711995576
H,0,-4.6462135864,-1.9240013416,1.384616826
H,0,-2.8133937826,-1.8571551371,-0.2639904384
H,0,1.6158158212,1.3334835339,3.2172249754
H,0,2.1287885857,-0.1604668386,4.0576739759
H,0,2.8755917942,0.31630341,2.4927911433
H,0,-1.1083424199,0.4740960383,3.3864642495
H,0,-1.5911514314,-1.1515225279,2.9049752682
H,0,-0.4741636797,-0.9324704199,4.2867754792
H,0,1.8800230371,-2.6406863876,-2.2817241797
H,0,2.703915992,-2.7177594479,-0.724877819
H,0,1.8609986404,-4.1638029883,-1.3417082468
H,0,-1.2726651024,-3.0815104606,-2.2164535206
H,0,-0.5673732863,-4.5607668587,-1.4850032327
H,0,-1.8591356828,-3.6658760914,-0.6559923755

dmpeBpin2PhHBinRotTS13
E(RB+HF-LYP) = -2019.76042936

Zero-point correction= 0.523546 (Hartree/Particle)
Thermal correction to Energy= 0.558287
Thermal correction to Enthalpy= 0.559232
Thermal correction to Gibbs Free Energy= 0.457245
Sum of electronic and zero-point Energies= -2019.236884
Sum of electronic and thermal Energies= -2019.202142
Sum of electronic and thermal Enthalpies= -2019.201198
Sum of electronic and thermal Free Energies= -2019.303185

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	350.331	127.897	214.650

C,0,4.351997731,0.2437421785,1.3298526185
C,0,2.9520534567,0.2012598651,1.2930583825
C,0,2.2086771934,-0.0381570776,0.1166168091
C,0,2.9992833601,-0.2364327636,-1.0395931552
C,0,4.3968426995,-0.1968715232,-1.0242494884
C,0,5.088675068,0.0440485315,0.1639733062
Ir,0,-0.0229912657,-0.0717433124,-0.0298533948
B,0,0.2085315234,-1.8567694328,-1.1252451354
O,0,0.1597731858,-3.1638896489,-0.6282994637
C,0,0.3060199031,-4.0886940343,-1.7166303303
C,0,0.7623023156,-3.2168154426,-2.9036296626
O,0,0.4927321576,-1.8744865717,-2.4870561316
B,0,-2.1144061207,-0.2242558828,-0.4402926021
O,0,-3.170455635,0.0488289861,0.4551024364
C,0,-4.4249947936,-0.2596584317,-0.1733214966
C,0,-4.0667036726,-0.4605420006,-1.6570604107
O,0,-2.6473102721,-0.6369084153,-1.6602112815
P,0,-0.2453115883,1.8071725297,1.5022959709
C,0,1.0409872717,3.1294546584,1.5983184091
P,0,-0.3782756367,-1.3752671039,1.8661461249
C,0,1.0275086506,-2.375166556,2.5141500409
B,0,-0.0219172533,1.6643179565,-1.4797442533
O,0,-1.1942863753,2.2131564115,-1.9697452588
C,0,-0.8700388016,3.4227604893,-2.6713652943
C,0,0.6044140702,3.7036964189,-2.3005917982
O,0,1.0636131242,2.4895426375,-1.6927710767
C,0,-0.213504103,1.0947832969,3.2313355824
C,0,-0.9082584433,-0.2698051335,3.2780543875
C,0,-1.8023918092,2.8014839486,1.4916993323
C,0,-1.7301755672,-2.6266161576,1.8521825276
H,0,0.2174041688,0.352652029,-1.6398256977
H,0,-0.7312338932,-0.7775933936,4.233142876
H,0,-1.9906739314,-0.1464669611,3.1642849114
H,0,-0.6764751191,1.7998842614,3.9313390162
H,0,0.8392412521,0.9994520421,3.5169612667
H,0,0.7033434798,4.5258578753,-1.5803737566
H,0,1.2294963795,3.9326441798,-3.1683737554
H,0,-1.5501024292,4.2208847036,-2.3576304276
H,0,-1.0055063539,3.2547851022,-3.7459470937
H,0,0.2131610586,-3.4331124022,-3.8253773738
H,0,1.8358302643,-3.3223287809,-3.1045372932
H,0,-0.6593941002,-4.5742642116,-1.9066735903
H,0,1.0352482661,-4.8591245775,-1.4468868768
H,0,-4.3224855074,0.4171761041,-2.2643558975

H,0,-4.55072114,-1.337969589,-2.0980768749
H,0,-5.1319913466,0.5599502891,-0.0088407041
H,0,-4.8425279142,-1.1691395775,0.2797674271
H,0,2.5112198732,-0.4323495922,-1.9906669779
H,0,4.9473729804,-0.3556377591,-1.9498365455
H,0,6.1751347487,0.074871735,0.1800786738
H,0,4.8616220916,0.4344837115,2.2729129876
H,0,2.4360153505,0.3681356302,2.2373505659
H,0,-1.5011576616,-3.3622137969,1.0805810843
H,0,-1.8022160175,-3.1189258639,2.8274941655
H,0,-2.6722969403,-2.1296125579,1.6176843882
H,0,1.2739861651,-3.114601477,1.7488140034
H,0,1.9066639494,-1.7524676633,2.6780728917
H,0,0.7439833836,-2.8831556704,3.4415164732
H,0,-1.8819523634,3.3198308964,0.5327451765
H,0,-2.6530342594,2.1224515587,1.5686826466
H,0,-1.8165385846,3.5343007064,2.30516314
H,0,0.970154641,3.7662967744,0.7142207718
H,0,0.9070541593,3.7425051492,2.4954685202
H,0,2.030323437,2.6691528922,1.5988392161

dmpeBpin2PhHBinRotTSPar
E(RB+HF-LYP) = -2019.75561076

Zero-point correction= 0.524111 (Hartree/Particle)
Thermal correction to Energy= 0.558614
Thermal correction to Enthalpy= 0.559559
Thermal correction to Gibbs Free Energy= 0.458170
Sum of electronic and zero-point Energies= -2019.231500
Sum of electronic and thermal Energies= -2019.196996
Sum of electronic and thermal Enthalpies= -2019.196052
Sum of electronic and thermal Free Energies= -2019.297441

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	350.536	127.768	213.390

C,0,4.3327897286,0.1114674991,1.2436928794
C,0,2.935281133,0.066132237,1.1858355068
C,0,2.206748804,0.0237338295,-0.0258933098
C,0,3.0158971141,0.0064313068,-1.1837330755
C,0,4.4140403692,0.0571096812,-1.1477769955
C,0,5.0879725361,0.1164918119,0.0715748525
Ir,0,-0.0338915653,-0.0666645354,-0.058877448

B,0,0.1250281134,-1.165407497,1.7248366539
O,0,0.1255064072,-0.6526805914,3.0278992008
C,0,0.4429445089,-1.7116642468,3.9452434935
C,0,0.2856652084,-2.9979159291,3.1116923026
O,0,0.2939489427,-2.5446535983,1.7550651938
B,0,-2.1378965715,-0.3964405143,0.1191832257
O,0,-3.1606538002,0.5737903466,0.0551875451
C,0,-4.4269574274,-0.0405598556,0.3446479359
C,0,-4.1376734107,-1.5517221552,0.2872799659
O,0,-2.7116084957,-1.6457754328,0.3537838483
P,0,-0.3303207086,1.4216296507,-1.9966697383
C,0,0.8344294268,1.5616465754,-3.4311306268
P,0,-0.2868706171,1.9113204387,1.162766074
C,0,1.189285271,2.7284551647,1.90991271
B,0,0.0405359383,-1.623452448,-1.7358259765
O,0,-1.0789260797,-1.797407602,-2.5334511232
C,0,-0.7222643372,-2.6673567395,-3.6211356265
C,0,0.8196543809,-2.736289879,-3.5687752785
O,0,1.1579811461,-2.2129608346,-2.2783085905
C,0,-0.2855709306,3.1675267077,-1.3387840876
C,0,-0.9626474582,3.2296145275,0.0313283082
C,0,-1.9519690056,1.3564869153,-2.8802392261
C,0,-1.484960054,1.9653095907,2.5595539516
H,0,0.0200855467,-1.7088434136,-0.4095389557
H,0,-0.8405064896,4.2139732226,0.4977887254
H,0,-2.0349613887,3.029560924,-0.0608057816
H,0,-0.7590750722,3.8505025136,-2.0536426939
H,0,0.7703377257,3.4521292621,-1.261452635
H,0,1.2924884452,-2.1164719435,-4.3409184819
H,0,1.2079922057,-3.7545370126,-3.6589822307
H,0,-1.1027504256,-2.2533408274,-4.5599930334
H,0,-1.1893461113,-3.645069243,-3.4569915057
H,0,-0.663989021,-3.5088221841,3.3156438633
H,0,1.103457232,-3.7081264628,3.2677077586
H,0,-0.2347276892,-1.6691913545,4.8038265223
H,0,1.4705983321,-1.5756076316,4.3048170019
H,0,-4.4869245628,-2.0028662473,-0.6504043594
H,0,-4.5840441135,-2.103237418,1.1210087229
H,0,-5.1707126042,0.283092054,-0.3907884052
H,0,-4.765228867,0.2800100035,1.3389260839
H,0,2.5522204186,-0.0900940782,-2.1586846341
H,0,4.9762067017,0.0388621134,-2.0800988522
H,0,6.1738827334,0.153506411,0.1075745373
H,0,4.8297404333,0.1387990082,2.2120974042

H,0,2.4024678741,0.0575819729,2.1333958522
H,0,-1.1543389046,1.2648632253,3.3269733187
H,0,-1.5382672252,2.9792046555,2.9691541428
H,0,-2.4658644722,1.6641330074,2.1892745898
H,0,1.5558991995,2.119499544,2.7372491762
H,0,1.9923071457,2.8152076949,1.176611165
H,0,0.9121102545,3.7182769166,2.287384114
H,0,-2.0595511909,0.3660430776,-3.3275208697
H,0,-2.7541512086,1.481382118,-2.151299479
H,0,-2.0154287737,2.1274352732,-3.655221677
H,0,0.8460984662,0.6269185196,-3.9981976183
H,0,0.5186967333,2.3711932287,-4.0973245363
H,0,1.8461901061,1.7576866466,-3.0729947745

Ir(dmpe)(BPin)$_2$(H)(η^2-PhBPin)
E(RB+HF-LYP) = -2019.79892754

Zero-point correction= 0.522787 (Hartree/Particle)
Thermal correction to Energy= 0.559141
Thermal correction to Enthalpy= 0.560086
Thermal correction to Gibbs Free Energy= 0.449410
Sum of electronic and zero-point Energies= -2019.276141
Sum of electronic and thermal Energies= -2019.239786
Sum of electronic and thermal Enthalpies= -2019.238842
Sum of electronic and thermal Free Energies= -2019.349518

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	350.867	130.060	232.937

C,0,-4.3189210515,-2.2507777429,1.0531167713
C,0,-4.6020063533,-2.0054477829,-0.2942294314
C,0,-4.1342564758,-0.8397953451,-0.9019108131
C,0,-3.3825921942,0.1063586065,-0.1807210259
C,0,-3.1044204651,-0.1581286261,1.1741071697
C,0,-3.568517446,-1.327129889,1.7845287383
Ir,0,0.4575433037,-0.1034602725,-0.0747645751
B,0,-2.8796624009,1.4112899627,-0.8696923236
O,0,-2.8697411668,1.5714483779,-2.234091932
C,0,-2.3220864062,2.8673393413,-2.5244990972
C,0,-1.9613662318,3.4719960757,-1.1424383888
O,0,-2.4599748433,2.5236117535,-0.1817580919
B,0,0.3497876858,1.6327363381,1.0804226653
O,0,0.8652254072,2.9054684161,0.8148639206

C,0,0.5948338818,3.7651092358,1.9295924307
C,0,-0.4778626643,3.0143130666,2.735016072
O,0,-0.3393539029,1.6505679774,2.307989795
B,0,2.1855030139,0.6419590108,-0.7607446709
O,0,2.3393109035,1.3402210598,-1.9568955173
C,0,3.7259806869,1.611724714,-2.1690314609
C,0,4.3981195269,1.2810309029,-0.8207190269
O,0,3.4305828363,0.4822194513,-0.1297517688
P,0,0.5016139384,-2.1405121323,-1.3569377013
C,0,1.8084563478,-2.2781771259,-2.6605077861
P,0,1.328688149,-1.4432200167,1.6760869471
C,0,2.7704287725,-0.9413463713,2.710690065
C,0,-0.9799922528,-2.8010341632,-2.2438003921
C,0,0.9339297688,-3.5421319277,-0.1774120578
C,0,1.8922804526,-3.0719454759,0.9322187917
C,0,0.1076504035,-1.9670944412,2.9674396177
H,0,-0.1750348449,0.7722457179,-1.2846873709
H,0,1.9999920093,-3.8392331615,1.708496237
H,0,2.891010622,-2.8886215143,0.5179068074
H,0,1.3504564175,-4.3976140648,-0.7226732115
H,0,-0.0138321138,-3.8760720556,0.2633020042
H,0,-1.442552929,2.7455076787,-3.1630962308
H,0,-3.0727964899,3.4573677856,-3.0629623073
H,0,-0.8818201922,3.5686186864,-0.9982867129
H,0,-2.4411001875,4.4407279715,-0.9664904774
H,0,1.5174342055,3.9136534536,2.507179573
H,0,0.254129131,4.7414235969,1.5694517919
H,0,-0.3300953839,3.0808720674,3.817861665
H,0,-1.4888685439,3.3624401465,2.4914003015
H,0,4.1015611418,0.976156491,-2.9829541801
H,0,3.8581932792,2.6578497198,-2.4635415305
H,0,5.3320781374,0.7200229065,-0.9323137259
H,0,4.6041460869,2.1848876363,-0.2335056487
H,0,-2.5140156764,0.5523409994,1.745614829
H,0,-3.3522494654,-1.512117725,2.8335332703
H,0,-4.6885473711,-3.154409665,1.5311775846
H,0,-5.1914473038,-2.7187685514,-0.8645195965
H,0,-4.356684983,-0.6499202142,-1.9484660053
H,0,2.4661797398,-0.1021475411,3.3423896084
H,0,3.1203140339,-1.7616228539,3.3463662565
H,0,3.5673622649,-0.5998878559,2.0482368926
H,0,-0.2398627357,-1.0684947333,3.4841326584
H,0,-0.7593355008,-2.4393902296,2.4985463742
H,0,0.5518455514,-2.65938593,3.6905431658

H,0,1.6336207542,-1.5053344795,-3.413294078
H,0,2.7899909427,-2.0963521522,-2.2149142765
H,0,1.8040912662,-3.2637303882,-3.1379800026
H,0,-1.2143593762,-2.1273904671,-3.072645532
H,0,-0.8091753029,-3.8094918427,-2.6355611219
H,0,-1.8404780466,-2.8091073741,-1.570034073

dmpeBpin2Hη2PhBin
E(RB+HF-LYP) = -2019.79908239

Zero-point correction= 0.522932 (Hartree/Particle)
Thermal correction to Energy= 0.559216
Thermal correction to Enthalpy= 0.560160
Thermal correction to Gibbs Free Energy= 0.449291
Sum of electronic and zero-point Energies= -2019.276151
Sum of electronic and thermal Energies= -2019.239867
Sum of electronic and thermal Enthalpies= -2019.238923
Sum of electronic and thermal Free Energies= -2019.349791

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	350.913	129.995	233.342

C,0,-4.735273632,-1.6283398293,0.5762622349
C,0,-4.1624565981,-1.009423025,-0.5353393473
C,0,-3.3591542183,0.1377618575,-0.3970235494
C,0,-3.13914326,0.6430968937,0.8987674575
C,0,-3.7083981571,0.0225864482,2.014767115
C,0,-4.5080798759,-1.1116111606,1.8557494923
Ir,0,0.4489240713,-0.1719223898,0.0402554115
B,0,0.4555459173,1.9156522018,0.067727561
O,0,-0.2723236411,2.626898877,1.0414738955
C,0,-0.3145664134,4.0103062894,0.6599707112
C,0,0.8452892668,4.1536744643,-0.3387690686
O,0,1.0866302014,2.8164771916,-0.7946489907
B,0,2.2505573998,-0.0296301609,-0.8216180854
O,0,3.4677130172,-0.1355842385,-0.12207734
C,0,4.5433560842,-0.1270589902,-1.0691909139
C,0,3.889483311,0.3521527128,-2.3797003713
O,0,2.4927195118,0.124048685,-2.184047975
P,0,0.3563417567,-2.5787755697,0.078167496
C,0,-1.1518473463,-3.5384901614,-0.3938812457
P,0,1.1709219592,-0.3860947154,2.2886596329
C,0,-0.1117675945,-0.0534276161,3.5831416143

B,0,-2.7382782659,0.8264942055,-1.6503845058
O,0,-2.2494405295,2.1100697,-1.6517985113
C,0,-1.6464571373,2.3476966699,-2.936887602
C,0,-2.0354251189,1.1147573236,-3.7931910179
O,0,-2.6825432041,0.2147386981,-2.879346512
C,0,0.6534917173,-3.127820628,1.8532199534
C,0,1.6274602762,-2.1822008552,2.5793275825
C,0,1.6775766425,-3.4799991852,-0.8535828267
C,0,2.6251256671,0.5273396243,2.9601967931
H,0,-0.0772324064,-0.0554622448,-1.4895828475
H,0,1.6694732829,-2.4084774568,3.6516569631
H,0,2.6413879137,-2.3028418401,2.1796486331
H,0,1.0107274467,-4.1641468967,1.886010274
H,0,-0.3250632699,-3.1120495577,2.3493037872
H,0,-1.1605160607,0.6176787272,-4.2215944012
H,0,-2.733966275,1.3626023525,-4.6009735123
H,0,-0.5655081241,2.4334428735,-2.796124186
H,0,-2.0371640218,3.2860976064,-3.3444249581
H,0,1.7546013304,4.5460685165,0.1367999612
H,0,0.5992477014,4.7959414134,-1.1907875573
H,0,-0.202259781,4.6433992031,1.5462138707
H,0,-1.2839785217,4.2209180641,0.1923428232
H,0,4.2380537376,-0.2008227822,-3.2582777993
H,0,4.0603048127,1.4225833505,-2.5533022338
H,0,4.9539414572,-1.1421784183,-1.1611768462
H,0,5.3415853769,0.5356590259,-0.7194877492
H,0,-2.5112961669,1.5198649343,1.029292025
H,0,-3.5353035548,0.4302766748,3.0073671921
H,0,-4.9589694334,-1.5874749287,2.7229158107
H,0,-5.3626839458,-2.5066822264,0.4482389513
H,0,-4.341358796,-1.4114262941,-1.5289184903
H,0,2.3773734344,1.5917885422,2.9978012687
H,0,2.8937753277,0.1846074829,3.9650080332
H,0,3.4611569516,0.3906325481,2.272341115
H,0,-0.4018186244,0.9977224086,3.5044858157
H,0,-1.0017394021,-0.6602736009,3.3981152683
H,0,0.2642077478,-0.257595363,4.5912932068
H,0,1.5709187937,-3.2576325261,-1.9185476834
H,0,2.6578597395,-3.1205658315,-0.530600519
H,0,1.6177905206,-4.5625386863,-0.6990117173
H,0,-1.3157896522,-3.418093335,-1.4682869546
H,0,-1.0496066116,-4.6040574618,-0.1619535705
H,0,-2.0253292186,-3.132115491,0.1221115396

dmpeBpin2HeqA
E(RB+HF-LYP) = -1534.11389776

Zero-point correction= 0.360084 (Hartree/Particle)
Thermal correction to Energy= 0.385198
Thermal correction to Enthalpy= 0.386142
Thermal correction to Gibbs Free Energy= 0.304221
Sum of electronic and zero-point Energies= -1533.753814
Sum of electronic and thermal Energies= -1533.728700
Sum of electronic and thermal Enthalpies= -1533.727755
Sum of electronic and thermal Free Energies= -1533.809677

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	241.716	90.457	172.419

C,0,-3.082276667,-0.0355396578,1.6074034677
C,0,-2.1533346121,-0.727030741,2.6194204028
P,0,-0.3583799847,-0.6536365075,2.0591474899
Ir,0,-0.2865234999,-0.5786322999,-0.3113048161
B,0,-0.1762312857,1.4151351611,-0.4728927447
O,0,0.612018666,2.1348896327,-1.3600688887
C,0,0.2883729923,3.5225892273,-1.264771828
C,0,-0.5520786629,3.6395051546,0.0233942274
O,0,-0.9621610573,2.2933176186,0.3032071075
P,0,-2.6942255484,-0.5665143261,-0.1475037457
B,0,1.7985180214,-0.6157277293,-0.3987283372
O,0,2.6849566113,0.1869972276,0.3355982057
C,0,4.0253343623,-0.0987466382,-0.0854041357
C,0,3.9098588666,-1.4320451575,-0.8485766217
O,0,2.5141914458,-1.5514824429,-1.1479933042
H,0,-0.2356783914,-0.5032344833,-1.9339370232
C,0,-3.7242934105,0.5978898709,-1.1460129625
C,0,-3.6446642703,-2.1524169236,-0.3262541151
H,0,-4.1368184577,-0.2136905875,1.8509538945
H,0,-2.9062037321,1.0452179288,1.6213671389
C,0,0.349133086,0.7848640614,2.9715512354
C,0,0.390191209,-2.0804546676,2.9753213077
H,0,-2.2626472557,-0.2896569413,3.6186340756
H,0,-2.412436306,-1.789796248,2.7071755863
H,0,-1.4335668953,4.2783009142,-0.0947557283
H,0,0.0386423723,4.0191725489,0.8673523017
H,0,-0.2797702229,3.8243688802,-2.1546264014
H,0,1.2074610404,4.116181442,-1.2265546336

H,0,4.227251923,-2.2876879877,-0.2368553972
H,0,4.4882678664,-1.443734712,-1.77818881
H,0,4.6837735121,-0.1604338197,0.7879451263
H,0,4.3834953617,0.7143673589,-0.7300741394
H,0,-4.7728272784,0.5956958705,-0.8296503342
H,0,-3.3113404191,1.6030814022,-1.0351859278
H,0,-3.6640994229,0.3138752369,-2.2000540508
H,0,-4.7045740943,-2.0226522564,-0.0822930888
H,0,-3.5570159417,-2.5073508789,-1.356989096
H,0,-3.2218027214,-2.9194651609,0.3288968746
H,0,0.2438390545,0.6730191023,4.0556419226
H,0,1.4056585167,0.860792489,2.7012751382
H,0,-0.1556225654,1.6929177691,2.6361238198
H,0,0.1634680364,-2.0445278442,4.0462118273
H,0,0.0187042173,-3.0228432954,2.5627509283
H,0,1.4748965416,-2.0545785908,2.8408220522

dmpeBpin2Hn2HBPinaxBest15
E(RB+HF-LYP) = -1788.74091500

Zero-point correction= 0.439746 (Hartree/Particle)
Thermal correction to Energy= 0.470561
Thermal correction to Enthalpy= 0.471505
Thermal correction to Gibbs Free Energy= 0.376217
Sum of electronic and zero-point Energies= -1788.301169
Sum of electronic and thermal Energies= -1788.270354
Sum of electronic and thermal Enthalpies= -1788.269410
Sum of electronic and thermal Free Energies= -1788.364698

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.281	110.324	200.551

C,0,2.022029144,-2.3052553126,-1.7094167201
P,0,1.3491853815,-0.5937535339,-1.6959529333
Ir,0,-0.0707049973,0.1935817192,0.0407706391
B,0,-1.9927383959,1.2779917053,-0.2642291357
O,0,-2.1361592527,2.6398507049,0.0044649713
C,0,-3.5340384423,2.923723732,0.1324511164
C,0,-4.2029214129,1.5358191285,0.2204862719
O,0,-3.2245654977,0.6371490438,-0.3092688123
C,0,0.6759608594,-0.4338760582,-3.4097449699
C,0,2.8825314184,0.4829432647,-1.7243827333
C,0,2.5434124298,1.9497889768,-1.4049167345

P,0,1.4295042043,2.0910766748,0.0996634549
C,0,2.6409081156,2.174443748,1.4962400108
C,0,0.8615769405,3.8466086019,0.000856433
B,0,0.9429390505,-0.7846951437,1.5836761813
O,0,1.7482805685,-1.9273100237,1.4580260209
C,0,2.1250541312,-2.3872494806,2.762385908
C,0,1.7692401385,-1.2154709394,3.699330386
O,0,0.9244574733,-0.369634471,2.915477135
B,0,-1.1724813896,-1.5949937215,0.0441796078
O,0,-1.8298833327,-2.1575787686,1.134311341
C,0,-2.581276003,-3.2948028116,0.7005442804
C,0,-2.0486233474,-3.5973655024,-0.7148074295
O,0,-1.3256389379,-2.4155418438,-1.0846543968
H,0,-0.9183201533,0.6436961289,1.3508007494
H,0,3.3956177504,0.3983155952,-2.6898530894
H,0,3.559779667,0.0757863809,-0.9641234731
H,0,3.4548717156,2.5449140898,-1.2720294999
H,0,1.9870807812,2.3957224423,-2.2386953832
H,0,1.555947487,-3.294295479,3.0013010989
H,0,3.1914102639,-2.637052239,2.7735363907
H,0,1.235833067,-1.5383757473,4.5992210724
H,0,2.6588827518,-0.6520224397,4.0131028178
H,0,-2.4328234273,-4.1259438745,1.398225095
H,0,-3.6485278026,-3.0389930649,0.6913450155
H,0,-1.3653854901,-4.4571698097,-0.7246838998
H,0,-2.8471143412,-3.7843314904,-1.440361541
H,0,1.1809690065,-2.9868896945,-1.8555732293
H,0,2.7545305307,-2.4426740245,-2.5115115011
H,0,2.4659893238,-2.5159278684,-0.7353780488
H,0,-0.2253896068,-1.0487253773,-3.4724997735
H,0,0.3960916185,0.6048082198,-3.6036548881
H,0,1.3987840842,-0.7634458835,-4.1636791852
H,0,0.298489496,4.0834323261,0.9066479077
H,0,1.7033094981,4.5400977543,-0.1001920296
H,0,0.1784354089,3.9609228999,-0.8431368994
H,0,2.0899704962,2.1813579939,2.439511826
H,0,3.2679752725,1.2787216797,1.4890728556
H,0,3.2789941934,3.0616765682,1.4280497218
H,0,-1.1219059002,0.9272296796,-1.2119577324
H,0,-5.1243180613,1.4644018597,-0.3659297095
H,0,-4.4268014693,1.2554673722,1.257886953
H,0,-3.8696434874,3.4893678514,-0.7471002655
H,0,-3.7074035193,3.5360764616,1.0232417527

dmpeBpin2Hn2HBPinax2ndBestRev
E(RB+HF-LYP) = -1788.74085531

Zero-point correction=	0.439952 (Hartree/Particle)
Thermal correction to Energy=	0.470563
Thermal correction to Enthalpy=	0.471507
Thermal correction to Gibbs Free Energy=	0.377398
Sum of electronic and zero-point Energies=	-1788.300903
Sum of electronic and thermal Energies=	-1788.270292
Sum of electronic and thermal Enthalpies=	-1788.269348
Sum of electronic and thermal Free Energies=	-1788.363457

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.283	110.351	198.070

C,0,1.0100061783,2.9591849596,-1.6041473159
P,0,1.3760584956,1.6389256522,-0.3674018122
Ir,0,-0.0286292414,-0.3305222484,-0.172983524
B,0,1.3032996833,-1.7318359429,-1.2905001578
O,0,2.2573697429,-1.2489410331,-2.1898315721
C,0,2.677173744,-2.3396309982,-3.0193080706
C,0,1.6417242465,-3.4493620172,-2.7442562584
O,0,1.0502565433,-3.0776150227,-1.496609201
C,0,3.2087426277,1.4451639965,-0.5489555598
C,0,1.2097810376,2.5365021632,1.2648816289
C,0,1.2551342236,1.5457133688,2.4421076154
P,0,0.0829875349,0.1080904055,2.1633073958
C,0,-1.4585159689,0.6044346372,3.041713896
C,0,0.7473523405,-1.2104169568,3.2685155863
B,0,-1.7508213009,0.8350542077,-0.4058757388
O,0,-1.8947051069,2.1388606912,0.1199352435
C,0,-3.228548816,2.6059225234,-0.1316225044
C,0,-3.7888444219,1.6110268975,-1.1653357858
O,0,-2.9037716678,0.4905147997,-1.1019127457
B,0,-1.4249881541,-1.8770457808,0.1032274677
O,0,-1.9165910166,-2.2702089178,1.3658046302
C,0,-2.7751462259,-3.4070262747,1.2003292774
C,0,-3.0214557187,-3.4812614114,-0.3203095248
O,0,-2.0197921576,-2.639702138,-0.8900632889
H,0,-0.3154047345,-0.5065356351,-1.7614140767
H,0,1.9809410617,3.3091418047,1.3703422461
H,0,0.2322803297,3.0280796473,1.227276811
H,0,1.0277033742,2.047334489,3.3899657001

H,0,2.260498581,1.1170163409,2.539798255
H,0,-3.1972383801,3.6369713386,-0.4986581494
H,0,-3.7986669859,2.5923362752,0.8068234382
H,0,-3.7780240778,2.0235602275,-2.1826806147
H,0,-4.8103675504,1.2897992867,-0.9375991507
H,0,-3.6957911997,-3.2642325384,1.7766359748
H,0,-2.2666494391,-4.3026005396,1.5810609141
H,0,-4.0140793842,-3.1007165218,-0.5953609424
H,0,-2.9219424759,-4.4979264656,-0.7159317159
H,0,1.1867509737,2.5613111469,-2.6071647901
H,0,1.6339811002,3.8465447974,-1.4538339888
H,0,-0.0437767858,3.2313985202,-1.5178387201
H,0,3.4081103866,0.8875477985,-1.4664841659
H,0,3.5951486939,0.854632422,0.2867027375
H,0,3.7230609595,2.4118827155,-0.5733512128
H,0,0.0625058038,-2.0595366174,3.2104088973
H,0,0.830953588,-0.8722789142,4.3067464713
H,0,1.7281962324,-1.5303407961,2.9073698178
H,0,-2.1650059455,-0.2242102935,2.9523166178
H,0,-1.8786791959,1.4828340393,2.5483458771
H,0,-1.2684297178,0.8208720267,4.0979309205
H,0,1.3967751843,-1.3866138099,0.0010677561
H,0,0.8628111026,-3.4840478966,-3.5166568433
H,0,2.0901707861,-4.4439087115,-2.6571513598
H,0,2.6946250591,-2.0219631496,-4.0666737784
H,0,3.6931170543,-2.641800548,-2.7312966065

dmpeBpin2Hn2HBPinax3rdBest
E(RB+HF-LYP) = -1788.73990099

Zero-point correction= 0.439821 (Hartree/Particle)
Thermal correction to Energy= 0.470593
Thermal correction to Enthalpy= 0.471537
Thermal correction to Gibbs Free Energy= 0.375995
Sum of electronic and zero-point Energies= -1788.300080
Sum of electronic and thermal Energies= -1788.269308
Sum of electronic and thermal Enthalpies= -1788.268364
Sum of electronic and thermal Free Energies= -1788.363906

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.301	110.358	201.085

C,0,-1.3536125954,-2.3817545502,2.2080413906

P,0,-1.1183551736,-0.5878068093,1.8749303592
Ir,0,0.0704528988,0.1893674822,-0.0302587927
B,0,1.7336410529,1.6670126812,-0.0518148896
O,0,1.6009316693,2.9488498692,-0.5893381587
C,0,2.9136683712,3.4689913653,-0.8275934424
C,0,3.844099173,2.2471248798,-0.6825122684
O,0,3.0701464865,1.3012272252,0.0599163982
C,0,-0.5117649997,0.0298840404,3.5073470131
C,0,-2.8665441626,0.0630213296,1.7607380491
C,0,-2.8866384338,1.5066224825,1.2309749193
P,0,-1.8040563448,1.7038357986,-0.2917805079
C,0,-2.979225678,1.370638383,-1.6811058701
C,0,-1.6188003684,3.5401158222,-0.3976245121
B,0,-0.8100467129,-1.2181361186,-1.2946514887
O,0,-1.9481828657,-1.9882482332,-0.9706445038
C,0,-2.2114819883,-2.9120043662,-2.036497092
C,0,-1.333158457,-2.4109359022,-3.2013019557
O,0,-0.4215685879,-1.491321883,-2.599824288
B,0,1.557267131,-1.2780740813,0.2251577011
O,0,2.3498267934,-1.8571709533,-0.7568551805
C,0,3.3716108303,-2.6423112234,-0.1375589153
C,0,2.901985347,-2.8111561449,1.3208454534
O,0,1.8918024413,-1.8071186754,1.4852047951
H,0,0.7709212182,0.5684900176,-1.4451138386
H,0,-3.3759245767,-0.0087739912,2.7292575417
H,0,-3.3836172456,-0.6041616255,1.0622450876
H,0,-3.9109381953,1.8360163727,1.0194352275
H,0,-2.4800945259,2.1908887825,1.9860973239
H,0,-1.934525929,-3.9243904908,-1.7151088691
H,0,-3.2810350417,-2.909529439,-2.2727415954
H,0,-0.7767277793,-3.2175374318,-3.6900069296
H,0,-1.9227120486,-1.8901904474,-3.967780693
H,0,3.4788818266,-3.5958847645,-0.6653361693
H,0,4.3258029729,-2.1034106669,-0.199208188
H,0,2.4629270519,-3.8017828811,1.50287815
H,0,3.7033855001,-2.6523530913,2.049829357
H,0,-0.3689110877,-2.8205804405,2.3816601616
H,0,-1.9922515862,-2.5458741778,3.082114723
H,0,-1.7988921324,-2.8395823736,1.3234751228
H,0,0.5088522853,-0.3373763312,3.6404615066
H,0,-0.4839965239,1.1225516861,3.505270889
H,0,-1.1390957615,-0.3173717909,4.3352187166
H,0,-1.0757766843,3.7876681537,-1.3124699225
H,0,-2.5902691438,4.0459418932,-0.3964932302

H,0,-1.0169123825,3.8941534605,0.4424421843
H,0,-2.4517001238,1.5129232619,-2.6285349681
H,0,-3.3029853141,0.3285033685,-1.6284671824
H,0,-3.8526321495,2.0306261158,-1.6504358674
H,0,0.9632296924,1.3611841384,0.9961972114
H,0,4.7684903583,2.4722978386,-0.1413642426
H,0,4.1061385663,1.8148785052,-1.6569447158
H,0,3.1351228673,4.2464307957,-0.0839462153
H,0,2.957768378,3.9213466825,-1.8235970358

Ir(dmpe)(BPin)$_2$(H)(η^2-BPinH) axial BPinH
E(RB+HF-LYP) = -1788.73351004

Zero-point correction= 0.441293 (Hartree/Particle)
Thermal correction to Energy= 0.471952
Thermal correction to Enthalpy= 0.472896
Thermal correction to Gibbs Free Energy= 0.377827
Sum of electronic and zero-point Energies= -1788.292218
Sum of electronic and thermal Energies= -1788.261558
Sum of electronic and thermal Enthalpies= -1788.260614
Sum of electronic and thermal Free Energies= -1788.355683

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.154	109.812	200.089

C,0,1.6089528706,1.7419401038,-2.8485866407
P,0,1.8322979142,0.6910185751,-1.3460108948
Ir,0,-0.1121988345,-0.2395367816,-0.2914585452
B,0,0.792703331,0.656587749,1.7036071846
O,0,1.941172376,0.1360395765,2.2846510273
C,0,2.4849111916,1.1197069975,3.1806347973
C,0,1.5912665248,2.3706302961,2.987132923
O,0,0.5420665019,1.9463862941,2.1078079076
C,0,3.1173946772,1.6821713214,-0.4444839865
C,0,2.8165679091,-0.7652983509,-1.9854087564
C,0,2.8524612304,-1.9015753549,-0.9499672963
P,0,1.1287825259,-2.2815156837,-0.3096447165
C,0,0.5545816803,-3.6537776144,-1.4012791724
C,0,1.4819669797,-3.180406383,1.2675723018
B,0,-0.9047910269,-0.4893045929,-2.2087989937
O,0,-0.2314911185,-1.0699220186,-3.3034418366
C,0,-1.1343917451,-1.1863658411,-4.4124428031
C,0,-2.3538839022,-0.3336740019,-4.0059915121

O,0,-2.1740194831,-0.0838585743,-2.6109932271
B,0,-1.9621186886,-1.1536765415,0.1695210715
O,0,-2.9371106708,-0.5958450514,0.9881144597
C,0,-4.0964142877,-1.4334456209,0.9954605724
C,0,-3.6393771806,-2.7421781328,0.3157131927
O,0,-2.3674821036,-2.423741495,-0.2637972321
H,0,-0.9688160829,1.1283794933,-0.3750452026
H,0,3.8286612973,-0.4544086521,-2.2716555188
H,0,2.2918354564,-1.0963716301,-2.8872069329
H,0,3.3125548535,-2.8025170273,-1.3728159756
H,0,3.45273466,-1.6078399492,-0.0803465367
H,0,-0.6463704141,-0.8284038296,-5.325468265
H,0,-1.3951845024,-2.2426990096,-4.5542780298
H,0,-2.3882866571,0.6229065308,-4.5433700044
H,0,-3.3050022604,-0.8510528659,-4.1698678307
H,0,-4.435392043,-1.5861554855,2.0258999812
H,0,-4.9018982722,-0.9382949579,0.4390743505
H,0,-3.5137573143,-3.5627095496,1.0343270406
H,0,-4.3275515853,-3.0771340733,-0.4677923538
H,0,1.1028788813,2.6673411475,-2.5603506788
H,0,2.5692872262,1.9851268581,-3.3152316286
H,0,0.9803372303,1.2077782844,-3.5624340021
H,0,2.6527689619,2.5877605216,-0.0443770409
H,0,3.5125715423,1.0983144619,0.3892591439
H,0,3.9395815845,1.9671040006,-1.1089661841
H,0,0.541275076,-3.5709329706,1.666223276
H,0,2.1751838949,-4.0145393544,1.1143356556
H,0,1.9013305415,-2.4792550871,1.9926087326
H,0,-0.4485517,-3.9418803882,-1.0782770242
H,0,0.4845515079,-3.2785216288,-2.424043487
H,0,1.2291824196,-4.5151675851,-1.3579841425
H,0,-0.1993928333,-0.136360042,1.4589531541
H,0,2.1335565787,3.2034400414,2.5251640496
H,0,1.1517970098,2.7261207554,3.9243961789
H,0,3.5331391484,1.3060714746,2.9240032629
H,0,2.4457111235,0.727499642,4.202689188

IrDMPEBpin2Hη2BpinH
E(RB+HF-LYP) = -1788.73462397

Zero-point correction= 0.440155 (Hartree/Particle)
Thermal correction to Energy= 0.471004
Thermal correction to Enthalpy= 0.471948
Thermal correction to Gibbs Free Energy= 0.375644

Sum of electronic and zero-point Energies= -1788.294469
Sum of electronic and thermal Energies= -1788.263620
Sum of electronic and thermal Enthalpies= -1788.262676
Sum of electronic and thermal Free Energies= -1788.358980

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.559	110.182	202.689

C,0,-3.0583677491,1.8599640225,-0.6047588609
P,0,-2.2838804597,0.4053436263,0.2174360081
C,0,-3.4306662776,-0.9603087001,-0.2838620553
C,0,-2.7065268401,0.6692926608,2.0290041947
C,0,-1.7564538132,-0.1058076871,2.9562192164
P,0,0.0288995818,0.1790682092,2.4655229669
C,0,0.9320530735,-1.1175227239,3.4189035036
Ir,0,0.1027615545,0.2553462775,0.0596607319
B,0,0.1765231769,0.5222319442,-2.0249161612
O,0,1.2197180582,0.0923297798,-2.8437681868
C,0,0.8842741097,0.326759162,-4.2137738091
C,0,-0.3491995244,1.2495715365,-4.1562692722
O,0,-0.8093863198,1.1467997822,-2.8026741324
B,0,2.1269562945,0.8479297076,-0.0170152105
O,0,2.5913649698,2.111477488,-0.373251676
C,0,4.0132053823,2.156293004,-0.2143763987
C,0,4.4260100425,0.6881240278,0.0124072781
O,0,3.1987689818,0.0177097601,0.3270692459
C,0,0.4772064544,1.7220935748,3.3817242028
H,0,-0.0794410929,1.8611363063,0.0801948256
H,0,-3.7526154203,0.4007535254,2.2171483402
H,0,-2.614388674,1.7466042897,2.2120580666
H,0,-1.9278429627,0.1610027528,4.0062128574
H,0,-1.9241142884,-1.1840564641,2.854927214
H,0,-1.145157738,0.9415683724,-4.842918453
H,0,-0.094015664,2.2953386653,-4.3715953093
H,0,0.6611139345,-0.6313969313,-4.7011122282
H,0,1.7342262478,0.7853842651,-4.7302360405
H,0,5.1374442905,0.5649919025,0.8360047878
H,0,4.8604073129,0.2378237616,-0.8889494842
H,0,4.2618515534,2.7939166982,0.6448602401
H,0,4.4707467793,2.5942572216,-1.1075792418
H,0,-2.8354241415,1.7989826347,-1.6719973243
H,0,-4.1395931261,1.8979755208,-0.4361679867
H,0,-2.5908809858,2.769726681,-0.2201585532

H,0,-3.2778893922,-1.1740574088,-1.3450316267
H,0,-3.1966330536,-1.861208345,0.2882123532
H,0,-4.4782744748,-0.6891993158,-0.1174378848
H,0,2.0059962239,-0.9781791761,3.2678428973
H,0,0.7082885225,-1.0768266587,4.4903160291
H,0,0.6528959279,-2.093539628,3.0162562161
H,0,1.5313867107,1.9466097554,3.1982207069
H,0,-0.1095711785,2.5583063349,2.9932908126
H,0,0.3107397482,1.6254816686,4.4598915133
B,0,-0.2282467413,-1.9452550862,-0.2116877468
H,0,0.9216179161,-1.2377026117,-0.0893763634
O,0,-0.4634627153,-2.5566277355,-1.4309710351
O,0,-0.5946798481,-2.7803623016,0.8485141707
C,0,-1.1007747384,-3.8184294993,-1.2070150456
C,0,-0.9714503679,-4.0585111131,0.3136274833
H,0,-2.1479146081,-3.7561944546,-1.5286757302
H,0,-0.6034859691,-4.5892198052,-1.8035746497
H,0,-1.9072965689,-4.3900970687,0.7752021221
H,0,-0.1907095338,-4.7902799869,0.5536767956

DMPE_BPinH_rotTS
E(RB+HF-LYP) = -1788.72079115

Zero-point correction= 0.439968 (Hartree/Particle)
Thermal correction to Energy= 0.469688
Thermal correction to Enthalpy= 0.470633
Thermal correction to Gibbs Free Energy= 0.379299
Sum of electronic and zero-point Energies= -1788.280823
Sum of electronic and thermal Energies= -1788.251103
Sum of electronic and thermal Enthalpies= -1788.250159
Sum of electronic and thermal Free Energies= -1788.341492

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	294.734	108.419	192.227

Ir,0,0.0705124255,-0.0205829459,-0.4375441744
P,0,1.4490321462,1.817153812,-0.113275942
C,0,0.4053829467,3.2790322898,0.3921797062
C,0,-0.9155947675,3.2893331948,-0.3820808916
P,0,-1.7075480378,1.5962023982,-0.3528222335
C,0,2.3840587348,2.4107970318,-1.5859498767
C,0,2.7381880799,1.7768653683,1.1980965816
C,0,-2.809423565,1.6632045393,1.1297516807

C,0,-2.9038921054,1.7247655978,-1.753167045
B,0,-1.7050218654,-1.3853332553,-0.5491979796
O,0,-2.3332605707,-1.8843851644,0.5801468576
C,0,-3.527707129,-2.5662081387,0.1736142976
C,0,-3.7323365591,-2.1441830362,-1.2982672838
O,0,-2.4809347674,-1.5619743575,-1.6842882241
B,0,1.8043261096,-1.1716868336,-0.7685775994
O,0,3.1290316809,-0.7088228071,-0.760537033
C,0,4.0186577274,-1.8184632905,-0.9447644793
C,0,3.1027204122,-2.973720447,-1.3956782353
O,0,1.7817984469,-2.5287880977,-1.0797739746
B,0,0.1672689975,-0.4552486576,1.6676359128
O,0,-0.0604813973,0.4767056888,2.705702587
C,0,0.1882911236,-0.1486681234,3.9747581248
C,0,0.3061739969,-1.6482141179,3.644057123
O,0,0.4932386704,-1.6893459161,2.2267907378
H,0,0.0938647692,0.2099986281,-2.1164017279
H,0,-0.3833297793,-1.5982228345,-0.7624850631
H,0,0.9646147654,4.2111344047,0.2500611712
H,0,0.2177171701,3.1597233303,1.4647342918
H,0,-1.6097378071,4.0384142517,0.0158086489
H,0,-0.739924258,3.5326212254,-1.436256679
H,0,-4.5280362765,-1.3954946945,-1.4085262454
H,0,-3.9609036536,-2.9856259629,-1.9588126548
H,0,-4.3579849212,-2.2714992936,0.823000601
H,0,-3.3728055587,-3.6465539817,0.2789069256
H,0,3.312881992,-3.9109131515,-0.8702071926
H,0,3.1744254781,-3.1593051004,-2.4753455617
H,0,4.5227765961,-2.0376152876,0.0052902474
H,0,4.7802200495,-1.5606402035,-1.6882486988
H,0,-0.6066304378,-2.1995470795,3.9049217913
H,0,1.1527346929,-2.1300455408,4.1445772104
H,0,-0.6320606188,0.0749561231,4.6649181392
H,0,1.1154152075,0.2558181036,4.4035692321
H,0,3.4413916382,0.9798836326,0.9528204855
H,0,3.2632609953,2.7356888826,1.2584792997
H,0,2.255503036,1.5564445802,2.1517477163
H,0,3.0649966917,1.6115568198,-1.8849852164
H,0,1.6875086565,2.5946999653,-2.4066525336
H,0,2.952643622,3.3198690614,-1.3629371752
H,0,-3.378055899,0.7311908443,1.1845747065
H,0,-2.1803149169,1.7128730839,2.021292322
H,0,-3.4997681187,2.5126498939,1.0969684448
H,0,-3.465862199,0.7935950151,-1.840022787

H,0,-3.5935642515,2.5644165553,-1.6183725831
H,0,-2.3378111387,1.8514561624,-2.6789705426

dmpeBpin3HHint17
E(RB+HF-LYP) = -1788.73274845

Zero-point correction= 0.439466 (Hartree/Particle)
Thermal correction to Energy= 0.469802
Thermal correction to Enthalpy= 0.470746
Thermal correction to Gibbs Free Energy= 0.378039
Sum of electronic and zero-point Energies= -1788.293282
Sum of electronic and thermal Energies= -1788.262946
Sum of electronic and thermal Enthalpies= -1788.262002
Sum of electronic and thermal Free Energies= -1788.354710

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	294.805	110.508	195.120

C,0,2.6541172174,2.3484341115,-1.3188889605
P,0,1.4306561402,1.8461387463,-0.0362744508
C,0,2.4862685693,1.6939887951,1.463373627
Ir,0,-0.0295106697,0.117625319,-0.6498280867
B,0,-0.0543972632,-0.4628607477,1.4359339043
O,0,0.9302709865,-1.2453237777,2.0305975712
C,0,0.5830248785,-1.4954421602,3.3954000129
C,0,-0.5329782901,-0.4761464146,3.7004848565
O,0,-0.9561311533,-0.0136054711,2.4095973753
P,0,-1.723876939,1.8608697954,-0.6748975706
C,0,-2.816731864,2.0302296773,-2.152812493
B,0,-1.5118837642,-1.3709763804,-0.2291739627
O,0,-2.8855528736,-1.088490893,-0.3096350122
C,0,-3.604370586,-2.1813281247,0.2724842126
C,0,-2.5793580922,-3.329742234,0.298563335
O,0,-1.3116424942,-2.6740144087,0.2162082773
B,0,1.5815153808,-1.2002356565,-0.904045944
O,0,1.5022034724,-2.4730424992,-1.4533867134
C,0,2.8144761568,-3.0221335617,-1.5906193907
C,0,3.7273168037,-2.0540435525,-0.8096988636
O,0,2.9197178841,-0.8877838032,-0.6079151405
C,0,0.4318044598,3.3962000921,0.27564712
C,0,-0.7756965319,3.4766991698,-0.6718311649
C,0,-2.9290182402,2.0838089007,0.7090371446
H,0,0.3734299581,0.6226723199,-2.1902938973

H,0,-0.8481069556,-1.0067267479,-1.5438376865
H,0,1.0731957397,4.2808845554,0.1854772051
H,0,0.0925152931,3.3468052454,1.3172928606
H,0,-1.4299583432,4.313885556,-0.401938568
H,0,-0.4368078145,3.6440449145,-1.7008194213
H,0,-3.933842077,-1.9027845478,1.2824575613
H,0,-4.4883540032,-2.406205085,-0.3328363073
H,0,-2.6279504659,-3.9283309768,1.2137712533
H,0,-2.6938017218,-4.0022125656,-0.5618151246
H,0,2.8335648593,-4.0398418993,-1.186714845
H,0,3.0779392809,-3.0699751742,-2.6555199039
H,0,4.0216474924,-2.4616791117,0.1658467855
H,0,4.6357126059,-1.7856770634,-1.3602784291
H,0,0.234055418,-2.5311448956,3.4925632378
H,0,1.4645268411,-1.3677347648,4.0325413103
H,0,-1.383178187,-0.9161696722,4.2317597372
H,0,-0.1682476214,0.3767136049,4.2884680021
H,0,3.0753579047,0.7820241104,1.3506055506
H,0,3.1443982877,2.5617401349,1.5733435797
H,0,1.8595447226,1.5976218242,2.352345331
H,0,3.2835246222,1.4805322192,-1.5261381517
H,0,2.1254329871,2.6198379252,-2.2350350469
H,0,3.2714544111,3.1867545881,-0.9797239916
H,0,-3.6039633771,1.2255536231,0.7026323656
H,0,-2.3940588667,2.0736817828,1.6606970565
H,0,-3.5045273695,3.0098766315,0.6038225811
H,0,-3.4760681766,1.1591791399,-2.1874370883
H,0,-3.4227188562,2.9418349182,-2.115806468
H,0,-2.202378776,2.0313714886,-3.0564311711

dmpeBpin2PhHtoHTS
E(RB+HF-LYP) = -1766.33026375

Zero-point correction= 0.457835 (Hartree/Particle)
Thermal correction to Energy= 0.488028
Thermal correction to Enthalpy= 0.488972
Thermal correction to Gibbs Free Energy= 0.396770
Sum of electronic and zero-point Energies= -1765.872429
Sum of electronic and thermal Energies= -1765.842236
Sum of electronic and thermal Enthalpies= -1765.841292
Sum of electronic and thermal Free Energies= -1765.933494

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	306.242	112.348	194.055

C,0,0.1824238598,3.1912397834,0.9692583311
C,0,0.7373678804,1.8967739954,0.950533519
C,0,2.0775187522,1.7643169066,1.3579920074
C,0,2.843022073,2.884333038,1.6961520132
C,0,2.288989848,4.165176428,1.6609397247
C,0,0.9480586228,4.3118364386,1.3045756628
Ir,0,-0.4404849845,0.2101885934,0.1364035454
H,0,-1.8431665797,1.1359261052,0.3034314218
P,0,-1.9051170802,-1.314543836,-0.879918202
C,0,-2.3468410384,-0.6464429433,-2.5710783515
C,0,-1.1180676357,-0.0102661022,-3.2418064986
P,0,-0.3024666443,1.1899768262,-2.0698351783
B,0,-0.3635546673,-1.0648085272,1.8188932076
O,0,-0.9132010164,-2.3576150913,1.8575913774
C,0,-0.7495448688,-2.8929832304,3.1792545794
C,0,0.2676659535,-1.9491530335,3.845910145
O,0,0.2337556257,-0.7701101279,3.0395355774
B,0,1.3134845163,-0.9785812922,-0.272189674
O,0,2.3231903485,-1.3678524802,0.6102928325
C,0,3.3709206986,-2.0364096653,-0.1027032816
C,0,2.7496982036,-2.3671324485,-1.4698329894
O,0,1.598134974,-1.5120118294,-1.5496591578
H,0,-0.3905860507,0.8949771625,1.5889867397
H,0,4.2328919449,-1.3626140535,-0.1929095844
H,0,3.6857824224,-2.9256702286,0.4521345789
H,0,3.4227361134,-2.1625356421,-2.3086931778
H,0,2.4267809351,-3.4146018842,-1.5345409159
H,0,-0.3984637992,-3.9279964817,3.1171074152
H,0,-1.7194919417,-2.8858396491,3.6939612293
H,0,1.2831663069,-2.3650937128,3.8332239189
H,0,0.0069175757,-1.6985452087,4.8789724077
H,0,-0.8696804822,3.3177261104,0.7319236081
H,0,0.4877746663,5.2973079598,1.3002490362
H,0,2.5235051274,0.7785224614,1.4128970233
H,0,3.8799337359,2.7497293657,1.9959846204
H,0,2.8870488544,5.0326865331,1.9270225185
C,0,-1.3576594684,-3.0372191705,-1.2446734144
C,0,-3.5421198484,-1.5731111857,-0.0799562764
C,0,1.3333880291,1.5338324246,-2.8441610074
C,0,-1.2097137939,2.7707792327,-2.3725293943
H,0,-0.3663311441,-0.7771208975,-3.4577442888
H,0,-1.3852179976,0.4779923335,-4.1862203323

H,0,-2.7707458105,-1.4437167596,-3.1923861307
H,0,-3.1315326398,0.1042967819,-2.4211858683
H,0,-1.1515491318,3.0725859448,-3.4236240513
H,0,-2.2552987992,2.6522216964,-2.0788192564
H,0,-0.7711308226,3.5538907624,-1.7492747614
H,0,1.228357586,1.9140080783,-3.8653416601
H,0,1.858134297,2.2753058913,-2.2352002566
H,0,1.9129493825,0.6092598627,-2.8447236828
H,0,-4.1888586841,-2.2203152978,-0.6814241677
H,0,-3.3658293938,-2.0333146429,0.894343827
H,0,-4.0196865505,-0.6030492793,0.0727429268
H,0,-2.1332871411,-3.5967064827,-1.7776368481
H,0,-0.4437673789,-2.9996263723,-1.8406843919
H,0,-1.1355872263,-3.5214644814,-0.292195509

dmpeBpin3HHTSforn2H2form18
E(RB+HF-LYP) = -1788.72215537

Zero-point correction= 0.436230 (Hartree/Particle)
Thermal correction to Energy= 0.466972
Thermal correction to Enthalpy= 0.467916
Thermal correction to Gibbs Free Energy= 0.372940
Sum of electronic and zero-point Energies= -1788.285925
Sum of electronic and thermal Energies= -1788.255183
Sum of electronic and thermal Enthalpies= -1788.254239
Sum of electronic and thermal Free Energies= -1788.349216

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	293.029	110.807	199.895

C,0,-1.0749873519,-3.6607987997,-0.6074233405
P,0,-0.4168062761,-2.3232923504,0.4840888702
C,0,-1.5259007428,-2.4617804818,1.9476965832
Ir,0,0.0154898299,-0.2071356539,-0.5198800063
B,0,-0.2235884283,0.6264818662,1.4403921289
O,0,-1.4296087291,1.0550337915,1.9855567147
C,0,-1.1846305845,1.7097837069,3.2327080646
C,0,0.2513379527,1.2945647537,3.6070563909
O,0,0.801313558,0.7793054919,2.386471907
P,0,2.3438720513,-0.8626036641,-0.3550253654
C,0,3.3666203096,-0.8591400859,-1.8934332613
B,0,0.5775307696,1.8375183636,-0.6936364219
O,0,1.7982376448,2.2242294384,-1.2693483357

C,0,1.9650421496,3.6394207221,-1.10894505
C,0,0.5740589094,4.1384022128,-0.6729964006
O,0,-0.11363341,2.9562591232,-0.2509382634
B,0,-2.0279079043,0.22207254,-0.7583981465
O,0,-2.5574851318,1.2369177185,-1.5484840404
C,0,-3.9825721374,1.1266533603,-1.5824785192
C,0,-4.317326806,0.0916013085,-0.4901082438
O,0,-3.0675997283,-0.5536990117,-0.219231814
C,0,1.2127539247,-2.9969335556,1.1104417665
C,0,2.3649499191,-2.672663973,0.1454138754
C,0,3.4946662631,-0.0663041984,0.8500914267
H,0,-0.0783117836,-0.9795456813,-2.0192535682
H,0,0.1357033627,0.2021495492,-2.1038411083
H,0,1.1378562915,-4.0753261637,1.2952482071
H,0,1.3857516917,-2.5095866568,2.0773467843
H,0,3.3317366359,-2.9447233958,0.5850006937
H,0,2.2571698538,-3.2541759031,-0.7784699489
H,0,2.7308130266,3.8301190821,-0.3451825385
H,0,2.3026684477,4.0803489257,-2.0523695979
H,0,0.6164175427,4.8555555452,0.1531738874
H,0,0.0209244421,4.5981876368,-1.5016198051
H,0,-4.4346190987,2.1056895213,-1.3918620491
H,0,-4.2970592024,0.7916391516,-2.5802361306
H,0,-4.6830585952,0.5680623753,0.4286215374
H,0,-5.056393416,-0.6494030665,-0.8140321602
H,0,-1.2759880681,2.7941992212,3.0925907592
H,0,-1.9284226856,1.3929068798,3.9714314348
H,0,0.8609998802,2.1316545969,3.9625604721
H,0,0.2708116765,0.5079158884,4.3736197697
H,0,-2.4993367856,-2.0631044391,1.6551462786
H,0,-1.6212502742,-3.4998054144,2.2824147715
H,0,-1.1373059904,-1.8488878502,2.7639606951
H,0,-2.0566188456,-3.3425160262,-0.9674872543
H,0,-0.4185696341,-3.784621578,-1.472103499
H,0,-1.1717325125,-4.6142967689,-0.0770793096
H,0,3.632258046,0.9732409108,0.5418445802
H,0,3.0323006325,-0.0597341372,1.838256773
H,0,4.4666694482,-0.5703257941,0.8784578039
H,0,3.4621442199,0.1772510932,-2.2266361215
H,0,4.3623150502,-1.2851559393,-1.7302265793
H,0,2.8522145924,-1.4242671859,-2.6752692968

Ir(dmpe)(BPin)$_3$(η^2-H$_2$) axial H$_2$
E(RB+HF-LYP) = -1788.73068328

Zero-point correction= 0.438508 (Hartree/Particle)
Thermal correction to Energy= 0.469795
Thermal correction to Enthalpy= 0.470739
Thermal correction to Gibbs Free Energy= 0.374074
Sum of electronic and zero-point Energies= -1788.292176
Sum of electronic and thermal Energies= -1788.260889
Sum of electronic and thermal Enthalpies= -1788.259945
Sum of electronic and thermal Free Energies= -1788.356610

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	294.801	112.233	203.449

C,0,2.2635846974,2.70917707,-1.7479508981
P,0,1.9223522527,1.5065246089,-0.3854427897
C,0,3.50921314,0.5046350044,-0.3085582933
C,0,3.294317879,-0.8207356306,0.4419003416
P,0,1.7682523708,-1.7107548525,-0.1757672469
C,0,1.539885396,-3.0486941719,1.071260827
Ir,0,0.0729132878,-0.043006033,-0.5239791707
B,0,-1.4782511907,-1.4637294529,-0.5182476673
O,0,-2.2442226676,-1.7740198229,-1.6442763968
C,0,-3.1160146582,-2.8686035788,-1.3471650955
C,0,-3.0030917494,-3.0496022488,0.1804647441
O,0,-1.8356503439,-2.3038103234,0.5438039891
C,0,2.0229476151,2.5933395293,1.1018459633
B,0,-0.3139122053,0.0965745252,1.5081617317
O,0,-1.5003451737,0.5182197755,2.1040113812
C,0,-1.338292085,0.5906372733,3.5207023076
C,0,-0.0002162559,-0.1237201431,3.7957947738
O,0,0.6329810079,-0.2001426885,2.5114924981
B,0,-1.3432510521,1.5289777865,-0.561868245
O,0,-2.6824050221,1.4386095347,-0.9188375084
C,0,-3.3290204187,2.6904779376,-0.6795060281
C,0,-2.1747643263,3.6888031661,-0.4538332316
O,0,-1.0221366015,2.8626293612,-0.2482075349
C,0,2.4050592736,-2.6612769047,-1.6355277419
H,0,0.4208412236,-0.1685692998,-2.3518638002
H,0,4.3122274631,1.0917595886,0.1524018901
H,0,3.8107301427,0.3092777252,-1.3453850628
H,0,4.1786425895,-1.4653025129,0.3683104631
H,0,3.1070579679,-0.6254936024,1.5031417458
H,0,-2.3318396638,4.3303367752,0.419969175

H,0,-2.0072344834,4.3335283924,-1.3270382613
H,0,-3.9728858993,2.6003322111,0.2045059498
H,0,-3.9572480216,2.952342048,-1.5375995697
H,0,-2.8821790726,-4.0965164821,0.4797694876
H,0,-3.8728747123,-2.6393056965,0.7092514713
H,0,-2.7813047923,-3.7600302797,-1.8949658423
H,0,-4.13377883,-2.6294713264,-1.672813706
H,0,1.4208610869,3.4031653262,-1.8004205662
H,0,3.187319249,3.2739177511,-1.5822822007
H,0,2.331504388,2.1776001397,-2.7012534074
H,0,1.1370586895,3.232424928,1.0955932276
H,0,1.993728184,1.9691852359,1.9974110679
H,0,2.9306060245,3.2059569582,1.1013986049
H,0,0.6735464923,-3.6514017286,0.7897216054
H,0,2.4270533729,-3.6855405927,1.1523167766
H,0,1.3263651474,-2.5786407231,2.0327373682
H,0,1.592102324,-3.2644366065,-2.0498474718
H,0,2.7361457594,-1.9672924235,-2.4129203842
H,0,3.2368534876,-3.320866607,-1.3651922876
H,0,-0.397161521,-0.0358366231,-2.2738703337
H,0,-1.3152633843,1.6436891508,3.8311834035
H,0,-2.1862280809,0.1051526232,4.0148700381
H,0,0.6429653205,0.4230887165,4.493586771
H,0,-0.1484270088,-1.1383958633,4.1865046514

dmpeBpin3η2H219
E(RB+HF-LYP) = -1788.73068328

Zero-point correction= 0.438508 (Hartree/Particle)
Thermal correction to Energy= 0.469795
Thermal correction to Enthalpy= 0.470739
Thermal correction to Gibbs Free Energy= 0.374074
Sum of electronic and zero-point Energies= -1788.292176
Sum of electronic and thermal Energies= -1788.260889
Sum of electronic and thermal Enthalpies= -1788.259945
Sum of electronic and thermal Free Energies= -1788.356610

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	294.801	112.233	203.449

C,0,2.2635846974,2.70917707,-1.7479508981
P,0,1.9223522527,1.5065246089,-0.3854427897
C,0,3.50921314,0.5046350044,-0.3085582933

C,0,3.294317879,-0.8207356306,0.4419003416
P,0,1.7682523708,-1.7107548525,-0.1757672469
C,0,1.539885396,-3.0486941719,1.071260827
Ir,0,0.0729132878,-0.043006033,-0.5239791707
B,0,-1.4782511907,-1.4637294529,-0.5182476673
O,0,-2.2442226676,-1.7740198229,-1.6442763968
C,0,-3.1160146582,-2.8686035788,-1.3471650955
C,0,-3.0030917494,-3.0496022488,0.1804647441
O,0,-1.8356503439,-2.3038103234,0.5438039891
C,0,2.0229476151,2.5933395293,1.1018459633
B,0,-0.3139122053,0.0965745252,1.5081617317
O,0,-1.5003451737,0.5182197755,2.1040113812
C,0,-1.338292085,0.5906372733,3.5207023076
C,0,-0.0002162559,-0.1237201431,3.7957947738
O,0,0.6329810079,-0.2001426885,2.5114924981
B,0,-1.3432510521,1.5289777865,-0.561868245
O,0,-2.6824050221,1.4386095347,-0.9188375084
C,0,-3.3290204187,2.6904779376,-0.6795060281
C,0,-2.1747643263,3.6888031661,-0.4538332316
O,0,-1.0221366015,2.8626293612,-0.2482075349
C,0,2.4050592736,-2.6612769047,-1.6355277419
H,0,0.4208412236,-0.1685692998,-2.3518638002
H,0,4.3122274631,1.0917595886,0.1524018901
H,0,3.8107301427,0.3092777252,-1.3453850628
H,0,4.1786425895,-1.4653025129,0.3683104631
H,0,3.1070579679,-0.6254936024,1.5031417458
H,0,-2.3318396638,4.3303367752,0.419969175
H,0,-2.0072344834,4.3335283924,-1.3270382613
H,0,-3.9728858993,2.6003322111,0.2045059498
H,0,-3.9572480216,2.952342048,-1.5375995697
H,0,-2.8821790726,-4.0965164821,0.4797694876
H,0,-3.8728747123,-2.6393056965,0.7092514713
H,0,-2.7813047923,-3.7600302797,-1.8949658423
H,0,-4.13377883,-2.6294713264,-1.672813706
H,0,1.4208610869,3.4031653262,-1.8004205662
H,0,3.187319249,3.2739177511,-1.5822822007
H,0,2.331504388,2.1776001397,-2.7012534074
H,0,1.1370586895,3.232424928,1.0955932276
H,0,1.993728184,1.9691852359,1.9974110679
H,0,2.9306060245,3.2059569582,1.1013986049
H,0,0.6735464923,-3.6514017286,0.7897216054
H,0,2.4270533729,-3.6855405927,1.1523167766
H,0,1.3263651474,-2.5786407231,2.0327373682
H,0,1.592102324,-3.2644366065,-2.0498474718

H,0,2.7361457594,-1.9672924235,-2.4129203842
H,0,3.2368534876,-3.320866607,-1.3651922876
H,0,-0.397161521,-0.0358366231,-2.2738703337
H,0,-1.3152633843,1.6436891508,3.8311834035
H,0,-2.1862280809,0.1051526232,4.0148700381
H,0,0.6429653205,0.4230887165,4.493586771
H,0,-0.1484270088,-1.1383958633,4.1865046514

dmpeBpin3H2rotTS
E(RB+HF-LYP) = -1788.72975859

Zero-point correction= 0.438165 (Hartree/Particle)
Thermal correction to Energy= 0.468791
Thermal correction to Enthalpy= 0.469735
Thermal correction to Gibbs Free Energy= 0.375094
Sum of electronic and zero-point Energies= -1788.291594
Sum of electronic and thermal Energies= -1788.260967
Sum of electronic and thermal Enthalpies= -1788.260023
Sum of electronic and thermal Free Energies= -1788.354665

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	294.171	110.427	199.190

C,0,1.6295710712,1.4257627731,-3.2722635071
P,0,1.7516811638,0.6954627073,-1.5782951755
C,0,2.7137208302,1.9956481183,-0.6885350432
C,0,2.9954513749,-0.692526472,-1.8050412119
C,0,2.9162348301,-1.7040789755,-0.6487060774
P,0,1.1432234248,-2.198742414,-0.3118677995
C,0,0.8456583558,-3.540103653,-1.5586306248
Ir,0,-0.182636691,-0.1960675422,-0.4578576442
B,0,-1.1786520339,1.6662344266,-0.483138757
O,0,-0.5703359353,2.8638849931,-0.8996857059
C,0,-1.5363456465,3.9221251241,-0.8734548879
C,0,-2.758018069,3.3129318203,-0.1542644044
O,0,-2.5043522538,1.9060914696,-0.1403593539
C,0,1.2754736598,-3.1672062184,1.2517264998
B,0,-1.7963688085,-0.9308162118,0.6825684226
O,0,-1.8476813797,-1.078620862,2.0710101734
C,0,-3.1650728112,-1.4858559787,2.4552685679
C,0,-3.8384885589,-1.9176188982,1.1352910999
O,0,-2.976097771,-1.4165826817,0.1094594724
B,0,0.5062904121,0.5017849244,1.3720890204

O,0,1.6402649727,-0.0070081734,2.0380993975
C,0,1.734769491,0.6000814311,3.3335752813
C,0,0.7831493782,1.8104260937,3.2570982413
O,0,-0.0229028813,1.5602294374,2.1054353447
H,0,-0.9806947127,-0.3695123105,-2.115189113
H,0,4.0096158884,-0.2887420568,-1.9077975956
H,0,2.7485927041,-1.1833222998,-2.7549739401
H,0,3.5380026108,-2.5849985991,-0.8494287996
H,0,3.2698755997,-1.2446403791,0.2805428617
H,0,-1.1224428182,4.7888145619,-0.3468284248
H,0,-1.7701493544,4.2258702752,-1.9026940834
H,0,-2.8488002911,3.6732106045,0.8783050515
H,0,-3.7014211812,3.5138345498,-0.6734297034
H,0,-3.1022550378,-2.2977816706,3.1883112051
H,0,-3.6823639333,-0.6391032207,2.9238601708
H,0,-3.9136834447,-3.0099311658,1.0464294545
H,0,-4.8414979595,-1.4953285606,1.0134385237
H,0,0.9814809335,2.3033668302,-3.2073720623
H,0,2.6061816846,1.7230764222,-3.6691288902
H,0,1.1678744746,0.7045945559,-3.9527026331
H,0,2.0538986425,2.8559488598,-0.5529856539
H,0,2.9987876883,1.6167126593,0.295629153
H,0,3.609184833,2.2939894137,-1.2437803293
H,0,0.2958697501,-3.5869769879,1.4949597869
H,0,2.0082471584,-3.9768688918,1.168930503
H,0,1.5622436862,-2.4785375844,2.0478073469
H,0,-0.1614529897,-3.94170109,-1.4142394666
H,0,0.8983944461,-3.1252230225,-2.5690970146
H,0,1.5716213677,-4.3551575643,-1.4671851926
H,0,-1.203632041,-1.0606828925,-1.7215121579
H,0,1.3266727573,2.7554123381,3.1226762866
H,0,0.1455691108,1.9042060481,4.1421689549
H,0,2.7737748332,0.8818538026,3.5359489706
H,0,1.4178326765,-0.1234664262,4.0951683621

Ir(dmpe)(BPin)$_3$(H$_2$) axial Variational TS for loss of H$_2$
E(RB+HF-LYP) = -1788.71478555

Zero-point correction= 0.434422 (Hartree/Particle)
Thermal correction to Energy= 0.466920
Thermal correction to Enthalpy= 0.467864
Thermal correction to Gibbs Free Energy= 0.369153
Sum of electronic and zero-point Energies= -1788.280364
Sum of electronic and thermal Energies= -1788.247866

Sum of electronic and thermal Enthalpies= -1788.246921
Sum of electronic and thermal Free Energies= -1788.345632

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	292.997	114.903	207.754

C,0,1.8446262685,-3.0828545762,0.1593887434
P,0,1.810680153,-1.4756047897,-0.7436307849
Ir,0,0.0165384058,0.090905304,-0.3576509368
B,0,-1.5227176251,-1.3178548049,-0.5715717202
O,0,-1.4625007019,-2.6672619558,-0.1867465285
C,0,-2.7454573207,-3.2699692447,-0.3972478265
C,0,-3.4774516853,-2.2890370926,-1.3314267071
O,0,-2.7391747964,-1.0679624073,-1.2124447582
C,0,2.2137143541,-2.002157527,-2.4774816463
C,0,3.3895828492,-0.6419163967,-0.1769479968
C,0,3.427961773,0.8315427823,-0.6151367817
P,0,1.8117868992,1.7041855036,-0.2092281357
C,0,2.1560456902,2.5148762034,1.4152180677
C,0,1.838328554,3.1467013501,-1.3684962125
B,0,-0.0452313694,-0.387438912,1.5924662677
O,0,1.120782011,-0.467368202,2.3895462989
C,0,0.7233984162,-0.6884121816,3.7506697777
C,0,-0.7484576133,-1.1347496834,3.6481016432
O,0,-1.1607687204,-0.7093749808,2.3501454753
B,0,-1.5004995694,1.5098843299,-0.1064549795
O,0,-2.2980864785,1.8228585489,0.9895155615
C,0,-3.1469995466,2.9265164741,0.6585096769
C,0,-3.0160725515,3.072127221,-0.8693585484
O,0,-1.8193861188,2.3508020074,-1.1889190422
H,0,4.2731571401,-1.1846566661,-0.5341484439
H,0,3.3707559131,-0.7056394235,0.9162721301
H,0,4.2766175263,1.3570567841,-0.161676472
H,0,3.5548124627,0.8994662196,-1.7031136533
H,0,-2.9207857811,4.1135544129,-1.1954363295
H,0,-3.8640464784,2.6194442525,-1.3992278908
H,0,-2.8012672274,3.8245029556,1.18943734
H,0,-4.1717092389,2.7132295637,0.9801786385
H,0,-4.5196012001,-2.1201585803,-1.0415246874
H,0,-3.4613348499,-2.6233925197,-2.377689495
H,0,-3.2567707308,-3.3767735701,0.5682010463
H,0,-2.6209671841,-4.2665462525,-0.8345562249
H,0,-1.3863650098,-0.6741760636,4.4092727898

H,0,-0.8520820519,-2.2255354338,3.7229921666
H,0,0.829468976,0.2482074207,4.3139920172
H,0,1.372115034,-1.4420416237,4.2092727296
H,0,2.7317046046,-3.6773171606,-0.0828465264
H,0,1.8251225835,-2.8703765867,1.2305936208
H,0,0.935071547,-3.6326401305,-0.0918556246
H,0,3.1211506569,-2.6141422954,-2.5165810722
H,0,1.3765433904,-2.5819404122,-2.876403499
H,0,2.3487088114,-1.124175114,-3.1154900763
H,0,2.743027548,3.7531447647,-1.2539861912
H,0,1.7728132462,2.7872510003,-2.3990698624
H,0,0.9567534565,3.7639761591,-1.1776262062
H,0,3.0669602937,3.1217669025,1.3820453181
H,0,1.3066157591,3.1518472038,1.6775400813
H,0,2.2464501998,1.7371740195,2.1757529583
H,0,-0.3877472589,0.9071199399,-3.2160256608
H,0,-0.0156290325,0.2808499997,-3.0420140128

Ir(dmpe)(BPin)$_2$(H) equatorial H
E(RB+HF-LYP) = -1534.11454072

Zero-point correction= 0.359756 (Hartree/Particle)
Thermal correction to Energy= 0.385069
Thermal correction to Enthalpy= 0.386013
Thermal correction to Gibbs Free Energy= 0.302825
Sum of electronic and zero-point Energies= -1533.754785
Sum of electronic and thermal Energies= -1533.729472
Sum of electronic and thermal Enthalpies= -1533.728527
Sum of electronic and thermal Free Energies= -1533.811716

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	241.634	90.546	175.085

C,0,-3.0908270668,-0.2034950365,1.6085086627
C,0,-2.1125533729,-0.8864667766,2.5799144256
P,0,-0.3236234788,-0.6040937708,2.067610353
Ir,0,-0.2650876174,-0.4499660251,-0.3437365977
B,0,-0.1840587006,1.5485975777,-0.4002988167
O,0,0.8332082568,2.3164613763,-0.9505569214
C,0,0.4373082141,3.6888641044,-0.9345790761
C,0,-0.728894896,3.7416612346,0.0720774595
O,0,-1.1674407162,2.3793709901,0.1762893662
P,0,-2.6244103953,-0.5512189594,-0.1740050796

B,0,-0.1794673097,-0.393747027,-2.4248149469
O,0,-0.6900778638,0.5744651517,-3.2964764983
C,0,-0.2976614081,0.245732961,-4.6352188185
C,0,0.1482029132,-1.2261844841,-4.5517755781
O,0,0.3767077606,-1.4490242551,-3.1551437715
H,0,1.3570864299,-0.3767728445,-0.4399983812
C,0,-3.7013023135,0.6087963623,-1.1184174066
C,0,-3.4419015773,-2.1863648087,-0.498800391
H,0,-4.1245871196,-0.5089069842,1.8107442649
H,0,-3.0364617041,0.8849898502,1.7198320502
C,0,0.1510634362,0.9090674623,3.019785358
C,0,0.5620032129,-1.9312465997,3.0097266455
H,0,-2.2796579768,-0.5506940884,3.6102814901
H,0,-2.2702924111,-1.9726008907,2.5705928682
H,0,-1.5576134904,4.3740538143,-0.2623319461
H,0,-0.4038897167,4.0929960735,1.0609309444
H,0,0.120189174,3.9856935251,-1.9427526467
H,0,1.2842520929,4.3165882844,-0.6390932837
H,0,1.0668000611,-1.4275998554,-5.1124961164
H,0,-0.6302002917,-1.9139804942,-4.9101203809
H,0,0.5222868283,0.9065710756,-4.9456579557
H,0,-1.1405938965,0.4005488936,-5.3173710631
H,0,-4.7588977277,0.4876075889,-0.8616551459
H,0,-3.3747188269,1.6266455777,-0.8967106739
H,0,-3.5568559624,0.4308873887,-2.1868664146
H,0,-4.5147391619,-2.1540598826,-0.2809132468
H,0,-3.3002046203,-2.4550054918,-1.5493237247
H,0,-2.9785372206,-2.9668214462,0.1117355572
H,0,-0.0279125064,0.7919713731,4.0937773395
H,0,1.2115658525,1.113501586,2.8487670509
H,0,-0.4239778106,1.7557618975,2.6380877594
H,0,0.3121085519,-1.9171245893,4.0759691057
H,0,0.3072350908,-2.9109669289,2.5956791763
H,0,1.6394632846,-1.78683091,2.8923840049

IrDMPE_Bpin2_H
E(RB+HF-LYP) = -1534.10362895

Zero-point correction= 0.359390 (Hartree/Particle)
Thermal correction to Energy= 0.385038
Thermal correction to Enthalpy= 0.385982
Thermal correction to Gibbs Free Energy= 0.301400
Sum of electronic and zero-point Energies= -1533.744239
Sum of electronic and thermal Energies= -1533.718591

Sum of electronic and thermal Enthalpies= -1533.717647
Sum of electronic and thermal Free Energies= -1533.802229

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	241.615	91.251	178.017

C,0,-2.8648647651,0.4645886701,1.9304694162
P,0,-2.4166779648,0.0456416457,0.1522277106
Ir,0,-0.0274203529,-0.0453603326,0.022839083
B,0,2.0554028506,-0.0310732189,-0.094549144
O,0,2.8126376785,-1.1597712614,0.2557608872
C,0,4.1728548822,-0.9422125286,-0.1444136196
C,0,4.2593144817,0.5779431528,-0.3774916502
O,0,2.8969135319,0.9970930337,-0.5188233936
C,0,-1.9402784214,-0.2551487071,2.9276640442
P,0,-0.1353950232,-0.0988771989,2.4191850635
B,0,0.0879854698,0.1161112745,-2.0540531624
O,0,-0.3450070973,1.193319828,-2.8338373821
C,0,0.0402265426,0.9667317549,-4.1952856667
C,0,0.4001699879,-0.5302544997,-4.2485847001
O,0,0.5931775777,-0.8980597354,-2.8771703984
H,0,0.0536145534,1.4925392966,-0.0092783509
C,0,-3.3236315487,1.3384884024,-0.8043821065
C,0,-3.4458652578,-1.4635766875,-0.1800856203
H,0,-3.9183133872,0.2369022436,2.1330585072
H,0,-2.7461185075,1.5506934819,2.0263398021
C,0,0.4125874027,1.4339551444,3.2994377424
C,0,0.6782529759,-1.4240819422,3.4222831773
H,0,-2.0957311505,0.1153972158,3.9479815062
H,0,-2.1662552947,-1.3289951885,2.9403636723
H,0,-0.7857722575,1.232347869,-4.8639854237
H,0,0.89893424,1.6054251227,-4.439717054
H,0,-0.410017914,-1.1352256797,-4.6782274751
H,0,1.3141974109,-0.7309794192,-4.8171623802
H,0,4.8509711633,-1.2963568572,0.6393248466
H,0,4.3767673158,-1.5116293263,-1.0604021769
H,0,4.7150406308,1.1006812639,0.4747116824
H,0,4.822156964,0.840612544,-1.2792392193
H,0,-3.1645880762,1.1613006701,-1.8706534427
H,0,-4.3960528788,1.3431605121,-0.5829201495
H,0,-2.8958104325,2.3165918506,-0.5703218491
H,0,-3.3103581366,-1.7631979634,-1.2231132735
H,0,-3.1080063168,-2.2903158752,0.4514907394

H,0,-4.5104456844,-1.2850467482,0.005405727
H,0,1.7556345075,-1.3817245473,3.2428802606
H,0,0.4800648007,-1.3190604713,4.4942686853
H,0,0.3252786016,-2.40271384,3.0850101844
H,0,1.4786126278,1.585702418,3.1107724469
H,0,-0.1213785153,2.29647137,2.8923843205
H,0,0.2387249204,1.3742572119,4.3791351363

IrDMPE_Bpin2_H_n2Ph
E(RB+HF-LYP) = -1766.36443853

Zero-point correction= 0.461251 (Hartree/Particle)
Thermal correction to Energy= 0.492047
Thermal correction to Enthalpy= 0.492991
Thermal correction to Gibbs Free Energy= 0.396899
Sum of electronic and zero-point Energies= -1765.903187
Sum of electronic and thermal Energies= -1765.872392
Sum of electronic and thermal Enthalpies= -1765.871448
Sum of electronic and thermal Free Energies= -1765.967539

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	308.764	111.446	202.242

C,0,-3.3742302775,2.0381236017,-0.6916854346
P,0,-2.4603352407,0.4392279992,-0.8190744037
C,0,-2.7603394604,-0.008435641,-2.5976166904
C,0,-3.6030530002,-0.7445665267,0.0984236521
C,0,-2.8672691655,-2.0224602725,0.536331256
P,0,-1.225867761,-1.6052309456,1.3495980118
C,0,-0.3692589608,-3.2395167185,1.4416162101
Ir,0,-0.3143342984,0.3155361918,0.2407810248
B,0,0.4540203836,2.1071845655,-0.5212724195
O,0,1.6532516807,2.2135566889,-1.2442967219
C,0,1.8222712759,3.5650687033,-1.6895857863
C,0,0.7715814016,4.3628859025,-0.894027942
O,0,-0.1359992227,3.3697739815,-0.403099618
B,0,1.4056839768,0.3458902778,1.4365589429
O,0,1.8255951955,1.41228505,2.2376550277
C,0,2.963018415,1.0131627932,3.0086711899
C,0,3.4138605001,-0.3144654564,2.3707456266
O,0,2.2865115681,-0.7349689737,1.5919588314
C,0,-1.7084473963,-1.3430515981,3.1180288915
H,0,-0.8503568916,1.2556173211,1.350952472

H,0,-4.482654819,-0.9826522303,-0.5114982343
H,0,-3.9633378114,-0.2007676784,0.980065662
H,0,-3.4943414097,-2.6310573374,1.1992684626
H,0,-2.632891715,-2.6396672196,-0.3398887098
H,0,0.2302333681,5.0890128988,-1.5102114995
H,0,1.2172072979,4.8967251957,-0.0448454031
H,0,1.6485179094,3.616564405,-2.773013446
H,0,2.8477232846,3.8940916663,-1.4912767627
H,0,3.6618861542,-1.0838891202,3.1097976963
H,0,4.2811665506,-0.1818618835,1.7106234168
H,0,2.6649068878,0.8868657404,4.0584801299
H,0,3.732468602,1.7911872657,2.9647486769
H,0,-2.8331563128,2.7981155933,-1.2600113816
H,0,-4.4025645733,1.9582379065,-1.0596691979
H,0,-3.3803402529,2.357500317,0.353142478
H,0,-2.1913787909,0.6734926082,-3.2361076221
H,0,-2.4064547146,-1.0241014103,-2.7949243032
H,0,-3.8208775148,0.0565776555,-2.8635837542
H,0,0.5572651811,-3.1015924919,2.0050003154
H,0,-0.9855945657,-4.0050166425,1.9249144321
H,0,-0.0963017008,-3.5649490408,0.4350317264
H,0,-0.804516855,-1.1565110927,3.7040176748
H,0,-2.3435285998,-0.4571641804,3.1979344926
H,0,-2.2355792828,-2.2086339882,3.5333676012
H,0,0.3627104031,-0.3301119262,-1.742551174
C,0,1.0322915297,-1.1997071099,-1.8614929737
C,0,0.5106937504,-2.4576286501,-2.1807166905
C,0,1.3736007467,-3.5248529941,-2.4402539736
C,0,2.7560446074,-3.3302116799,-2.3816660963
C,0,3.274572124,-2.0698262137,-2.0741812925
C,0,2.4151403645,-1.0014475583,-1.8129254753
H,0,-0.5642668068,-2.6043746706,-2.238996077
H,0,0.9712311443,-4.5020864599,-2.6931875586
H,0,3.4283449176,-4.1596559607,-2.5840499546
H,0,4.3501689152,-1.9212324992,-2.0366284842
H,0,2.7948437007,-0.0138769949,-1.5770543037

IrDMPE_BPin2_H_PhH_CHAct_TS
E(RB+HF-LYP) = -1766.33811780

Zero-point correction= 0.457836 (Hartree/Particle)
Thermal correction to Energy= 0.488333
Thermal correction to Enthalpy= 0.489277
Thermal correction to Gibbs Free Energy= 0.396013

Sum of electronic and zero-point Energies= -1765.880282
Sum of electronic and thermal Energies= -1765.849785
Sum of electronic and thermal Enthalpies= -1765.848841
Sum of electronic and thermal Free Energies= -1765.942105

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	306.434	112.490	196.292

C,0,1.5420154597,-0.7795153375,-2.4609146449
C,0,0.4770124936,-1.1147522095,-1.6013719013
C,0,-0.372300773,-2.1516929149,-2.0354376221
C,0,-0.2118313725,-2.7768166649,-3.2760220027
C,0,0.8292112628,-2.3987879812,-4.1239361295
C,0,1.7091706596,-1.4018429138,-3.7015189706
Ir,0,-0.0112349356,0.1014950164,0.2310148249
B,0,1.4791835412,1.5176846634,-0.1768601656
O,0,1.262117465,2.8996590083,-0.2662047501
C,0,2.5214601882,3.5744280976,-0.3732600441
C,0,3.5368941426,2.4531244628,-0.673351253
O,0,2.8315619865,1.2427405117,-0.3842354531
P,0,-1.8808656913,-1.2374935909,1.0629337171
C,0,-1.9322258376,-3.078182102,1.2548103844
P,0,-1.7364684122,1.2848430421,-0.9631732499
C,0,-1.8149087222,1.132236249,-2.8001724123
B,0,1.1286100225,-0.4061450756,1.9340629166
O,0,0.9562430713,-1.5990468809,2.6488134469
C,0,1.752951371,-1.5472668022,3.8415097079
C,0,2.6855660352,-0.3395765636,3.6237937173
O,0,2.0761578911,0.392659501,2.555784125
C,0,-3.3647494919,-0.8565924436,-0.0152622596
C,0,-3.4031745031,0.6362462882,-0.3831375229
C,0,-2.458842511,-0.7209577516,2.742658665
C,0,-1.9147368007,3.0987980669,-0.7012598145
H,0,-2.7018721834,1.6303437274,-3.204666283
H,0,-0.9176925116,1.5885118972,-3.2261457182
H,0,-1.8167857913,0.0779707765,-3.0848174311
H,0,-0.9789525812,3.5800397003,-0.9907194941
H,0,-2.0643619534,3.2877835696,0.3646888909
H,0,-2.7538534659,3.5105190218,-1.2712386245
H,0,-3.6688741953,1.2307677077,0.4988815786
H,0,-4.1681328996,0.8347971688,-1.1427902544
H,0,-4.2968991926,-1.1605249693,0.4764971475
H,0,-3.2608333547,-1.4649251333,-0.9208230621

H,0,-2.6305944316,0.3576790664,2.7568910346
H,0,-3.3727727841,-1.2445074806,3.0426276922
H,0,-1.6610872978,-0.9438673427,3.4553235397
H,0,-2.9039695866,-3.4187132215,1.6277494786
H,0,-1.1509106424,-3.3492034832,1.9695710531
H,0,-1.7138275817,-3.5792242412,0.3097063047
H,0,-0.3873604862,1.1837287588,1.3906245382
H,0,2.2932671573,-2.4910580968,3.9640683788
H,0,1.0953138358,-1.4104960774,4.7102960523
H,0,3.6946857877,-0.6468328583,3.3209811379
H,0,2.7704250719,0.3000910226,4.5079933049
H,0,2.2601088492,-0.0330149914,-2.1432656176
H,0,2.5410515457,-1.1069929948,-4.3372044668
H,0,0.9609307469,-2.8831250582,-5.0876411692
H,0,-0.9014808594,-3.5637454687,-3.5735373272
H,0,-1.1897642591,-2.4789754732,-1.4038661007
H,0,4.4339688387,2.5137602506,-0.0487272104
H,0,3.8509872681,2.4484778207,-1.7258073517
H,0,2.7376596944,4.0848501223,0.5736627644
H,0,2.4716456343,4.3285369465,-1.1663429504
H,0,1.0184024836,-1.1269006318,-0.0485584519

IrDMPE_Bpin2_n2BpinH_Ph_goodgsC
E(RB+HF-LYP) = -2019.76524937

Zero-point correction= 0.524029 (Hartree/Particle)
Thermal correction to Energy= 0.559180
Thermal correction to Enthalpy= 0.560124
Thermal correction to Gibbs Free Energy= 0.456708
Sum of electronic and zero-point Energies= -2019.241220
Sum of electronic and thermal Energies= -2019.206069
Sum of electronic and thermal Enthalpies= -2019.205125
Sum of electronic and thermal Free Energies= -2019.308541

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	350.891	129.482	217.657

C,0,-4.5085209495,0.5984562211,-0.7243304511
C,0,-3.2012559851,0.6296480109,-0.2246578457
C,0,-2.223509312,-0.3221890556,-0.5817575985
C,0,-2.647496307,-1.2865601803,-1.5235440866
C,0,-3.9486257811,-1.3281495674,-2.0354202596
C,0,-4.8967691432,-0.3888314175,-1.6290528298

Ir,0,-0.1020143753,-0.2511605662,0.0441444351
B,0,-0.2755411531,1.7952799817,-0.326213911
O,0,-0.6908626553,2.7400208556,0.6244987775
C,0,-0.8674206802,4.0053652268,-0.0297902913
C,0,-0.2061831923,3.8175463653,-1.4100102687
O,0,-0.080987357,2.4005018847,-1.5572515772
P,0,-0.5779562199,0.0262224958,2.3383165355
C,0,-2.2937592455,0.4140686399,2.8988417457
P,0,-0.0652771697,-2.6817878967,0.6515663279
C,0,-1.0701241291,-3.9865110927,-0.1912994303
B,0,1.9147247177,0.2317284044,0.6604182226
O,0,2.4229380254,1.5259878746,0.6728863926
C,0,3.8016281614,1.5026532947,1.0517488901
C,0,4.0149637455,0.0914607899,1.6349649548
O,0,2.8585957994,-0.6480274909,1.2120096724
B,0,1.3243950285,-0.6920257931,-1.5339238898
O,0,2.2477203982,0.1665563103,-2.1156751461
C,0,3.007858877,-0.5659300966,-3.0813844479
C,0,2.7321906919,-2.0436197458,-2.74585903
O,0,1.5234448275,-2.007319147,-1.9763548903
C,0,-0.2196478577,-1.5798857209,3.2131264032
C,0,-0.7389217342,-2.7664552071,2.3926564785
C,0,0.390028253,1.2533269974,3.3134334016
C,0,1.5531196164,-3.5602534327,0.8259511055
H,0,4.0584026455,0.0956495956,2.7321497566
H,0,4.9206117262,-0.3960898349,1.2602601542
H,0,4.0000010501,2.2987111233,1.7769909288
H,0,4.420774359,1.6819402436,0.1641186974
H,0,3.534423585,-2.4842813158,-2.1392088295
H,0,2.5833081113,-2.6670203507,-3.6326782754
H,0,4.0657864195,-0.2977902395,-2.9991885828
H,0,2.6597458556,-0.299717058,-4.0874475764
H,0,-0.3995519108,4.7970786442,0.5644787928
H,0,-1.940795172,4.2198268791,-0.1120430105
H,0,0.7912247379,4.2730520518,-1.4530931323
H,0,-0.8094502244,4.2216680168,-2.2291029832
H,0,-0.0249372923,-0.309697713,-1.6232626274
H,0,-2.9360034466,1.4428526297,0.4431937472
H,0,-5.2205276405,1.3597473488,-0.4109282856
H,0,-1.9378136209,-2.0211465734,-1.8927578451
H,0,-4.2155857506,-2.0929437801,-2.762271742
H,0,-5.9096833815,-0.4156058818,-2.0222935492
H,0,-0.4696782452,-3.7201235955,2.8613438482
H,0,-1.8326660073,-2.7344669868,2.3216943644

H,0,0.8693855407,-1.6409810291,3.3175260771
H,0,-0.6511744962,-1.560836324,4.2205969997
H,0,0.0224732849,1.3009229003,4.343215481
H,0,1.4457946092,0.9776013137,3.320085887
H,0,0.2844319762,2.2245585898,2.8277348821
H,0,-2.3582514821,0.3005677749,3.985816684
H,0,-2.5305343739,1.4457470635,2.6327989784
H,0,-3.016878335,-0.2400634074,2.4099993575
H,0,1.4267434519,-4.5288289298,1.3214088918
H,0,1.9660926903,-3.7107947271,-0.1730747613
H,0,2.2472379902,-2.9297714317,1.3831172939
H,0,-0.9996118761,-4.9371628865,0.3476928654
H,0,-2.1146042344,-3.6755429927,-0.2508402395
H,0,-0.6920214385,-4.1258350597,-1.2074356363

IrDMPE_Bpin2_Ph_H2_TSlossH2
E(RB+HF-LYP) = -1766.31805399

Zero-point correction= 0.454522 (Hartree/Particle)
Thermal correction to Energy= 0.486964
Thermal correction to Enthalpy= 0.487908
Thermal correction to Gibbs Free Energy= 0.390236
Sum of electronic and zero-point Energies= -1765.863532
Sum of electronic and thermal Energies= -1765.831090
Sum of electronic and thermal Enthalpies= -1765.830146
Sum of electronic and thermal Free Energies= -1765.927818

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	305.574	117.466	205.568

C,0,0.3765703776,-2.2196092172,4.0295738812
C,0,-0.8595199694,-1.7477847153,3.5840957291
C,0,-0.9804021337,-1.0706019669,2.3683554896
C,0,0.139296253,-0.8353678842,1.5474750971
C,0,1.3763359362,-1.3201128436,2.0140822855
C,0,1.4974751794,-1.9989788375,3.2327599694
Ir,0,-0.0040846225,0.1520972388,-0.2351437242
P,0,1.8012694302,1.7509938514,0.1958612013
C,0,2.5008916861,1.985065517,1.892732493
B,0,-1.5373703099,-1.114326778,-0.8577451865
O,0,-1.8222244933,-2.4149303182,-0.4485449074
C,0,-3.0236905375,-2.8556982343,-1.0929068345
C,0,-3.2328284433,-1.8522525943,-2.2429465362

O,0,-2.410185567,-0.732629748,-1.8884812745
B,0,-1.563310143,1.4159257935,0.3252128761
O,0,-1.7317923175,2.5823625847,-0.4471761437
C,0,-3.0150260297,3.1507879974,-0.1469447539
C,0,-3.4071348023,2.4962399003,1.1893247306
O,0,-2.5841931353,1.3255776036,1.2662227164
P,0,1.740739464,-1.0899277898,-1.3819093447
C,0,3.4055310061,-0.2990684778,-1.007814814
C,0,3.2819994181,1.2271255812,-0.8504300066
C,0,1.6372220019,-0.9399868936,-3.2269262459
C,0,2.0653685539,-2.8958010762,-1.1691914496
C,0,1.5861291799,3.5067247701,-0.3476808061
H,0,3.4041477766,2.603417043,1.874152438
H,0,1.7426633719,2.4739342561,2.511025191
H,0,2.7196153465,1.0171366594,2.3463529546
H,0,0.7862247069,3.9609896238,0.2411293173
H,0,1.2764500618,3.5320526197,-1.3953036247
H,0,2.5071198395,4.0866038631,-0.2259955255
H,0,3.1242330868,1.6868545579,-1.8340796626
H,0,4.2076324434,1.6551916029,-0.44803905
H,0,4.1341657891,-0.5509904443,-1.7880832583
H,0,3.7691810767,-0.7496192535,-0.0774015314
H,0,1.5680208597,0.112854119,-3.5137220537
H,0,2.5037094071,-1.3907724847,-3.7219434422
H,0,0.7262380298,-1.4367338601,-3.571384857
H,0,2.9463087138,-3.2261253742,-1.7293234949
H,0,1.1852193175,-3.4446376648,-1.5144255522
H,0,2.1966172331,-3.1166428486,-0.1077315357
H,0,-0.3595517941,2.1877590316,-3.3511712688
H,0,-3.8503036987,-2.8326369178,-0.3710673994
H,0,-2.8997793108,-3.886737625,-1.4399786915
H,0,-4.2732294671,-1.5276199252,-2.3461175121
H,0,-2.9023093623,-2.2562515559,-3.2095583382
H,0,-1.9542241907,-0.7128790739,2.0646368151
H,0,-1.7510855963,-1.9070311961,4.1864903308
H,0,0.4630592815,-2.7472107933,4.9752744889
H,0,2.47624961,-2.3534613868,3.5493120214
H,0,2.2784269035,-1.1691352084,1.4292196445
H,0,-4.4621529727,2.2079108042,1.2319998875
H,0,-3.1918985827,3.1470710929,2.047131065
H,0,-3.7194328652,2.9001742425,-0.9503019368
H,0,-2.9318311459,4.2407323126,-0.0850611469
H,0,-0.7338410334,2.2932032659,-2.7140963019

IrDMPE_Bpin2_Ph
E(RB+HF-LYP) = -1765.13849868

Zero-point correction=	0.441653 (Hartree/Particle)
Thermal correction to Energy=	0.472381
Thermal correction to Enthalpy=	0.473325
Thermal correction to Gibbs Free Energy=	0.377284
Sum of electronic and zero-point Energies=	-1764.696845
Sum of electronic and thermal Energies=	-1764.666118
Sum of electronic and thermal Enthalpies=	-1764.665174
Sum of electronic and thermal Free Energies=	-1764.761214

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	296.423	110.797	202.134

C,0,-0.899171589,-1.2979418575,3.7409484584
C,0,-1.0078541597,-0.7643931448,2.4545616874
C,0,0.1179622943,-0.6433362758,1.6177390545
C,0,1.3464998803,-1.0880376993,2.1417556892
C,0,1.4552103345,-1.6230634482,3.4310682953
C,0,0.3288454678,-1.732894453,4.2431185358
Ir,0,-0.0057083248,0.1287077518,-0.26839179
B,0,-1.5517687629,-1.1754045996,-0.7644865066
O,0,-2.2923445192,-0.9651471061,-1.9389897408
C,0,-3.1657188525,-2.08335238,-2.1466906002
C,0,-3.1336550744,-2.8454591571,-0.8073665422
O,0,-1.9722844484,-2.3433589398,-0.1361161616
B,0,-1.550766814,1.4711937757,0.1270114247
O,0,-2.6070369634,1.4698680358,1.0338918395
C,0,-3.4007318635,2.6469495986,0.839041511
C,0,-2.9480716236,3.1878489175,-0.5289740963
O,0,-1.6682489103,2.5740509056,-0.7385505275
P,0,1.7396577681,-1.2469715785,-1.2518019456
C,0,1.6416769351,-1.2939905279,-3.1030219161
P,0,1.8048081884,1.7566752875,-0.0137668916
C,0,1.5911486331,3.4310594633,-0.7702228038
C,0,2.0653594555,-3.0197356328,-0.8455340758
C,0,3.4062592756,-0.4242930494,-0.9645342661
C,0,3.2886560002,1.1100933721,-0.9849019688
C,0,2.4984988472,2.1893096314,1.6463958189
H,0,3.4114127753,2.7877866091,1.5612711228
H,0,1.7441488218,2.7610179893,2.1944083474
H,0,2.7002002404,1.281066583,2.2172388098

H,0,0.8008105902,3.9611722996,-0.2347481962
H,0,1.2637238543,3.3213897394,-1.8072318374
H,0,2.5166568395,4.0153922635,-0.7387334509
H,0,3.1387003249,1.4545312559,-2.015750346
H,0,4.2138339213,1.5783330219,-0.6288762678
H,0,4.1361218526,-0.7678885782,-1.7077860148
H,0,3.7660451087,-0.7633932696,0.0133548511
H,0,1.5981065883,-0.2760558193,-3.5011464181
H,0,2.499288051,-1.8124370105,-3.5443524691
H,0,0.7201172374,-1.803722016,-3.3961810593
H,0,2.9592120867,-3.4010169244,-1.3501697676
H,0,1.1966851935,-3.6091333372,-1.1509222326
H,0,2.1757987414,-3.1272085788,0.2357556407
H,0,-4.0219472159,-2.6410657813,-0.1957660968
H,0,-3.0469868178,-3.9297103763,-0.9334644036
H,0,-4.1656957739,-1.726440169,-2.4137954278
H,0,-2.7865962174,-2.6928985428,-2.9783378883
H,0,-1.9758049667,-0.4352147997,2.1038928306
H,0,-1.7943319635,-1.3744319754,4.3541338711
H,0,0.4048492815,-2.1483085955,5.2440789859
H,0,2.4277238097,-1.9530281543,3.7904851385
H,0,2.2499085295,-1.0182807248,1.5442644219
H,0,-4.4628291639,2.3837126138,0.8661488184
H,0,-3.2001165297,3.3578972009,1.6515217203
H,0,-3.6299065428,2.8893585029,-1.335598009
H,0,-2.8440641452,4.2776948664,-0.5487988431

IrDMPE_Bpin_H2_PhH_CHActTS
E(RB+HF-LYP) = -1512.92216087

Zero-point correction= 0.395459 (Hartree/Particle)
Thermal correction to Energy= 0.420876
Thermal correction to Enthalpy= 0.421821
Thermal correction to Gibbs Free Energy= 0.339893
Sum of electronic and zero-point Energies= -1512.526702
Sum of electronic and thermal Energies= -1512.501284
Sum of electronic and thermal Enthalpies= -1512.500340
Sum of electronic and thermal Free Energies= -1512.582268

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	264.104	94.985	172.430

C,0,2.3803112119,-3.6466652298,0.3265114665

C,0,2.0628586366,-2.3285888691,-0.0100310435
C,0,0.8986579449,-1.7004213235,0.4774622658
C,0,0.0999251664,-2.4499140048,1.3626978807
C,0,0.4110370725,-3.7710334412,1.700681502
C,0,1.55264979,-4.3800179977,1.1790964848
Ir,0,0.2756931128,0.2695282191,-0.3609733101
B,0,1.4603895874,1.8340878865,0.4043050326
O,0,2.7278334372,2.1779810189,-0.0369176457
C,0,3.2396734665,3.2407999791,0.7743452391
C,0,2.0202063938,3.7398717019,1.57647638
O,0,1.0451122109,2.6985653133,1.4252165279
H,0,1.4912438798,0.0711003283,-1.3987024314
P,0,-1.6413619117,0.8212615051,0.9608915831
C,0,-2.2392357714,2.559924656,0.7799479953
P,0,-1.3106990988,-0.7660436386,-1.8241801035
C,0,-1.3364411155,-0.2691753712,-3.5996099563
C,0,-1.7606805586,0.6058923826,2.7943224437
C,0,-3.0833442457,-0.1838012012,0.3068999181
C,0,-3.0246396135,-0.2854072048,-1.2281503008
C,0,-1.3813239649,-2.6074653675,-1.9312949733
H,0,-2.2046800638,-2.9415189086,-2.5707084966
H,0,-0.4342354752,-2.9729073481,-2.3368266631
H,0,-1.4923261242,-3.030714758,-0.9308388877
H,0,-0.4041967994,-0.5957132484,-4.0679532753
H,0,-1.3815774895,0.8204602164,-3.6645830754
H,0,-2.1838260298,-0.7075236283,-4.136713088
H,0,-3.2449951994,0.6907528901,-1.6763868153
H,0,-3.7731851627,-0.9902511553,-1.6082259458
H,0,-4.0396763981,0.2421704737,0.6332280355
H,0,-3.0026900518,-1.1824826794,0.7536456849
H,0,-2.4030343624,2.778640808,-0.2780324678
H,0,-3.163124211,2.7380819908,1.3403031961
H,0,-1.4470123503,3.2184248149,1.1426354336
H,0,-2.7613930728,0.8466190251,3.1682010721
H,0,-1.0333557322,1.2796812989,3.255351268
H,0,-1.5046818805,-0.41639839,3.0807840575
H,0,-0.0514914741,1.5893422672,-1.2686032351
H,0,2.2379094286,3.8899877421,2.6388649078
H,0,1.6144560499,4.6762593913,1.1718433194
H,0,4.030561491,2.8483773655,1.426373015
H,0,3.6750165565,4.0157054384,0.1354062759
H,0,2.725389424,-1.7710043031,-0.6639267415
H,0,3.2829247149,-4.0993113098,-0.0772837057
H,0,1.8006300804,-5.4043981437,1.4431111158

H,0,-0.239911886,-4.3206994898,2.3769585622
H,0,-0.7935516005,-2.0054267954,1.7906246957
H,0,1.2299196079,-0.1759971067,0.8816788366

dmpe Bpin3 Para Toluene CH Activation Transition Structure
E(RB+HF-LYP) = -2059.07157717

Zero-point correction= 0.547979 (Hartree/Particle)
Thermal correction to Energy= 0.585395
Thermal correction to Enthalpy= 0.586339
Thermal correction to Gibbs Free Energy= 0.476339
Sum of electronic and zero-point Energies= -2058.523598
Sum of electronic and thermal Energies= -2058.486182
Sum of electronic and thermal Enthalpies= -2058.485238
Sum of electronic and thermal Free Energies= -2058.595238

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.341	135.820	231.516

C,0,0.38701651,-3.4759758873,-0.6564136945
C,0,-0.603165575,-2.9436645948,-1.7029375922
P,0,-0.3362049001,-1.1211300039,-2.0351536361
Ir,0,0.123920817,-0.0623684474,0.0745081106
B,0,0.0553971415,1.8087145399,-0.8872805345
O,0,-0.2560433989,3.0486234946,-0.3476150132
C,0,-0.0650026755,4.0703205798,-1.3282457011
C,0,0.065678165,3.3073783574,-2.660721944
O,0,0.3030656515,1.9491381868,-2.2698226433
P,0,0.5157585162,-2.359784485,0.8514342141
B,0,0.9649604879,0.8163884048,1.8310516061
O,0,1.6941717123,0.0690913004,2.7669896864
C,0,2.0418253166,0.9201771901,3.869052581
C,0,1.7214572672,2.3408392683,3.3651703903
O,0,0.8716390014,2.1345104394,2.2345804881
B,0,2.1879914462,0.131790902,-0.4099773993
O,0,2.9849236247,-0.867897959,-0.9961099429
C,0,4.284413691,-0.3375320897,-1.2957303254
C,0,4.3290825541,1.0098187046,-0.5500079085
O,0,2.9675241459,1.2700065651,-0.1960553218
C,0,2.1795338863,-2.8324830054,1.5010631011
C,0,-0.5514146645,-3.1853780775,2.1278082213
H,0,0.1288103144,-4.4973281193,-0.3530047258
H,0,1.3950049825,-3.5112605679,-1.0844699944

C,0,0.9178729999,-1.1102744304,-3.3867263805
C,0,-1.861585658,-0.6266489328,-2.9436653379
H,0,-0.5279225633,-3.5094760476,-2.6395134702
H,0,-1.6333397722,-3.0496258501,-1.3467820204
H,0,0.8956680037,3.6656082958,-3.278866685
H,0,-0.8547113606,3.3575839663,-3.2580318047
H,0,0.8436501406,4.6354918051,-1.0853811966
H,0,-0.914794588,4.7610259081,-1.3138290707
H,0,2.6234446027,2.8761469945,3.04282189
H,0,1.2018169118,2s.9528941422,4.1090418765
H,0,3.0980590643,0.7825705793,4.1220999638
H,0,1.4379325418,0.642617503,4.7427769485
H,0,4.7111918972,1.8270692675,-1.1700825175
H,0,4.9361248931,0.9576821523,0.3628442525
H,0,4.380289791,-0.2140516686,-2.3820624441
H,0,5.0548766042,-1.0391676375,-0.9597262955
H,0,2.2361122149,-3.9070095604,1.7048799233
H,0,2.9322557264,-2.5510746913,0.7632296213
H,0,2.3600491426,-2.2642673637,2.4149822666
H,0,-0.2756216838,-4.2374087435,2.2567935451
H,0,-0.403851551,-2.6618813987,3.0770707112
H,0,-1.6095210834,-3.1177145996,1.8722652143
H,0,-2.044167737,-1.2849740808,-3.7992044497
H,0,-2.7171839215,-0.649151023,-2.2666178306
H,0,-1.7203418299,0.3975470521,-3.2961649491
H,0,0.569416414,-1.6900107283,-4.2475729063
H,0,1.0767942113,-0.0698318192,-3.6782494024
H,0,1.8585683723,-1.5139362819,-3.010512745
H,0,-0.7445539538,0.3395216136,1.3899772253
C,0,-2.1284508809,0.0935864486,0.4804152568
C,0,-2.9680997992,-1.03573609,0.4884972227
C,0,-4.3603221588,-0.9305321207,0.5711949438
C,0,-4.9878342402,0.3146236194,0.6837397081
C,0,-4.1626925661,1.4453453712,0.7049725889
C,0,-2.7727694721,1.3397596831,0.6122014841
H,0,-2.5450010491,-2.0303819952,0.4020519793
H,0,-4.9651037161,-1.8359365202,0.5502843734
C,0,-6.4882914622,0.4320317681,0.815206016
H,0,-4.6125794713,2.4322414573,0.8007910019
H,0,-2.1753744827,2.2445622635,0.6373497047
H,0,-6.863446256,1.3402551097,0.3323399975
H,0,-6.9991550464,-0.4251395086,0.3651406735
H,0,-6.7961016149,0.4767178524,1.8680559831

dmpeBpin3ParaTolHCHactTSParSptBack
E(RB+HF-LYP) = -2059.07268038

Zero-point correction= 0.547875 (Hartree/Particle)
Thermal correction to Energy= 0.585281
Thermal correction to Enthalpy= 0.586225
Thermal correction to Gibbs Free Energy= 0.476722
Sum of electronic and zero-point Energies= -2058.524806
Sum of electronic and thermal Energies= -2058.487399
Sum of electronic and thermal Enthalpies= -2058.486455
Sum of electronic and thermal Free Energies= -2058.595959

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	367.269	135.891	230.469

C,0,2.9062517144,1.1425164943,-0.2536046443
C,0,2.157395365,0.1266244391,0.372531151
C,0,2.8959320484,-0.7962087576,1.1325203947
C,0,4.2929540091,-0.7562703218,1.2070079466
C,0,5.0249037733,0.229267114,0.5395027551
C,0,4.2992122062,1.182794944,-0.1878140824
Ir,0,-0.0962193641,-0.0170884851,0.0428182541
P,0,0.2081436188,-0.5345311485,-2.300736162
C,0,-0.3335402527,-2.3002206923,-2.568838231
C,0,0.1615154049,-3.204998385,-1.4315579785
P,0,-0.2650245364,-2.4817777714,0.2421609887
B,0,-2.1913825842,0.1109782788,-0.3374624092
O,0,-3.1259687698,0.8238649669,0.4146076262
C,0,-4.443046177,0.6098443293,-0.1005285606
C,0,-4.2186022379,-0.0807103722,-1.4577818406
O,0,-2.8552043929,-0.5261589504,-1.40557639
B,0,-0.8967576193,0.2314097116,1.9975110731
O,0,-1.2527664047,-0.8651631079,2.7954482343
C,0,-1.7037261791,-0.3754496725,4.0682597653
C,0,-1.9086495463,1.1335119405,3.837398285
O,0,-1.1507960944,1.4169631109,2.6598978632
B,0,-0.2251597588,2.0473476204,-0.3022894823
O,0,0.3692975325,3.0232763485,0.4869877104
C,0,0.1439576899,4.3145770431,-0.082023751
C,0,-0.897738873,4.0710998211,-1.1927865561
O,0,-0.891508961,2.6496249976,-1.3824536804
H,0,-5.0066961167,-0.0235581812,0.5969186017
H,0,-4.9634741899,1.5684841639,-0.1914441821

H,0,-4.8810548991,-0.9372651348,-1.620049846
H,0,-4.3380097924,0.6138738857,-2.2988913857
H,0,-2.6225749504,-0.8946835448,4.3590238543
H,0,-0.9349643886,-0.5790845945,4.8248366338
H,0,-2.9620096025,1.3794882727,3.6522899453
H,0,-1.545845819,1.7480537708,4.6671552109
H,0,-1.903853174,4.388087092,-0.8907426361
H,0,-0.6469265292,4.571225353,-2.1344652145
H,0,-0.2129838548,5.0009000302,0.6924849846
H,0,1.0901352473,4.7065208541,-0.4789634575
H,0,0.7913250491,0.4551949751,1.3164823877
H,0,2.3934757707,1.9229217055,-0.8051502094
H,0,4.8329720036,1.9786214618,-0.7052413638
H,0,2.3751232226,-1.5548971128,1.7051004987
H,0,4.8170393859,-1.4985844291,1.8068668564
C,0,6.5313875154,0.2969978679,0.6336648987
C,0,-0.6884363523,0.3762759509,-3.6264128694
C,0,1.9371262105,-0.5405505333,-2.9545052879
C,0,-1.9651551388,-3.1468342667,0.5420767873
C,0,0.705949118,-3.5847745846,1.3728713338
H,0,-0.2530557875,-4.2159693163,-1.5235592935
H,0,1.2538163961,-3.2992113678,-1.4675843895
H,0,-1.4273307842,-2.271515383,-2.586407468
H,0,0.0145165939,-2.6609072982,-3.5441673185
H,0,1.9569690551,-0.9306712017,-3.977207183
H,0,2.3344677564,0.4764903334,-2.9491614607
H,0,2.5820860769,-1.1443977389,-2.3131140945
H,0,-0.4228447174,-0.0108880893,-4.6153737171
H,0,-1.7591555075,0.264528051,-3.4538587257
H,0,-0.4422040972,1.4367616176,-3.5548758741
H,0,0.3956102263,-4.6284138625,1.2556149345
H,0,1.7740435734,-3.5078956273,1.1613895132
H,0,0.5271175819,-3.2738720583,2.4054101466
H,0,-1.9840211171,-4.239699457,0.4730086803
H,0,-2.2744727017,-2.832781054,1.5415524195
H,0,-2.6529094761,-2.7167043976,-0.1880187061
H,0,6.9858242077,0.5241978383,-0.3369974313
H,0,6.8549975523,1.0814709166,1.3297729498
H,0,6.952907353,-0.6482644503,0.98902446

dmpeBpin3ParaTolHCHactTSSptSptBack
E(RB+HF-LYP) = -2059.07335991

Zero-point correction= 0.548090 (Hartree/Particle)

Thermal correction to Energy= 0.585419
Thermal correction to Enthalpy= 0.586363
Thermal correction to Gibbs Free Energy= 0.476856
Sum of electronic and zero-point Energies= -2058.525270
Sum of electronic and thermal Energies= -2058.487941
Sum of electronic and thermal Enthalpies= -2058.486997
Sum of electronic and thermal Free Energies= -2058.596504

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.356	135.742	230.477

C,0,3.0166580311,-0.7521370957,0.6671377335
C,0,2.0891921562,0.3067148105,0.6211297733
C,0,2.619854649,1.5915743157,0.8475770714
C,0,3.9853500332,1.8015351976,1.0596355734
C,0,4.8981877473,0.7412439938,1.0756812679
C,0,4.3834613733,-0.5438952101,0.8733939334
Ir,0,-0.105276116,-0.0411379711,0.04332239
P,0,0.5170667952,-0.782591758,-2.1729617878
C,0,0.2950782592,-2.6408848248,-2.2290473804
C,0,0.6832469173,-3.3200650097,-0.9060784409
P,0,-0.1258042553,-2.4474026465,0.5417272758
B,0,-2.1337102276,-0.0880707988,-0.6018716114
O,0,-2.6589852372,-1.0071813752,-1.5311767993
C,0,-4.0165996191,-0.656398351,-1.8387376196
C,0,-4.400464879,0.3657756693,-0.7531609573
O,0,-3.1515619247,0.7703720801,-0.1844910523
B,0,-1.20241937,0.3836118661,1.8177563786
O,0,-1.7865676762,-0.6345659619,2.5863138706
C,0,-2.3732436983,-0.0475785054,3.7574447202
C,0,-2.3772746434,1.4639737459,3.458535616
O,0,-1.4402291348,1.6175922955,2.3904991263
B,0,-0.2844905316,1.9599168903,-0.5785126337
O,0,-0.0620400382,3.0965781046,0.1923939234
C,0,-0.1724047708,4.2681321009,-0.6187503412
C,0,-0.8081019527,3.7678758334,-1.9288884076
O,0,-0.6337430566,2.3462333381,-1.8861566648
H,0,-4.0573347158,-0.2239023909,-2.8467256231
H,0,-4.6421170605,-1.5548006508,-1.8233638693
H,0,-4.9228137067,1.2395289007,-1.1553727967
H,0,-5.0266610696,-0.0802365374,0.0303046586
H,0,-3.3762990554,-0.4576675527,3.9133318473
H,0,-1.757868044,-0.2958830684,4.6320475822

H,0,-3.362387667,1.813962995,3.1249769106
H,0,-2.0635850728,2.070971096,4.3135885574
H,0,-1.8801372823,3.9977235818,-1.9803365174
H,0,-0.3243761774,4.1746862897,-2.8234311412
H,0,-0.7847646421,5.015518727,-0.1042315398
H,0,0.8274563542,4.6934488135,-0.7806643325
H,0,0.6273156159,0.3580997297,1.4398102193
H,0,2.6878263006,-1.7728244535,0.5080179972
H,0,5.0579858006,-1.3989602152,0.8769536365
H,0,1.9501072833,2.443822566,0.8651657024
H,0,4.3442953718,2.8163346405,1.2238718917
C,0,6.3682450585,0.9680284933,1.339727802
C,0,-0.3896569078,-0.2424094192,-3.6838261899
C,0,2.2673568254,-0.5218867095,-2.7037955712
C,0,-1.7673165994,-3.292262731,0.639336991
C,0,0.6964663968,-3.1836984873,2.0285664857
H,0,0.4042191993,-4.3805332867,-0.9159765412
H,0,1.7682283938,-3.2755933373,-0.7588264904
H,0,-0.7700175465,-2.7953474548,-2.4322939392
H,0,0.8581939246,-3.0613227418,-3.0707162022
H,0,2.4578517587,-1.0078981332,-3.6662784307
H,0,2.443107949,0.5526427458,-2.8035235674
H,0,2.9601610754,-0.9011825174,-1.9516852517
H,0,0.028071153,-0.7164856602,-4.5778961896
H,0,-1.4403791392,-0.5119167201,-3.5741430019
H,0,-0.3167178782,0.8434551859,-3.7573461296
H,0,0.6963793429,-4.2781149019,1.9895115684
H,0,1.7205680502,-2.8212432932,2.1309625931
H,0,0.1303772249,-2.8577519397,2.9052530355
H,0,-1.6508883643,-4.3741463268,0.7636814857
H,0,-2.3016776948,-2.8754839421,1.4958696144
H,0,-2.340316506,-3.0767453447,-0.2638301413
H,0,6.986046504,0.204894498,0.8553019909
H,0,6.6944603869,1.947516736,0.975712807
H,0,6.5929236946,0.9316292671,2.4137609971

dmpeBpin2ParaTolHBpinRotTS
E(RB+HF-LYP) = -2059.07985901

Zero-point correction= 0.551022 (Hartree/Particle)
Thermal correction to Energy= 0.587616
Thermal correction to Enthalpy= 0.588560
Thermal correction to Gibbs Free Energy= 0.482114
Sum of electronic and zero-point Energies= -2058.528837

Sum of electronic and thermal Energies= -2058.492243
Sum of electronic and thermal Enthalpies= -2058.491299
Sum of electronic and thermal Free Energies= -2058.597745

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	368.734	133.896	224.033

C,0,4.4173326201,0.3625978223,0.9954038387
C,0,3.0189540421,0.2918381615,1.0674860373
C,0,2.1927922792,0.0160734705,-0.0410520215
C,0,2.9049023598,-0.1863825636,-1.2473909909
C,0,4.2964521796,-0.1182001367,-1.3343681338
C,0,5.0882557663,0.1578672061,-0.2114657843
Ir,0,-0.0422756121,-0.0707471581,-0.0259483028
B,0,0.1548935098,-1.875536309,-1.0951196417
O,0,0.1655199896,-3.1710932648,-0.5662182407
C,0,0.2550458452,-4.119077823,-1.6404673606
C,0,0.6140830047,-3.2681919746,-2.8750738216
O,0,0.3466547243,-1.9212396738,-2.4723676336
B,0,-2.153200804,-0.2832414369,-0.2792510912
O,0,-3.1490832458,-0.0076588659,0.6820163637
C,0,-4.4371844583,-0.3633280624,0.1547586955
C,0,-4.1811731426,-0.5988759315,-1.3449690367
O,0,-2.7617887187,-0.7438816721,-1.4456223542
P,0,-0.1943425746,1.840092644,1.4737785905
C,0,1.0662640749,3.1896691296,1.4427413943
P,0,-0.2297724215,-1.3348952886,1.9209004081
C,0,1.2373970134,-2.2964079944,2.48362644
B,0,-0.185270502,1.6287048064,-1.5088412976
O,0,-1.4030705493,2.1455836941,-1.9167060092
C,0,-1.1585228042,3.3397806549,-2.6745247249
C,0,0.3371115528,3.6520795992,-2.4366372855
O,0,0.864386584,2.4647686064,-1.8314633578
C,0,-0.0172535106,1.1718226902,3.2118758403
C,0,-0.6759725127,-0.2049180393,3.3424892375
C,0,-1.7706879272,2.8000511092,1.5542592134
C,0,-1.5560834971,-2.6082896625,2.0352627171
H,0,0.0686603499,0.3171628443,-1.6578786268
H,0,-0.4172474151,-0.6848702959,4.2933527159
H,0,-1.7662932286,-0.1061122992,3.3077507474
H,0,-0.441928747,1.8844823499,3.9283265883
H,0,1.0559692152,1.105428495,3.4188469019
H,0,0.4828368445,4.4989043183,-1.7539633285

H,0,0.8842047784,3.8603890434,-3.3605526166
H,0,-1.8230311905,4.1365377198,-2.3258140837
H,0,-1.3806402481,3.1405147582,-3.7291501238
H,0,0.0091804462,-3.5166701096,-3.7527452443
H,0,1.6737511512,-3.3593494563,-3.144871641
H,0,-0.711882466,-4.6252966796,-1.7534714779
H,0,1.0149075429,-4.8705023696,-1.40353499
H,0,-4.500739249,0.2551645505,-1.9558467469
H,0,-4.6742501735,-1.4990819826,-1.7259829308
H,0,-5.151102878,0.4439947142,0.3476279409
H,0,-4.7980336704,-1.2688770893,0.6613298675
H,0,2.3562211837,-0.4088282862,-2.15887099
H,0,4.777441649,-0.2827158346,-2.2984070639
C,0,6.595008793,0.2231306798,-0.3079102633
H,0,4.9900170608,0.5820852331,1.8962061444
H,0,2.5779927809,0.4681219413,2.0477606575
H,0,-1.3749630047,-3.3539861605,1.2606748438
H,0,-1.5429323555,-3.0837602976,3.0214619213
H,0,-2.5222390676,-2.1310968448,1.8666627026
H,0,1.4259514596,-3.062114918,1.727702725
H,0,2.1190882781,-1.6595222548,2.5474299047
H,0,1.0401851194,-2.7715778471,3.4499622971
H,0,-1.934850087,3.2858633166,0.5890628395
H,0,-2.5967050447,2.1053567419,1.7151411549
H,0,-1.7412835804,3.5571169812,2.3447810565
H,0,0.9187196459,3.8001921601,0.5495811804
H,0,0.9834198983,3.8243907169,2.3309120614
H,0,2.0626429375,2.7485199378,1.384196502
H,0,7.0257208403,-0.7460040757,-0.5900140984
H,0,6.9212801104,0.9471392489,-1.0644322786
H,0,7.0434940554,0.5165113132,0.6465000638

dmpe Bpin3 Meta Toluene CH Activation Transition Structure
E(RB+HF-LYP) = -2059.07150335

Zero-point correction= 0.548183 (Hartree/Particle)
Thermal correction to Energy= 0.585458
Thermal correction to Enthalpy= 0.586403
Thermal correction to Gibbs Free Energy= 0.477453
Sum of electronic and zero-point Energies= -2058.523321
Sum of electronic and thermal Energies= -2058.486045
Sum of electronic and thermal Enthalpies= -2058.485101
Sum of electronic and thermal Free Energies= -2058.594050

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.381	135.728	229.304

C,0,-0.3985423567,-3.4603559903,0.0487040878
C,0,0.7138206953,-3.1505022413,1.0616679545
P,0,0.5511942421,-1.4162172205,1.7465151097
Ir,0,-0.0978247471,0.0197944133,-0.0678755992
B,0,0.1174454376,1.6779811135,1.2086001764
O,0,0.3892465443,2.9953495262,0.8690144324
C,0,0.3383786046,3.8221222427,2.0329928057
C,0,0.3369872271,2.8299686305,3.2126862307
O,0,0.0335746241,1.5644049499,2.6124690193
P,0,-0.6212750119,-2.0895268154,-1.2172588403
B,0,-1.0968155,1.2229036877,-1.5249928738
O,0,-1.9254553128,0.6715892204,-2.5118401677
C,0,-2.3593681084,1.7210003475,-3.3893877546
C,0,-1.9845735128,3.0144063547,-2.6417634273
O,0,-1.0260727254,2.5954536191,-1.6675054236
B,0,-2.0979160872,0.1203447804,0.6561987303
O,0,-2.8477073325,-0.9748460847,1.121360596
C,0,-4.1011603382,-0.5132994135,1.6468768567
C,0,-4.2033550605,0.9444812735,1.1615895721
O,0,-2.8762008944,1.2762022115,0.7418665171
C,0,-2.3426963628,-2.421611249,-1.8007158416
C,0,0.3206008084,-2.6857832152,-2.7027010991
H,0,-0.2189952437,-4.4182443292,-0.4537014457
H,0,-1.3607334525,-3.5410827901,0.566752846
C,0,-0.5485712628,-1.6278962634,3.2109157126
C,0,2.1824116306,-1.1223382841,2.5528128322
H,0,0.7152931139,-3.8793114166,1.8812481497
H,0,1.6966214732,-3.2066863257,0.5804643627
H,0,-0.4154131244,3.0695449506,3.9715410545
H,0,1.3166338388,2.7719544225,3.7056896607
H,0,-0.5749164264,4.4296364765,2.0024934983
H,0,1.2005842952,4.4974092818,2.0453350729
H,0,-2.8476668042,3.4567785771,-2.1283000448
H,0,-1.5404460472,3.7737449666,-3.2929067267
H,0,-3.4341975805,1.6266017342,-3.574704989
H,0,-1.8328787347,1.6285974985,-4.3483097441
H,0,-4.5250924532,1.6346287806,1.9479130753
H,0,-4.8876586493,1.0486216602,0.3097936114
H,0,-4.0807754534,-0.5856081371,2.7419421436
H,0,-4.9126521056,-1.1473147529,1.2751590556

H,0,-2.4433647336,-3.4453361002,-2.176753403
H,0,-3.0290820777,-2.2607556447,-0.9681500477
H,0,-2.5791221517,-1.705367325,-2.5892640365
H,0,0.0091694078,-3.695275906,-2.9915790559
H,0,0.11385613,-2.0014796387,-3.5308900364
H,0,1.396682384,-2.6769159688,-2.5256427221
H,0,2.4247739755,-1.9231370016,3.2589977254
H,0,2.9619612833,-1.0472313401,1.7928697063
H,0,2.1218524022,-0.1715579843,3.0869668814
H,0,-0.1258807353,-2.3494321237,3.9176334275
H,0,-0.645777562,-0.6505989277,3.6886582475
H,0,-1.5349457226,-1.953160358,2.8788075301
H,0,0.6383675979,0.6449334361,-1.3776136878
C,0,2.1051888847,0.2556744846,-0.6765188047
C,0,2.926236833,-0.8553543203,-0.9536962338
C,0,4.3086347145,-0.7522295313,-1.1692776748
C,0,4.8975338809,0.5181660393,-1.1389655323
C,0,4.1082090171,1.6403584592,-0.9000503631
C,0,2.733250137,1.5149910311,-0.6768773891
H,0,2.4955949147,-1.8510126396,-0.9867512986
C,0,5.1490762517,-1.9841510201,-1.4228153005
H,0,5.9662310389,0.6250526615,-1.3122918437
H,0,4.5622202144,2.6288136926,-0.8936217104
H,0,2.1412939093,2.4057285207,-0.5001925744
H,0,5.8645414042,-2.1578309377,-0.6095230601
H,0,4.5293771765,-2.8816887702,-1.5139713364
H,0,5.7332430008,-1.8882869815,-2.345330932

dmpe Bpin3 Meta Toluene CH Activation Transition Structure – Isomer 2
E(RB+HF-LYP) = -2059.07155341

Zero-point correction= 0.547854 (Hartree/Particle)
Thermal correction to Energy= 0.585338
Thermal correction to Enthalpy= 0.586282
Thermal correction to Gibbs Free Energy= 0.476260
Sum of electronic and zero-point Energies= -2058.523699
Sum of electronic and thermal Energies= -2058.486216
Sum of electronic and thermal Enthalpies= -2058.485272
Sum of electronic and thermal Free Energies= -2058.595294

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.305	135.935	231.561

C,0,-0.4156538602,-3.4311505041,-0.994954503
C,0,-1.3150937123,-2.6256883738,-1.9439596914
P,0,-0.7054858194,-0.865232959,-2.1162944108
Ir,0,0.0412098132,-0.1418082357,0.0563997757
B,0,0.3871985026,1.7735625205,-0.7401275115
O,0,0.3488218257,2.9984774768,-0.0886585425
C,0,0.7599924462,4.0394489637,-0.9763610029
C,0,0.7397900922,3.3873649822,-2.3727977249
O,0,0.6676043112,1.9812728018,-2.1068775588
P,0,-0.108159989,-2.5371366595,0.6257183471
B,0,1.1414866937,0.3748839209,1.8122851787
O,0,1.7314227102,-0.5864994187,2.644054458
C,0,2.314302943,0.0752253437,3.7760583787
C,0,2.304757523,1.5656504423,3.3870348659
O,0,1.3697095857,1.6447972161,2.3088055898
B,0,2.0703233108,-0.4390068583,-0.5155394067
O,0,2.5615661188,-1.5726813654,-1.1914248227
C,0,3.9433347777,-1.371905851,-1.525503945
C,0,4.3597900994,-0.1371444216,-0.7041434358
O,0,3.1237808978,0.4439782036,-0.2776733537
C,0,1.3837481663,-3.4298675191,1.249727081
C,0,-1.3821380943,-3.2361794871,1.7824304846
H,0,-0.8261221655,-4.4314609983,-0.8132208976
H,0,0.5765848834,-3.5555246958,-1.4422499123
C,0,0.4787369624,-0.9588751359,-3.5262322102
C,0,-2.1287592473,0.0129356549,-2.8912050226
H,0,-1.3719812209,-3.1007021491,-2.9308497736
H,0,-2.337927992,-2.5730535752,-1.5545596615
H,0,1.6375603983,3.6072563709,-2.9601336252
H,0,-0.1376385998,3.6916121882,-2.9592943647
H,0,1.7645766306,4.3777301694,-0.6926708846
H,0,0.0743394571,4.8895421613,-0.8931107806
H,0,3.2871984119,1.9045248478,3.0347472014
H,0,1.9829598708,2.2208146206,4.2026272851
H,0,3.3211255181,-0.3161290643,3.954130733
H,0,1.7025962569,-0.1258532486,4.6652616665
H,0,4.9271954705,0.5925869532,-1.2905150818
H,0,4.9546151165,-0.4082848887,0.1774613886
H,0,4.0300005618,-1.1990369542,-2.6059479332
H,0,4.5178180077,-2.2690453625,-1.2730059202
H,0,1.1995562759,-4.5072514455,1.3187124068
H,0,2.2130349252,-3.2366044218,0.5680974222
H,0,1.6409358936,-3.0263217795,2.2302968526
H,0,-1.3233031138,-4.3290911657,1.8215875593

H,0,-1.1892908904,-2.83658212,2.782502801
H,0,-2.3923826263,-2.9408042381,1.4971807637
H,0,-2.4638719377,-0.4988677562,-3.799247142
H,0,-2.9519498583,0.0842021938,-2.1785618779
H,0,-1.7992326216,1.023018776,-3.1460484078
H,0,-0.0115778752,-1.3519738378,-4.4226479053
H,0,0.8456881172,0.0524835138,-3.7135637416
H,0,1.3218049876,-1.5914340944,-3.2463008698
H,0,-0.6717570813,0.3111106686,1.4460599063
C,0,-2.0980330036,0.5003577052,0.595487077
C,0,-3.1806340509,-0.394098032,0.4988632114
C,0,-4.5010476292,0.0317589683,0.6719963393
C,0,-4.7786510535,1.3623444033,0.9796237197
C,0,-3.7285267035,2.2772532638,1.1192646819
C,0,-2.4114813011,1.8326750224,0.9259417615
H,0,-3.0086985792,-1.436451705,0.2575752418
H,0,-5.3153795383,-0.6818600255,0.5646701902
H,0,-5.8070102837,1.688732027,1.1183764717
C,0,-4.0023570658,3.7136521435,1.5050843414
H,0,-1.6037280022,2.5496589891,1.031335421
H,0,-3.1914118368,4.3740325328,1.1845799062
H,0,-4.9353735016,4.0782358408,1.06225249
H,0,-4.0981714105,3.8210674542,2.5933073961

dmpeBpin2MetaTolHBpinRotTS
E(RB+HF-LYP) = -2059.07961048

Zero-point correction= 0.551049 (Hartree/Particle)
Thermal correction to Energy= 0.586674
Thermal correction to Enthalpy= 0.587618
Thermal correction to Gibbs Free Energy= 0.483944
Sum of electronic and zero-point Energies= -2058.528562
Sum of electronic and thermal Energies= -2058.492937
Sum of electronic and thermal Enthalpies= -2058.491992
Sum of electronic and thermal Free Energies= -2058.595666

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	368.143	131.833	218.200

C,0,-4.1460399052,-0.4854612355,1.0118661644
C,0,-2.7424137976,-0.4327919401,1.0427544049
C,0,-1.9357820076,0.0296790346,-0.0196091343
C,0,-2.6565473734,0.4511848551,-1.1593800965

C,0,-4.052160338,0.4069539181,-1.2250887954
C,0,-4.8029325732,-0.0589057878,-0.1467842273
Ir,0,0.2977849334,0.0831420357,-0.0149713723
B,0,0.1057874788,2.0518761055,-0.7361700184
O,0,0.085128705,3.2272029322,0.0240985919
C,0,-0.0128141141,4.3568919106,-0.8564285702
C,0,-0.3683531111,3.7459902976,-2.2263022399
O,0,-0.0812602439,2.3515403779,-2.0819054552
B,0,2.4100717364,0.3007536825,-0.2574112724
O,0,3.404101031,-0.1124727475,0.658138195
C,0,4.6949966754,0.2995665172,0.1803130587
C,0,4.4405615899,0.7286774885,-1.2757113504
O,0,3.0231495647,0.9053904311,-1.3525746959
P,0,0.4554153145,-2.0653467994,1.1276682246
C,0,-0.81657511,-3.3817031928,0.8811126971
P,0,0.5350977133,0.9830438796,2.1233572401
C,0,-0.912627095,1.8266615865,2.8908784209
B,0,0.3790834836,-1.3334122227,-1.7704596064
O,0,1.5810278311,-1.8118728187,-2.2648691903
C,0,1.2976450829,-2.8393597584,-3.2267120279
C,0,-0.2057886639,-3.1438639219,-3.0370356839
O,0,-0.6966556064,-2.0608481689,-2.2369060537
C,0,0.3183401124,-1.7089769617,2.9568208476
C,0,1.007390719,-0.3857789494,3.3054384215
C,0,2.0265988081,-3.0306664344,1.0129539408
C,0,1.8681212108,2.2159189529,2.4325318987
H,0,0.167699124,-0.0067432429,-1.6873888348
H,0,0.7939235479,-0.080009719,4.3360448488
H,0,2.0928691171,-0.4907296524,3.2056566283
H,0,0.7447920711,-2.5409536565,3.5292888951
H,0,-0.7490843109,-1.6636334101,3.1973226556
H,0,-0.3753727435,-4.0889899145,-2.5054355357
H,0,-0.7598964613,-3.1776860316,-3.9793904573
H,0,1.9379278831,-3.7062939748,-3.0357067789
H,0,1.5228110902,-2.4567911731,-4.2289053085
H,0,0.2273806394,4.161718629,-3.0449334387
H,0,-1.4309996927,3.8706719435,-2.4696383137
H,0,0.9503473602,4.8824576378,-0.874938774
H,0,-0.7772992579,5.0461644166,-0.4842036798
H,0,4.7470345361,-0.0447876212,-1.9916564854
H,0,4.945690878,1.6632623548,-1.5401920268
H,0,5.4037726646,-0.5303587549,0.2669717118
H,0,5.0616754385,1.1299903688,0.7990686749
H,0,-2.1187690485,0.8235604699,-2.0271369546

H,0,-4.5579097332,0.7371235398,-2.1308288305
H,0,-5.8891907416,-0.0923819201,-0.203094161
C,0,-4.9326016291,-0.9714959508,2.2097799404
H,0,-2.2724975646,-0.784261897,1.9615414739
H,0,1.6674337205,3.0917647871,1.8144102372
H,0,1.8837127869,2.5008991519,3.4895565109
H,0,2.8275134783,1.7796646791,2.1523018597
H,0,-1.1189143559,2.7169224032,2.2928812389
H,0,-1.7945883731,1.1873980225,2.8635523622
H,0,-0.6864500116,2.1178366359,3.9217052856
H,0,2.1761704424,-3.3360269872,-0.0256552543
H,0,2.8583913909,-2.3789559117,1.2860921542
H,0,2.0003688495,-3.915873047,1.656832073
H,0,-0.6944542947,-3.8206215604,-0.1114113726
H,0,-0.7218771275,-4.1689717226,1.6361417752
H,0,-1.8102281076,-2.9325007012,0.9264252422
H,0,-5.3965276511,-0.138274254,2.7538800725
H,0,-5.7428750718,-1.6473407321,1.9137528399
H,0,-4.2938948933,-1.5076202715,2.9199224103

dmpeBpin3MetaTolHCHactTSParSptBackA
E(RB+HF-LYP) = -2059.07262857

Zero-point correction= 0.547885 (Hartree/Particle)
Thermal correction to Energy= 0.585245
Thermal correction to Enthalpy= 0.586190
Thermal correction to Gibbs Free Energy= 0.477328
Sum of electronic and zero-point Energies= -2058.524744
Sum of electronic and thermal Energies= -2058.487383
Sum of electronic and thermal Enthalpies= -2058.486439
Sum of electronic and thermal Free Energies= -2058.595301

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.247	135.944	229.119

C,0,4.3165615883,1.6686453645,0.4078675601
C,0,2.9461795443,1.4706397645,0.1908883317
C,0,2.2550356315,0.334145006,0.652213992
C,0,2.9973120743,-0.5776331054,1.4230244243
C,0,4.3647399663,-0.3992400457,1.6583017532
C,0,5.027988365,0.7118471332,1.1441279134
Ir,0,0.0737828891,-0.0047389304,0.0750360624
B,0,-0.24874126,2.0483649431,-0.18493918

O,0,-0.8585741556,2.6336466415,-1.3073222953
C,0,-1.0503363369,4.0326636466,-1.0573163304
C,0,-0.1753498652,4.3259494998,0.1783901515
O,0,0.1367427672,3.0371068398,0.7106345261
H,0,6.0900065586,0.8522528536,1.333210728
P,0,0.6727616416,-0.3486204272,-2.2468939106
C,0,2.4457470645,-0.1090033643,-2.7119837933
P,0,0.1448597008,-2.4879127404,0.1325057987
C,0,1.0669102124,-3.5739415295,1.3201704667
B,0,-1.9716413276,-0.0561234079,-0.5287178832
O,0,-2.4519702949,-0.7083663795,-1.6818194356
C,0,-3.839288594,-0.3941068879,-1.8714359463
C,0,-4.2723656868,0.2361714953,-0.5348096197
O,0,-3.0450905629,0.5392447692,0.1343021538
B,0,-0.9597729163,0.0397493512,1.9319840702
O,0,-1.3846227305,1.1526534414,2.6323640734
C,0,-2.2324419503,0.7296025978,3.701879648
C,0,-1.927021631,-0.7718268679,3.8591468017
O,0,-1.306182586,-1.1340696272,2.615866479
C,0,0.386119296,-2.1477721425,-2.6550596326
C,0,0.8479424076,-3.0558588262,-1.5065648783
C,0,-0.1894200333,0.5246954605,-3.6204640896
C,0,-1.5067728049,-3.3192924618,0.1742537559
H,0,-4.858443747,-0.4591160025,0.0800677885
H,0,-4.855595757,1.1531172583,-0.6665816384
H,0,-4.3935373516,-1.3061229343,-2.1164993838
H,0,-3.9383666127,0.3064123565,-2.7102269741
H,0,-2.8241429541,-1.3796481655,4.0147725349
H,0,-1.2266486532,-0.9687984152,4.681006862
H,0,-3.2785955863,0.9076948497,3.4219778
H,0,-2.008078035,1.3097447584,4.6023999612
H,0,-2.1137779199,4.2196182269,-0.8622718958
H,0,-0.7548579077,4.6103026257,-1.9398394233
H,0,-0.6953685826,4.920959199,0.935990494
H,0,0.7557580995,4.8454491335,-0.0858044702
H,0,0.7672464004,0.4771286453,1.4590814757
H,0,2.4019273539,2.240662648,-0.3465497876
C,0,5.016655612,2.8876677851,-0.1501032493
H,0,2.4987938079,-1.4246709637,1.878416453
H,0,4.9071542292,-1.1238146699,2.261939579
H,0,0.5732596227,-4.1001740637,-1.6975585598
H,0,1.9399972257,-3.0214961694,-1.4100208285
H,0,-0.6923221211,-2.2472558964,-2.8125511536
H,0,0.8912514688,-2.4058872797,-3.5935239261

H,0,2.614021597,-0.4181629815,-3.748652071
H,0,2.7134075558,0.9437969152,-2.6015939404
H,0,3.0923913573,-0.6814241381,-2.0445057224
H,0,0.2137631704,0.2185120804,-4.5910980965
H,0,-1.2524539036,0.2892819068,-3.5638121663
H,0,-0.0718692544,1.600749411,-3.483330666
H,0,0.8770894469,-4.6301343632,1.1016266966
H,0,2.1410498339,-3.3891158882,1.2616247187
H,0,0.7248800605,-3.3544902219,2.3348316594
H,0,-1.4129508603,-4.4048357487,0.064416337
H,0,-1.970510552,-3.0812906822,1.1342630236
H,0,-2.1322047676,-2.9156708949,-0.6236246125
H,0,5.7468673777,3.2906259899,0.5598237422
H,0,5.5632282304,2.6517205664,-1.0726542728
H,0,4.3031791445,3.6829180584,-0.3864969827

dmpeBpin3MetaTolHCHactTSSptSptBackA
E(RB+HF-LYP) = -2059.07295561

Zero-point correction= 0.548271 (Hartree/Particle)
Thermal correction to Energy= 0.585473
Thermal correction to Enthalpy= 0.586417
Thermal correction to Gibbs Free Energy= 0.478173
Sum of electronic and zero-point Energies= -2058.524684
Sum of electronic and thermal Energies= -2058.487482
Sum of electronic and thermal Enthalpies= -2058.486538
Sum of electronic and thermal Free Energies= -2058.594783

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.390	135.717	227.820

C,0,3.1785021226,-0.7314130814,0.8103514527
C,0,2.2780651627,0.3371141176,0.6257708354
C,0,2.8304831789,1.630105123,0.6725375008
C,0,4.2053870078,1.8293756282,0.8348073285
C,0,5.072083038,0.7489063993,0.9774906526
C,0,4.5602340822,-0.5542969571,0.9758157716
Ir,0,0.0744872766,-0.0065311865,0.0798464901
P,0,0.7212552516,-0.7319488384,-2.1312237477
C,0,0.5177066866,-2.592740408,-2.2089068753
C,0,0.8828497351,-3.2740039531,-0.8794130665
P,0,0.0300357787,-2.4198442714,0.5524371992
B,0,-1.9533989456,-0.0341476348,-0.56629976

O,0,-2.467849904,-0.8915834932,-1.5569183001
C,0,-3.8264744069,-0.5302983248,-1.8468667531
C,0,-4.2246625721,0.4063366244,-0.6917684403
O,0,-2.9820703617,0.7801838285,-0.0896164501
B,0,-1.0086345129,0.3809719573,1.8723043435
O,0,-1.5548071172,-0.6592290671,2.6397613564
C,0,-2.1438764445,-0.0972577499,3.8219512847
C,0,-2.1940025324,1.4155604776,3.5340449248
O,0,-1.2741042213,1.6034262717,2.4563795334
B,0,-0.1513522405,1.9948884705,-0.5257787162
O,0,0.081821458,3.1276294397,0.2475144527
C,0,-0.0984224118,4.306165966,-0.5407921606
C,0,-0.7656080377,3.8044927368,-1.8356215852
O,0,-0.5628935692,2.3860083237,-1.8132845263
H,0,-3.8647429291,-0.0252407759,-2.8204709676
H,0,-4.4442455016,-1.4326122913,-1.9014913389
H,0,-4.753839974,1.3020275274,-1.0320461607
H,0,-4.8497242758,-0.101205646,0.0543218368
H,0,-3.1330876244,-0.5366449999,3.9863370912
H,0,-1.5113848179,-0.3344496706,4.6874154064
H,0,-3.1925158663,1.7394720955,3.2143479837
H,0,-1.8876546179,2.0250074042,4.3899823372
H,0,-1.8428245378,4.0141441768,-1.8518657106
H,0,-0.3182639627,4.228697992,-2.7409529883
H,0,-0.7166355105,5.0237920081,0.0079006391
H,0,0.8793966917,4.7689484458,-0.7313635381
H,0,0.8090506234,0.4318946101,1.4651510571
H,0,2.8157477319,-1.7534715827,0.8097609019
C,0,5.4777843357,-1.7420758325,1.1652902417
H,0,2.1776744761,2.4912035128,0.5982533011
H,0,4.5985879284,2.8434351979,0.8568746608
H,0,6.1401142153,0.9131866815,1.1036355875
C,0,-0.1546588558,-0.175188845,-3.6535242817
C,0,2.4838527099,-0.4674825704,-2.6175610197
C,0,-1.6288781854,-3.2353120652,0.5633476616
C,0,0.7685195533,-3.2133431728,2.0546903539
H,0,0.6207991807,-4.3386767784,-0.9019501392
H,0,1.9627540883,-3.2084589638,-0.7038719535
H,0,-0.5380203178,-2.7663248228,-2.4439748323
H,0,1.1111606291,-2.9988150347,-3.0366407304
H,0,2.6906140732,-0.9270718428,-3.5895106769
H,0,2.6746100523,0.6071538554,-2.6779895274
H,0,3.1528882258,-0.8775730408,-1.8599393826
H,0,0.2814860358,-0.6376459078,-4.5448236733

H,0,-1.2075491067,-0.4440788617,-3.5669024839
H,0,-0.0806544077,0.9117145596,-3.7131945201
H,0,0.7303180166,-4.3059678231,1.9907420879
H,0,1.800404791,-2.8946505122,2.2088714907
H,0,0.1777955499,-2.8829155839,2.9129116024
H,0,-1.5377096859,-4.3228466758,0.6562832712
H,0,-2.1855672716,-2.8368912109,1.4147028292
H,0,-2.1654259736,-2.9788557503,-0.3512880398
H,0,6.3391821807,-1.6977463965,0.4890572866
H,0,5.8762341944,-1.7814305471,2.1867299568
H,0,4.9567976379,-2.6867962606,0.9804566352

dmpeBpin3MetaTolHCHactTSSptSptBackS
E(RB+HF-LYP) = -2059.07327815

Zero-point correction= 0.548025 (Hartree/Particle)
Thermal correction to Energy= 0.585359
Thermal correction to Enthalpy= 0.586303
Thermal correction to Gibbs Free Energy= 0.476661
Sum of electronic and zero-point Energies= -2058.525253
Sum of electronic and thermal Energies= -2058.487919
Sum of electronic and thermal Enthalpies= -2058.486975
Sum of electronic and thermal Free Energies= -2058.596617

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	367.318	135.851	230.762

C,0,2.998928971,-0.9724501502,0.5379430825
C,0,2.1666197986,0.1560018674,0.4077302461
C,0,2.8116301577,1.4069474644,0.3819005765
C,0,4.2072803138,1.5459658967,0.4328205643
C,0,4.9989175286,0.3954905592,0.5221724962
C,0,4.3917822029,-0.8572893049,0.5806048055
Ir,0,-0.1001266906,-0.0335255111,0.0618482305
P,0,0.2618572704,-0.9889419992,-2.1256726904
C,0,-0.1029437903,-2.8223425894,-2.0110431718
C,0,0.3385875074,-3.4259764986,-0.6682193871
P,0,-0.2909031481,-2.3821813212,0.7543654173
B,0,-2.1783401257,0.0618067904,-0.3923851069
O,0,-2.8658979713,-0.8589423835,-1.2049883337
C,0,-4.2160329875,-0.4137196517,-1.4032283621
C,0,-4.4032374871,0.7098613956,-0.3664628909
O,0,-3.0757928456,1.0298213758,0.0606467588

B,0,-0.9711629058,0.6094560686,1.8967873638
O,0,-1.5455204393,-0.3036549496,2.7945788471
C,0,-1.9704617418,0.4082040344,3.9661806083
C,0,-1.8932051468,1.8908979147,3.5536082272
O,0,-1.0598419365,1.8947466294,2.3926042
B,0,-0.18756882,1.923216815,-0.7039992805
O,0,0.1616848353,3.0946601138,-0.0392614294
C,0,0.0587076133,4.211527104,-0.9245303204
C,0,-0.6953155966,3.661622307,-2.1498593888
O,0,-0.6061601064,2.2382138857,-2.0104447468
H,0,-4.328343075,-0.0506121437,-2.4327963806
H,0,-4.9053284529,-1.2517542307,-1.2567811404
H,0,-4.8802547725,1.6013978769,-0.7857349659
H,0,-4.9918499135,0.3791187192,0.4989105971
H,0,-2.9810484156,0.0918458164,4.2440991515
H,0,-1.2929808733,0.1720372492,4.7971778521
H,0,-2.8785644638,2.2948251759,3.2890606202
H,0,-1.4514831927,2.5284567842,4.3258316628
H,0,-1.752205299,3.9577759993,-2.1491807145
H,0,-0.2509107756,3.9699695391,-3.1022377236
H,0,-0.4736096354,5.0280516416,-0.4262583758
H,0,1.0662015508,4.5652513402,-1.1834013609
H,0,0.7906630166,0.4148973203,1.3499066247
H,0,2.5749200251,-1.9685966669,0.5829632757
H,0,5.003574803,-1.7537091954,0.6583239629
H,0,2.2065430702,2.3058810028,0.3338482075
C,0,4.8399180371,2.919720832,0.4292830987
H,0,6.0828064857,0.4810338393,0.5568378891
C,0,-0.730809478,-0.4911906605,-3.5961919986
C,0,1.9758952637,-0.9147580693,-2.8089633304
C,0,-1.9865963713,-3.0695986321,1.0190661228
C,0,0.5610110922,-3.0822594406,2.2427318843
H,0,-0.0160106311,-4.4591235785,-0.5701497932
H,0,1.4321877651,-3.4516515718,-0.6038118839
H,0,-1.1895579458,-2.9064299419,-2.1194829736
H,0,0.3569704583,-3.3512805983,-2.8541868638
H,0,2.0436898438,-1.473933009,-3.7477035699
H,0,2.231572473,0.1319913907,-2.9933375282
H,0,2.6935253513,-1.30753183,-2.0875804675
H,0,-0.4273858523,-1.0584754497,-4.4820320519
H,0,-1.7844232578,-0.6704133584,-3.3796510571
H,0,-0.5877755562,0.5779272267,-3.7587933096
H,0,0.4635467702,-4.1720778251,2.2880828518
H,0,1.6173590395,-2.8098586627,2.2589675194

H,0,0.0825415629,-2.6428311145,3.1219488982
H,0,-1.9495128534,-4.1455770287,1.2200817611
H,0,-2.4243871569,-2.5484077425,1.8732697148
H,0,-2.6023018881,-2.8720626451,0.1404152977
H,0,5.7979360065,2.9206048385,-0.1014959457
H,0,4.1875227737,3.6589816419,-0.0447155286
H,0,5.0365210119,3.2687162981,1.451254656

dmpeBpin3MetaTolHCHactTSSptSptFrntA
E(RB+HF-LYP) = -2059.07150335

Zero-point correction= 0.548183 (Hartree/Particle)
Thermal correction to Energy= 0.585458
Thermal correction to Enthalpy= 0.586403
Thermal correction to Gibbs Free Energy= 0.477453
Sum of electronic and zero-point Energies= -2058.523321
Sum of electronic and thermal Energies= -2058.486045
Sum of electronic and thermal Enthalpies= -2058.485101
Sum of electronic and thermal Free Energies= -2058.594050

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	367.381	135.728	229.304

C,0,-0.3985423567,-3.4603559903,0.0487040878
C,0,0.7138206953,-3.1505022413,1.0616679545
P,0,0.5511942421,-1.4162172205,1.7465151097
Ir,0,-0.0978247471,0.0197944133,-0.0678755992
B,0,0.1174454376,1.6779811135,1.2086001764
O,0,0.3892465443,2.9953495262,0.8690144324
C,0,0.3383786046,3.8221222427,2.0329928057
C,0,0.3369872271,2.8299686305,3.2126862307
O,0,0.0335746241,1.5644049499,2.6124690193
P,0,-0.6212750119,-2.0895268154,-1.2172588403
B,0,-1.0968155,1.2229036877,-1.5249928738
O,0,-1.9254553128,0.6715892204,-2.5118401677
C,0,-2.3593681084,1.7210003475,-3.3893877546
C,0,-1.9845735128,3.0144063547,-2.6417634273
O,0,-1.0260727254,2.5954536191,-1.6675054236
B,0,-2.0979160872,0.1203447804,0.6561987303
O,0,-2.8477073325,-0.9748460847,1.121360596
C,0,-4.1011603382,-0.5132994135,1.6468768567
C,0,-4.2033550605,0.9444812735,1.1615895721
O,0,-2.8762008944,1.2762022115,0.7418665171

C,0,-2.3426963628,-2.421611249,-1.8007158416
C,0,0.3206008084,-2.6857832152,-2.7027010991
H,0,-0.2189952437,-4.4182443292,-0.4537014457
H,0,-1.3607334525,-3.5410827901,0.566752846
C,0,-0.5485712628,-1.6278962634,3.2109157126
C,0,2.1824116306,-1.1223382841,2.5528128322
H,0,0.7152931139,-3.8793114166,1.8812481497
H,0,1.6966214732,-3.2066863257,0.5804643627
H,0,-0.4154131244,3.0695449506,3.9715410545
H,0,1.3166338388,2.7719544225,3.7056896607
H,0,-0.5749164264,4.4296364765,2.0024934983
H,0,1.2005842952,4.4974092818,2.0453350729
H,0,-2.8476668042,3.4567785771,-2.1283000448
H,0,-1.5404460472,3.7737449666,-3.2929067267
H,0,-3.4341975805,1.6266017342,-3.574704989
H,0,-1.8328787347,1.6285974985,-4.3483097441
H,0,-4.5250924532,1.6346287806,1.9479130753
H,0,-4.8876586493,1.0486216602,0.3097936114
H,0,-4.0807754534,-0.5856081371,2.7419421436
H,0,-4.9126521056,-1.1473147529,1.2751590556
H,0,-2.4433647336,-3.4453361002,-2.176753403
H,0,-3.0290820777,-2.2607556447,-0.9681500477
H,0,-2.5791221517,-1.705367325,-2.5892640365
H,0,0.0091694078,-3.695275906,-2.9915790559
H,0,0.11385613,-2.0014796387,-3.5308900364
H,0,1.396682384,-2.6769159688,-2.5256427221
H,0,2.4247739755,-1.9231370016,3.2589977254
H,0,2.9619612833,-1.0472313401,1.7928697063
H,0,2.1218524022,-0.1715579843,3.0869668814
H,0,-0.1258807353,-2.3494321237,3.9176334275
H,0,-0.645777562,-0.6505989277,3.6886582475
H,0,-1.5349457226,-1.953160358,2.8788075301
H,0,0.6383675979,0.6449334361,-1.3776136878
C,0,2.1051888847,0.2556744846,-0.6765188047
C,0,2.926236833,-0.8553543203,-0.9536962338
C,0,4.3086347145,-0.7522295313,-1.1692776748
C,0,4.8975338809,0.5181660393,-1.1389655323
C,0,4.1082090171,1.6403584592,-0.9000503631
C,0,2.733250137,1.5149910311,-0.6768773891
H,0,2.4955949147,-1.8510126396,-0.9867512986
C,0,5.1490762517,-1.9841510201,-1.4228153005
H,0,5.9662310389,0.6250526615,-1.3122918437
H,0,4.5622202144,2.6288136926,-0.8936217104
H,0,2.1412939093,2.4057285207,-0.5001925744

H,0,5.8645414042,-2.1578309377,-0.6095230601
H,0,4.5293771765,-2.8816887702,-1.5139713364
H,0,5.7332430008,-1.8882869815,-2.345330932

dmpeBpin3MetaTolHCHactTSSptSptFrntS
E(RB+HF-LYP) = -2059.07155341

Zero-point correction= 0.547854 (Hartree/Particle)
Thermal correction to Energy= 0.585338
Thermal correction to Enthalpy= 0.586282
Thermal correction to Gibbs Free Energy= 0.476260
Sum of electronic and zero-point Energies= -2058.523699
Sum of electronic and thermal Energies= -2058.486216
Sum of electronic and thermal Enthalpies= -2058.485272
Sum of electronic and thermal Free Energies= -2058.595294

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.305	135.935	231.561

C,0,-0.4156538602,-3.4311505041,-0.994954503
C,0,-1.3150937123,-2.6256883738,-1.9439596914
P,0,-0.7054858194,-0.865232959,-2.1162944108
Ir,0,0.0412098132,-0.1418082357,0.0563997757
B,0,0.3871985026,1.7735625205,-0.7401275115
O,0,0.3488218257,2.9984774768,-0.0886585425
C,0,0.7599924462,4.0394489637,-0.9763610029
C,0,0.7397900922,3.3873649822,-2.3727977249
O,0,0.6676043112,1.9812728018,-2.1068775588
P,0,-0.108159989,-2.5371366595,0.6257183471
B,0,1.1414866937,0.3748839209,1.8122851787
O,0,1.7314227102,-0.5864994187,2.644054458
C,0,2.314302943,0.0752253437,3.7760583787
C,0,2.304757523,1.5656504423,3.3870348659
O,0,1.3697095857,1.6447972161,2.3088055898
B,0,2.0703233108,-0.4390068583,-0.5155394067
O,0,2.5615661188,-1.5726813654,-1.1914248227
C,0,3.9433347777,-1.371905851,-1.525503945
C,0,4.3597900994,-0.1371444216,-0.7041434358
O,0,3.1237808978,0.4439782036,-0.2776733537
C,0,1.3837481663,-3.4298675191,1.249727081
C,0,-1.3821380943,-3.2361794871,1.7824304846
H,0,-0.8261221655,-4.4314609983,-0.8132208976
H,0,0.5765848834,-3.5555246958,-1.4422499123

C,0,0.4787369624,-0.9588751359,-3.5262322102
C,0,-2.1287592473,0.0129356549,-2.8912050226
H,0,-1.3719812209,-3.1007021491,-2.9308497736
H,0,-2.337927992,-2.5730535752,-1.5545596615
H,0,1.6375603983,3.6072563709,-2.9601336252
H,0,-0.1376385998,3.6916121882,-2.9592943647
H,0,1.7645766306,4.3777301694,-0.6926708846
H,0,0.0743394571,4.8895421613,-0.8931107806
H,0,3.2871984119,1.9045248478,3.0347472014
H,0,1.9829598708,2.2208146206,4.2026272851
H,0,3.3211255181,-0.3161290643,3.954130733
H,0,1.7025962569,-0.1258532486,4.6652616665
H,0,4.9271954705,0.5925869532,-1.2905150818
H,0,4.9546151165,-0.4082848887,0.1774613886
H,0,4.0300005618,-1.1990369542,-2.6059479332
H,0,4.5178180077,-2.2690453625,-1.2730059202
H,0,1.1995562759,-4.5072514455,1.3187124068
H,0,2.2130349252,-3.2366044218,0.5680974222
H,0,1.6409358936,-3.0263217795,2.2302968526
H,0,-1.3233031138,-4.3290911657,1.8215875593
H,0,-1.1892908904,-2.83658212,2.782502801
H,0,-2.3923826263,-2.9408042381,1.4971807637
H,0,-2.4638719377,-0.4988677562,-3.799247142
H,0,-2.9519498583,0.0842021938,-2.1785618779
H,0,-1.7992326216,1.023018776,-3.1460484078
H,0,-0.0115778752,-1.3519738378,-4.4226479053
H,0,0.8456881172,0.0524835138,-3.7135637416
H,0,1.3218049876,-1.5914340944,-3.2463008698
H,0,-0.6717570813,0.3111106686,1.4460599063
C,0,-2.0980330036,0.5003577052,0.595487077
C,0,-3.1806340509,-0.394098032,0.4988632114
C,0,-4.5010476292,0.0317589683,0.6719963393
C,0,-4.7786510535,1.3623444033,0.9796237197
C,0,-3.7285267035,2.2772532638,1.1192646819
C,0,-2.4114813011,1.8326750224,0.9259417615
H,0,-3.0086985792,-1.436451705,0.2575752418
H,0,-5.3153795383,-0.6818600255,0.5646701902
H,0,-5.8070102837,1.688732027,1.1183764717
C,0,-4.0023570658,3.7136521435,1.5050843414
H,0,-1.6037280022,2.5496589891,1.031335421
H,0,-3.1914118368,4.3740325328,1.1845799062
H,0,-4.9353735016,4.0782358408,1.06225249
H,0,-4.0981714105,3.8210674542,2.5933073961

dmpe Bpin3 Ortho Toluene CH Activation Transition Structure
E(RB+HF-LYP) = -2059.06117747

Zero-point correction= 0.548851 (Hartree/Particle)
Thermal correction to Energy= 0.585660
Thermal correction to Enthalpy= 0.586604
Thermal correction to Gibbs Free Energy= 0.480423
Sum of electronic and zero-point Energies= -2058.512326
Sum of electronic and thermal Energies= -2058.475518
Sum of electronic and thermal Enthalpies= -2058.474574
Sum of electronic and thermal Free Energies= -2058.580755

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	367.507	135.615	223.477

C,0,-0.1259625702,-3.5302254527,0.1976803156
C,0,0.8790992451,-3.13280587,1.288091278
P,0,0.6598240132,-1.3526506238,1.8314906892
Ir,0,0.0252025606,-0.0527960806,-0.1056054856
B,0,-0.0576037293,1.6662195753,1.1083311229
O,0,-0.5748972786,2.9167550822,0.8057702326
C,0,-0.66045866,3.7076814448,1.9899084941
C,0,0.2069895763,2.9576531143,3.01805566
O,0,0.3545884003,1.6459872877,2.4585431194
P,0,-0.249252284,-2.2637672122,-1.1828084051
B,0,-1.0562778646,0.9805911686,-1.63034072
O,0,-2.069616229,0.3788539616,-2.386036246
C,0,-2.526652273,1.3064083077,-3.381438808
C,0,-1.9003859954,2.6503420356,-2.9642372321
O,0,-0.8578401764,2.283974023,-2.0570487336
B,0,-2.0127965645,-0.1731962849,0.5322857249
O,0,-2.676993,-1.3732204281,0.8542258142
C,0,-3.9923155842,-1.0789594524,1.3489360084
C,0,-4.2006627769,0.4065212553,1.0054780436
O,0,-2.8865531003,0.8951107443,0.7213826082
C,0,-1.8621988643,-2.7434834145,-1.9472171785
C,0,0.8884421766,-2.9005278585,-2.5080729775
H,0,0.1071363257,-4.520521625,-0.2112987528
H,0,-1.1334235458,-3.5752770582,0.6236936557
C,0,-0.5126801436,-1.4832046532,3.2500539686
C,0,2.2390864821,-0.9761730471,2.7018607369
H,0,0.7929107855,-3.7940476573,2.1587429137
H,0,1.9061342255,-3.2284141827,0.9199183161

H,0,-0.2595796558,2.8897461775,4.0066751742
H,0,1.1986342233,3.4142887184,3.1357496865
H,0,-1.7101907519,3.7717831294,2.3055885491
H,0,-0.299216935,4.721629892,1.7868012325
H,0,-2.6170914312,3.2969773616,-2.4433522537
H,0,-1.476539576,3.2065956268,-3.8061130726
H,0,-3.6209653436,1.3270047283,-3.3893837719
H,0,-2.1797045683,0.9745360055,-4.3687715004
H,0,-4.637892041,0.9794818658,1.8292319634
H,0,-4.8326447061,0.5388911052,0.1181366355
H,0,-4.0192599028,-1.2631696854,2.4311131498
H,0,-4.723021396,-1.7381724815,0.8696322163
H,0,-1.8492381358,-3.7954475678,-2.2517823187
H,0,-2.6563091679,-2.5737772563,-1.2203369189
H,0,-2.0477155126,-2.104933753,-2.8117877699
H,0,0.6709144326,-3.9481855273,-2.7413680824
H,0,0.7265539769,-2.299993256,-3.4085403343
H,0,1.9374766466,-2.8009702874,-2.2304064343
H,0,2.4442518536,-1.7194358811,3.4793087118
H,0,3.0607772459,-0.9494805779,1.985043576
H,0,2.131429778,0.0136851421,3.148773617
H,0,-0.1117252298,-2.137241408,4.0308746257
H,0,-0.6572260736,-0.4780072828,3.6521219566
H,0,-1.4695361688,-1.8668810898,2.8941238937
H,0,0.7470412272,0.5476925434,-1.4246137799
C,0,2.266668319,0.2664380191,-0.5912747861
C,0,3.0808587135,-0.8838335474,-0.6520189172
C,0,4.4694513706,-0.8416461311,-0.7983884998
C,0,5.1062987231,0.3899063346,-0.9207127813
C,0,4.3283269443,1.5430422245,-0.9009600308
C,0,2.9296475609,1.5133912897,-0.7460482239
H,0,2.6293737657,-1.8632594436,-0.5604972362
H,0,5.0396002682,-1.7676918208,-0.8201751145
H,0,6.1840984037,0.4535971417,-1.0439424368
H,0,4.8117608094,2.5108135266,-1.0178244614
C,0,2.2212918895,2.8495279545,-0.7566525713
H,0,2.8416198269,3.6024569494,-1.2543560506
H,0,1.2529252357,2.8106953323,-1.255437716
H,0,2.0342850745,3.2085253615,0.2615162715

dmpeBpin3OrthoTolHCHactTSParSptBackA
E(RB+HF-LYP) = -2059.05413039

Zero-point correction= 0.549152 (Hartree/Particle)

Thermal correction to Energy= 0.585794
Thermal correction to Enthalpy= 0.586739
Thermal correction to Gibbs Free Energy= 0.480885
Sum of electronic and zero-point Energies= -2058.504978
Sum of electronic and thermal Energies= -2058.468336
Sum of electronic and thermal Enthalpies= -2058.467392
Sum of electronic and thermal Free Energies= -2058.573245

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.591	135.286	222.787

C,0,-1.8754277568,2.4018444124,-0.4949547452
C,0,-1.6667776111,1.0797234463,-0.9389136755
C,0,-2.6331637454,0.5339125833,-1.8248808188
C,0,-3.789629958,1.2846194989,-2.1072135088
C,0,-4.0059275469,2.5621571699,-1.5982218117
C,0,-3.0224101934,3.1358741087,-0.7979766037
Ir,0,0.1111872461,0.0178537492,-0.0040746273
B,0,1.6001959174,1.4806938225,-0.6936627691
O,0,1.4387361325,2.8648634166,-0.640341189
C,0,2.6497160632,3.5092933614,-1.0598534435
C,0,3.4934103254,2.3735070415,-1.6688426342
O,0,2.8569412647,1.170636466,-1.208814075
P,0,1.731943389,-1.1893474125,1.1982052559
C,0,2.0127167681,-0.3575005925,2.8476050736
C,0,0.7010555121,0.2051403776,3.4154561134
P,0,-0.1656413486,1.2576618642,2.139654531
B,0,0.6022395804,-1.1953805242,-1.6341890852
O,0,1.081426162,-2.5122125046,-1.5537522098
C,0,1.5306767122,-2.9366204932,-2.8464187764
C,0,0.9778651811,-1.8711268008,-3.8110705165
O,0,0.6342020091,-0.7704867756,-2.9653233148
B,0,-1.2815752597,-1.4769725264,0.752379769
O,0,-1.8208907971,-2.5478272052,0.0448434287
C,0,-2.8025000047,-3.2287205529,0.8345406013
C,0,-2.6015814489,-2.675218922,2.2575664921
O,0,-1.7633413927,-1.5234342818,2.0762958307
H,0,-0.0653175612,1.0756484021,-1.2435480885
H,0,-3.801456719,-3.0054865844,0.4396226297
H,0,-2.6404786495,-4.3093958957,0.7692235892
H,0,-3.5387192624,-2.3769468029,2.7382280589
H,0,-2.0922595865,-3.3925524702,2.9146693292
H,0,4.5365469005,2.3876859385,-1.337310676

H,0,3.4773154071,2.386861302,-2.7650417844
H,0,3.1351610206,3.9674857688,-0.1880632356
H,0,2.4132033004,4.3007203199,-1.7771533483
H,0,1.1527993235,-3.9422691695,-3.0563830826
H,0,2.6286844106,-2.970027927,-2.8559742988
H,0,0.0780510218,-2.2203933343,-4.3350831206
H,0,1.7095699405,-1.5484438619,-4.5584928391
H,0,-1.094565894,2.8874492424,0.077407362
H,0,-3.1319418055,4.1490663846,-0.4188994918
C,0,-2.4938984248,-0.7910716412,-2.5367866974
H,0,-4.5364922753,0.8441080595,-2.7641787149
H,0,-4.913948386,3.1054391586,-1.8459329017
C,0,1.3458622673,-2.930859429,1.6754417596
C,0,3.4419200863,-1.3906593299,0.5423054041
C,0,-1.8147709054,1.5636480011,2.9144253017
C,0,0.6661841328,2.896317191,2.4108555544
H,0,0.0081810096,-0.6066977914,3.6559221123
H,0,0.8837027451,0.7795095166,4.3313229595
H,0,2.4787570806,-1.0654141293,3.5433370171
H,0,2.7351064364,0.4506805812,2.6794971274
H,0,0.5338122442,3.2345185789,3.4440541882
H,0,1.7329430428,2.8081762268,2.1921857273
H,0,0.2579080823,3.6443442109,1.7287734492
H,0,-1.711748988,1.9905471185,3.9175835717
H,0,-2.3854769768,2.2504199435,2.284863246
H,0,-2.3447545003,0.6121118617,2.9621754871
H,0,4.0931846056,-1.8254738752,1.3076253157
H,0,3.3950180797,-2.0619519196,-0.3174897046
H,0,3.8270875411,-0.428614226,0.2059075322
H,0,2.1974549121,-3.3866123959,2.1909831447
H,0,0.4717889721,-2.9510603053,2.3287395501
H,0,1.1229490357,-3.4838712738,0.7612706156
H,0,-3.4346546518,-1.0581761155,-3.0291262815
H,0,-1.7168427122,-0.7249719002,-3.3036272533
H,0,-2.2173206402,-1.5954414648,-1.855523447

dmpeBpin3OrthoTolHCHactTSSptSptBack
E(RB+HF-LYP) = -2059.06343158

Zero-point correction= 0.548427 (Hartree/Particle)
Thermal correction to Energy= 0.585310
Thermal correction to Enthalpy= 0.586254
Thermal correction to Gibbs Free Energy= 0.479921
Sum of electronic and zero-point Energies= -2058.515005

Sum of electronic and thermal Energies= -2058.478122
Sum of electronic and thermal Enthalpies= -2058.477177
Sum of electronic and thermal Free Energies= -2058.583511

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.288	135.740	223.797

C,0,3.149868173,-0.7022192723,0.5344583738
C,0,2.2569510986,0.3816714867,0.6635881627
C,0,2.8150010289,1.6118093183,1.1009126148
C,0,4.2013300628,1.7077184296,1.321052608
C,0,5.062073287,0.6289897564,1.1435802164
C,0,4.5253645796,-0.5943251874,0.7505017362
Ir,0,0.0419675857,0.0140006615,0.0501397041
P,0,0.6298586747,-0.6901572117,-2.1778101742
C,0,0.3736901435,-2.54330127,-2.2651291842
C,0,0.7691180049,-3.2552262208,-0.9606554566
P,0,0.0370688177,-2.3893867437,0.5341776395
B,0,-2.0114851074,-0.1006028054,-0.5050644537
O,0,-2.5200490217,-0.938231401,-1.5214309039
C,0,-3.9245200222,-0.6923090678,-1.6885506072
C,0,-4.3155698483,0.1221704583,-0.4423109931
O,0,-3.0705003197,0.583978261,0.0856868061
B,0,-0.9759012401,0.4565432941,1.8743073984
O,0,-1.566199809,-0.5494162788,2.6506751794
C,0,-2.1207044957,0.0463170808,3.8329162257
C,0,-2.0609881158,1.562070824,3.5587255096
O,0,-1.1323489299,1.6898757083,2.4786297176
B,0,-0.1407202094,1.978962465,-0.6887151187
O,0,-1.0172182935,2.980873322,-0.2965415225
C,0,-0.7362425295,4.1825724069,-1.0144074658
C,0,0.1835242038,3.7383110924,-2.1684254332
O,0,0.6325651236,2.4343698527,-1.7781503132
H,0,-4.0846674104,-0.1298580625,-2.6176103857
H,0,-4.459278541,-1.6445066804,-1.7667020933
H,0,-4.9578300036,0.9774504101,-0.6747382965
H,0,-4.8222193354,-0.4958772593,0.3105576716
H,0,-3.1411067752,-0.3194255402,3.9858469263
H,0,-1.514289611,-0.2442465684,4.7006391127
H,0,-3.0320771429,1.961091409,3.2420589638
H,0,-1.7079094724,2.1402918044,4.4183219308
H,0,-0.3559313973,3.6667918054,-3.1231272224
H,0,1.0445584044,4.3996152454,-2.3114201867

H,0,-1.6715318137,4.6342358341,-1.3615448318
H,0,-0.2392818254,4.8967532967,-0.3444289649
H,0,0.755562398,0.3776577258,1.4656721554
H,0,2.7738111579,-1.6720294851,0.2310166057
H,0,5.1650163825,-1.4637143584,0.6161935214
C,0,1.9979415444,2.8599210629,1.3582094389
H,0,4.6064488824,2.6612363271,1.6539527885
H,0,6.1276792531,0.7390607324,1.3259838689
C,0,-0.309898963,-0.0932628673,-3.6474352542
C,0,2.3615928458,-0.4176098849,-2.7545765787
C,0,-1.6013392707,-3.2256001788,0.7100858721
C,0,0.9421998734,-3.1436963689,1.9625621303
H,0,0.4516049522,-4.3048135336,-0.9794678104
H,0,1.8585696363,-3.2552498766,-0.842559138
H,0,-0.6968476947,-2.6741721479,-2.4542037751
H,0,0.9175714264,-2.9600018652,-3.1211614076
H,0,2.5152570118,-0.8658933874,-3.7416963222
H,0,2.5185746653,0.6622060451,-2.8115255748
H,0,3.0818059444,-0.8251639094,-2.0453299062
H,0,0.02255975,-0.6056196356,-4.5559104348
H,0,-1.3721872765,-0.2732835554,-3.4840359526
H,0,-0.1305776723,0.9789496009,-3.7459301359
H,0,0.9386560736,-4.2376014093,1.9097748275
H,0,1.9710631243,-2.7819472074,2.0025135439
H,0,0.4334656781,-2.8293802486,2.8779581011
H,0,-1.4855631988,-4.3073726848,0.8347963539
H,0,-2.097353873,-2.8002638591,1.5851926666
H,0,-2.2083867614,-3.0139453402,-0.1717023625
H,0,2.527587776,3.5266597654,2.0467127097
H,0,1.8382386267,3.4172969294,0.4285431415
H,0,1.0160007897,2.6408919615,1.7805400373

dmpeBpin2OrthoTolHBpinRotTS
E(RB+HF-LYP) = -2059.05413039

Zero-point correction= 0.549152 (Hartree/Particle)
Thermal correction to Energy= 0.585794
Thermal correction to Enthalpy= 0.586739
Thermal correction to Gibbs Free Energy= 0.480885
Sum of electronic and zero-point Energies= -2058.504978
Sum of electronic and thermal Energies= -2058.468336
Sum of electronic and thermal Enthalpies= -2058.467392
Sum of electronic and thermal Free Energies= -2058.573245

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	367.591	135.286	222.787

C,0,-1.875427757,2.4018444122,-0.4949547449
C,0,-1.6667776116,1.079723446,-0.938913675
C,0,-2.6331637462,0.5339125828,-1.8248808177
C,0,-3.789629959,1.2846194983,-2.1072135073
C,0,-4.0059275477,2.5621571694,-1.5982218104
C,0,-3.0224101938,3.1358741085,-0.797976603
Ir,0,0.1111872461,0.0178537492,-0.0040746273
B,0,1.6001959171,1.4806938223,-0.6936627702
O,0,1.4387361322,2.8648634164,-0.6403411906
C,0,2.6497160627,3.5092933612,-1.0598534458
C,0,3.4934103248,2.373507041,-1.6688426362
O,0,2.8569412643,1.1706364656,-1.2088140764
P,0,1.7319433896,-1.1893474123,1.1982052553
C,0,2.0127167695,-0.3575005918,2.8476050726
C,0,0.7010555139,0.2051403785,3.415456113
P,0,-0.1656413475,1.2576618648,2.1396545308
B,0,0.6022395796,-1.1953805246,-1.6341890852
O,0,1.0814261611,-2.5122125051,-1.5537522097
C,0,1.5306767105,-2.936620494,-2.8464187765
C,0,0.9778651792,-1.8711268018,-3.8110705165
O,0,0.6342020077,-0.7704867763,-2.9653233149
B,0,-1.2815752593,-1.4769725261,0.75237977
O,0,-1.8208907971,-2.5478272051,0.0448434303
C,0,-2.8025000044,-3.2287205526,0.8345406036
C,0,-2.6015814481,-2.6752189211,2.2575664941
O,0,-1.7633413918,-1.523434281,2.076295832
H,0,-0.0653175618,1.0756484018,-1.2435480888
H,0,-3.8014567189,-3.0054865841,0.4396226322
H,0,-2.6404786492,-4.3093958953,0.7692235918
H,0,-3.5387192614,-2.3769468017,2.738228061
H,0,-2.0922595855,-3.392552469,2.9146693313
H,0,4.5365469,2.3876859382,-1.3373106781
H,0,3.4773154063,2.3868613011,-2.7650417864
H,0,3.1351610203,3.967485769,-0.1880632383
H,0,2.4132032996,4.3007203192,-1.777153351
H,0,1.1527993216,-3.9422691703,-3.0563830822
H,0,2.6286844089,-2.970027928,-2.8559742994
H,0,0.0780510196,-2.2203933352,-4.3350831201
H,0,1.7095699382,-1.5484438631,-4.5584928395
H,0,-1.094565894,2.8874492424,0.0774073618

H,0,-3.1319418057,4.1490663844,-0.4188994914
C,0,-2.493898426,-0.7910716419,-2.536786696
H,0,-4.5364922767,0.8441080587,-2.7641787129
H,0,-4.9139483869,3.1054391581,-1.8459329001
C,0,1.3458622678,-2.9308594286,1.6754417598
C,0,3.4419200865,-1.39065933,0.5423054027
C,0,-1.8147709038,1.563648002,2.9144253022
C,0,0.6661841341,2.8963171917,2.4108555532
H,0,0.0081810114,-0.6066977904,3.6559221125
H,0,0.8837027474,0.7795095177,4.3313229588
H,0,2.4787570824,-1.0654141284,3.5433370161
H,0,2.7351064378,0.4506805818,2.6794971259
H,0,0.5338122461,3.2345185798,3.444054187
H,0,1.732943044,2.8081762274,2.1921857256
H,0,0.2579080832,3.6443442114,1.7287734481
H,0,-1.7117489859,1.9905471196,3.9175835721
H,0,-2.3854769755,2.2504199442,2.2848632466
H,0,-2.3447544987,0.6121118625,2.9621754882
H,0,4.0931846061,-1.8254738752,1.3076253142
H,0,3.3950180794,-2.0619519201,-0.3174897057
H,0,3.8270875412,-0.4286142263,0.2059075303
H,0,2.1974549129,-3.3866123954,2.1909831446
H,0,0.471788973,-2.9510603046,2.3287395507
H,0,1.1229490358,-3.4838712736,0.7612706161
H,0,-3.4346546533,-1.0581761163,-3.0291262796
H,0,-1.7168427138,-0.7249719011,-3.3036272523
H,0,-2.2173206411,-1.5954414653,-1.8555234455

dmpe Bpin3 Para Anisole CH Activation Transition Structure
E(RB+HF-LYP) = -2134.27375331

Zero-point correction= 0.552920 (Hartree/Particle)
Thermal correction to Energy= 0.591250
Thermal correction to Enthalpy= 0.592194
Thermal correction to Gibbs Free Energy= 0.479774
Sum of electronic and zero-point Energies= -2133.720834
Sum of electronic and thermal Energies= -2133.682504
Sum of electronic and thermal Enthalpies= -2133.681560
Sum of electronic and thermal Free Energies= -2133.793979

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	371.015	138.967	236.607

C,0,2.6256561976,1.276860249,0.2528065961
C,0,1.8894497623,0.149697513,0.6564995344
C,0,2.5859813595,-0.7871822271,1.4470554358
C,0,3.9388643503,-0.6512317718,1.7525243771
C,0,4.656187174,0.4575584976,1.2893806748
C,0,3.9874561249,1.431850552,0.5417287372
Ir,0,-0.281135342,-0.080335101,-0.0278391415
P,0,0.186945152,0.0729347164,-2.3878153658
C,0,-0.2380173617,-1.5847375271,-3.131660041
C,0,0.335379229,-2.7256324061,-2.2817305654
P,0,-0.0940463111,-2.5200567832,-0.4658721214
B,0,-2.3268431638,0.0758119623,-0.6174632136
O,0,-2.9812703863,1.2870001294,-0.8549999154
C,0,-4.3827983964,1.052231568,-1.0206189618
C,0,-4.483966858,-0.4607965154,-1.2870569372
O,0,-3.2181738183,-0.9810616221,-0.8575745417
B,0,-1.3532033011,-0.5419081436,1.7407984116
O,0,-1.0583527052,-1.6736785991,2.5149388382
C,0,-2.0512464054,-1.8062019173,3.5426859511
C,0,-2.7986020254,-0.458211003,3.5261556685
O,0,-2.437560214,0.1361383656,2.2747141124
B,0,-0.4873546217,1.9941406278,0.1992984332
O,0,-0.7730472347,2.6460391587,1.3916827938
C,0,-0.6674928288,4.0593953142,1.2080952557
C,0,-0.5344378443,4.2450167857,-0.317503612
O,0,-0.2272130556,2.9342231043,-0.8098242801
H,0,-4.9064142545,1.3439372667,-0.1020025753
H,0,-4.7662060313,1.6601466632,-1.8467737634
H,0,-5.2904349035,-0.9419550691,-0.7245350405
H,0,-4.6256122714,-0.6876045225,-2.3523526704
H,0,-2.7121725288,-2.6485321858,3.299270715
H,0,-1.5632584863,-2.0153742679,4.4996158807
H,0,-3.885945565,-0.5720988455,3.5799941535
H,0,-2.478580294,0.2028215232,4.341101984
H,0,-1.4703304453,4.5906806507,-0.7744272185
H,0,0.2646279976,4.9404579205,-0.5962733269
H,0,-1.5547812142,4.5527817925,1.6183965074
H,0,0.2134865776,4.4291912598,1.7486275982
H,0,0.4236998704,0.1615692262,1.4130905747
H,0,2.1346379953,2.0661276428,-0.3077817486
H,0,4.5045875322,2.3169403152,0.1868631858
H,0,2.0517404534,-1.6336870173,1.8643593173
H,0,4.4538649084,-1.3848111814,2.3661386387
O,0,5.9822988467,0.5048718219,1.6332342011

C,0,-0.7376000541,1.2490295579,-3.462492766
C,0,1.9284081971,0.3419667451,-2.9474365162
C,0,-1.5913509182,-3.5863084907,-0.2684308016
C,0,1.1781297324,-3.628742048,0.3003764416
H,0,-0.0091016298,-3.7012484803,-2.6438173029
H,0,1.4301327824,-2.7283693205,-2.3480317945
H,0,-1.3326603514,-1.6390318429,-3.1483081575
H,0,0.1154705152,-1.6413658824,-4.1682994541
H,0,1.1383530388,-4.6257347391,-0.151249947
H,0,2.1776922706,-3.2109533904,0.1676367411
H,0,0.976742811,-3.7165675667,1.3710262179
H,0,-1.4099628781,-4.5984258744,-0.6454721634
H,0,-1.8310977244,-3.6345951908,0.796735059
H,0,-2.4343380953,-3.1256083838,-0.7831276488
H,0,2.0168120728,0.2096821379,-4.0307928755
H,0,2.2363289687,1.3560833691,-2.6843484216
H,0,2.5969253254,-0.3506912765,-2.4321532652
H,0,-0.4895395411,1.0997522388,-4.5183263852
H,0,-1.8101623426,1.1179907038,-3.3069779997
H,0,-0.4816961526,2.261825159,-3.1480961656
C,0,6.7360965884,1.6285469836,1.2175395187
H,0,7.7482063131,1.473143942,1.5961750531
H,0,6.7722191465,1.7146208079,0.1229294458
H,0,6.337682687,2.5643959353,1.6320672937

dmpeBpin3ParaAnisCHactTSParSptBackA
E(RB+HF-LYP) = -2134.27585367

Zero-point correction= 0.553088 (Hartree/Particle)
Thermal correction to Energy= 0.591233
Thermal correction to Enthalpy= 0.592177
Thermal correction to Gibbs Free Energy= 0.481323
Sum of electronic and zero-point Energies= -2133.722766
Sum of electronic and thermal Energies= -2133.684620
Sum of electronic and thermal Enthalpies= -2133.683676
Sum of electronic and thermal Free Energies= -2133.794531

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	371.004	138.981	233.314

C,0,3.9590141604,1.6562994104,0.3834842086
C,0,2.5857277235,1.4599786227,0.1899621019
C,0,1.9218434143,0.285677192,0.5822092227

C,0,2.7144634009,-0.6591501417,1.264515773
C,0,4.0818804484,-0.4871660692,1.4735519659
C,0,4.7206321687,0.6720674671,1.0203387361
Ir,0,-0.2578238803,-0.0782294948,0.0185234413
B,0,-0.5966062085,1.9714020641,-0.2585890779
O,0,-1.207262474,2.5441019155,-1.3875655895
C,0,-1.4147045226,3.9424112713,-1.1484742214
C,0,-0.5443377821,4.2535129137,0.0856888524
O,0,-0.2253654138,2.9719232487,0.6313073402
O,0,6.067605846,0.7536735308,1.2624477088
P,0,0.3516207404,-0.4393030075,-2.2908544874
C,0,2.1311872508,-0.2015137547,-2.7276407202
P,0,-0.1991376057,-2.5548583269,0.0983514497
C,0,0.7021164315,-3.6337685481,1.3094364569
B,0,-2.3034914644,-0.1448236132,-0.5853128663
O,0,-2.774227359,-0.7630484521,-1.7606568672
C,0,-4.1686820408,-0.4704885717,-1.9329051001
C,0,-4.6102408861,0.0840723658,-0.5664955507
O,0,-3.3871980217,0.4016359232,0.1038194695
B,0,-1.2703802,-0.0183839302,1.8902011038
O,0,-1.7237935044,1.0949687433,2.5703773979
C,0,-2.5560871394,0.6679588477,3.6504341138
C,0,-2.20671245,-0.8208355972,3.8357279144
O,0,-1.5772128542,-1.1886343679,2.5981304019
C,0,0.0632831656,-2.2403497524,-2.6902466852
C,0,0.5077449982,-3.1463914237,-1.5324745849
C,0,-0.4917110952,0.4269439822,-3.6795433778
C,0,-1.8547853427,-3.3811985681,0.1342672825
H,0,-5.1627001809,-0.6602650415,0.021791918
H,0,-5.2285856808,0.9833349949,-0.6510647645
H,0,-4.7039099391,-1.3813974783,-2.2206146125
H,0,-4.2852975282,0.2680070643,-2.7361260229
H,0,-3.0858733725,-1.4510189185,4.0041848095
H,0,-1.5002880682,-0.9820495602,4.6602058715
H,0,-3.6073915123,0.8097965853,3.3694178995
H,0,-2.3466068909,1.2717723604,4.53888853
H,0,-2.4803765936,4.1195910012,-0.9560218395
H,0,-1.1244884002,4.5166679085,-2.034947205
H,0,-1.0689585067,4.853125616,0.8363408264
H,0,0.3842745322,4.7753857734,-0.1829242383
H,0,0.4299883159,0.3894792169,1.4134664709
H,0,2.0264663717,2.2656308594,-0.2721121752
H,0,4.4119534606,2.5825116892,0.0462198675
H,0,2.2527256784,-1.5503110899,1.6715409341

H,0,4.6692347401,-1.2330832797,2.0015025274
H,0,0.2187275774,-4.188110756,-1.7165184847
H,0,1.5997596023,-3.1282378232,-1.4316346533
H,0,-1.014140904,-2.3362016686,-2.8579994559
H,0,0.5758565239,-2.5082030436,-3.621952657
H,0,2.3244369349,-0.5350739108,-3.7523535076
H,0,2.3873380396,0.856380391,-2.6382757165
H,0,2.7676001452,-0.748816424,-2.029888333
H,0,-0.0817130284,0.1105151151,-4.6440460175
H,0,-1.5563814072,0.1988035462,-3.6288979981
H,0,-0.368496389,1.5032297366,-3.5497048167
H,0,0.4759668709,-4.6895932421,1.1278249274
H,0,1.7814363879,-3.4896699434,1.2338616701
H,0,0.3791299943,-3.3683995494,2.3191898802
H,0,-1.7588630809,-4.4683980981,0.0455442009
H,0,-2.332312256,-3.129275817,1.0836615381
H,0,-2.4698732599,-2.9956911326,-0.6805278965
C,0,6.743774658,1.9290284146,0.856369104
H,0,7.7878251963,1.7953157153,1.1462810554
H,0,6.6898800342,2.0770299819,-0.2308981033
H,0,6.3444285967,2.8228450409,1.3542185188

dmpeBpin3ParaAnisCHactTSSptSptBackA
E(RB+HF-LYP) = -2134.27646546

Zero-point correction= 0.553391 (Hartree/Particle)
Thermal correction to Energy= 0.591415
Thermal correction to Enthalpy= 0.592359
Thermal correction to Gibbs Free Energy= 0.482422
Sum of electronic and zero-point Energies= -2133.723074
Sum of electronic and thermal Energies= -2133.685050
Sum of electronic and thermal Enthalpies= -2133.684106
Sum of electronic and thermal Free Energies= -2133.794044

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	371.119	138.825	231.383

C,0,2.839403597,-0.7616116838,0.6240291087
C,0,1.9144704741,0.2948222778,0.5966940935
C,0,2.4501061561,1.5767706288,0.850892328
C,0,3.8096586963,1.7869217067,1.0673993046
C,0,4.7076642881,0.7130873113,1.0553136791
C,0,4.2134730034,-0.5745762153,0.8338889773

Ir,0,-0.2797538294,-0.0362679709,0.0115606724
P,0,0.336929885,-0.7648412316,-2.2085379109
C,0,0.1083847895,-2.622223059,-2.2780683217
C,0,0.4952025874,-3.3126410429,-0.9604814491
P,0,-0.3103005595,-2.4490380914,0.494981702
B,0,-2.3080546513,-0.069020007,-0.6347944013
O,0,-2.8411442785,-0.9939827271,-1.5539539198
C,0,-4.1966742745,-0.6373093972,-1.8639630381
C,0,-4.5693790924,0.4086053633,-0.7967207865
O,0,-3.3170759023,0.8054514767,-0.2302097593
B,0,-1.3752323296,0.3850758082,1.7868782146
O,0,-1.9663696991,-0.6351793339,2.547737052
C,0,-2.5482775713,-0.053740002,3.7237913574
C,0,-2.542361438,1.4601733084,3.4370071948
O,0,-1.6060888243,1.616142989,2.3686445507
B,0,-0.4340910453,1.9701378109,-0.5968421832
O,0,-0.2176131809,3.0978150808,0.1887288003
C,0,-0.2996753581,4.2775224919,-0.6138773369
C,0,-0.9093844605,3.7946365493,-1.9429270073
O,0,-0.7511687213,2.3707270609,-1.9082555272
H,0,-4.2372825206,-0.2242506371,-2.8800881589
H,0,-4.8296816124,-1.529967894,-1.8295320399
H,0,-5.0779105303,1.2827137143,-1.2156201848
H,0,-5.204839413,-0.0147424484,-0.0082120596
H,0,-3.5539480483,-0.4583689834,3.8772509738
H,0,-1.9340848575,-0.3131711224,4.5960428352
H,0,-3.5256591387,1.8196793332,3.1082584786
H,0,-2.2230321423,2.0579914113,4.2964268115
H,0,-1.9773752428,4.0365183383,-2.0179846567
H,0,-0.4000481413,4.2034416604,-2.8221895801
H,0,-0.91759612,5.0252419613,-0.1065217952
H,0,0.7070557711,4.6958337354,-0.7487588226
H,0,0.4483092987,0.3439531773,1.4158114211
H,0,2.5100342051,-1.779532486,0.4486084187
H,0,4.8726439633,-1.436061036,0.8234051456
H,0,1.7819009437,2.429602024,0.8882295365
H,0,4.1967541826,2.7835780189,1.2594890321
O,0,6.024717546,1.0213942171,1.2758047958
C,0,-0.5693331287,-0.2116103255,-3.7151239523
C,0,2.0870586832,-0.5030694861,-2.7389545443
C,0,-1.9523780739,-3.2923754828,0.5916813916
C,0,0.5169112232,-3.1939174786,1.9747749443
H,0,0.2134733163,-4.3723147458,-0.9786546786
H,0,1.5804679486,-3.2719012005,-0.8139220612

H,0,-0.9575520399,-2.7708297892,-2.4807517204
H,0,0.6687362415,-3.0389006104,-3.1234498743
H,0,2.2781314633,-0.9850698826,-3.703337978
H,0,2.2613175324,0.5720747445,-2.8341980614
H,0,2.7801191916,-0.8839845635,-1.9879695468
H,0,-0.1600965488,-0.687950531,-4.611936636
H,0,-1.6226103145,-0.4701143219,-3.6025794769
H,0,-0.4842754131,0.8735344024,-3.7858952669
H,0,0.5216538023,-4.2879685219,1.9280573375
H,0,1.5396387781,-2.8277792099,2.0780141801
H,0,-0.0488870916,-2.8766369712,2.8548608745
H,0,-1.8377934833,-4.375548457,0.7060899989
H,0,-2.4819774013,-2.8814271078,1.4538731871
H,0,-2.5291007084,-3.0675316829,-0.30688715
C,0,6.9611922757,-0.0394914062,1.2847473567
H,0,7.9349385062,0.4147567649,1.4778417214
H,0,6.7434715146,-0.7706760385,2.0751507292
H,0,6.9951694443,-0.5631299533,0.3194545317

dmpeBpin3ParaAnisCHactTSSptSptFrntS
E(RB+HF-LYP) = -2134.27536754

Zero-point correction= 0.553494 (Hartree/Particle)
Thermal correction to Energy= 0.591500
Thermal correction to Enthalpy= 0.592445
Thermal correction to Gibbs Free Energy= 0.482400
Sum of electronic and zero-point Energies= -2133.721874
Sum of electronic and thermal Energies= -2133.683867
Sum of electronic and thermal Enthalpies= -2133.682923
Sum of electronic and thermal Free Energies= -2133.792967

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	371.172	138.766	231.608

C,0,0.0418590209,-3.4592430759,-0.6226109997
C,0,-1.0301249323,-2.9092395683,-1.5756373618
P,0,-0.7483650742,-1.0971003797,-1.951267415
Ir,0,-0.0211741474,-0.0398809512,0.0823286188
B,0,-0.1131624935,1.8195285958,-0.895528921
O,0,-0.3183272168,3.0764411711,-0.3441988019
C,0,-0.1933199115,4.0801910026,-1.3533712505
C,0,-0.2241710491,3.2993778287,-2.6820097877
O,0,-0.0054149603,1.9362978545,-2.2979857444

P,0,0.334535089,-2.3427755274,0.8590847368
B,0,1.0563912662,0.8264438668,1.7109968902
O,0,1.8437623649,0.0615020572,2.5825474739
C,0,2.3558380947,0.9178195291,3.6138976945
C,0,2.0702818139,2.3410060774,3.0980440667
O,0,1.083371244,2.1580836026,2.0802852411
B,0,1.9882948243,0.032144191,-0.6214353643
O,0,2.6578017893,-1.0193644394,-1.2740607382
C,0,3.9442187318,-0.5676226949,-1.7218126332
C,0,4.1553001354,0.7678816446,-0.9851508312
O,0,2.8541826504,1.1217102116,-0.5061746855
C,0,2.0200170775,-2.8918797708,1.3812428953
C,0,-0.6666432709,-3.1120600067,2.2209942461
H,0,-0.2068385221,-4.4748445435,-0.2927151676
H,0,1.0058455483,-3.5120952729,-1.1407128004
C,0,0.3450966857,-1.1273279642,-3.4351340817
C,0,-2.3504554271,-0.5608094996,-2.6882182375
H,0,-1.0596699504,-3.4850778091,-2.5085608798
H,0,-2.0243126904,-2.985281323,-1.1221766701
H,0,0.5558007609,3.6167735987,-3.3821749277
H,0,-1.1952506329,3.382725681,-3.1884038701
H,0,0.753502664,4.6162878384,-1.2112137126
H,0,-1.0136103326,4.8003224751,-1.2630529336
H,0,2.961050077,2.8039510782,2.6548022694
H,0,1.6808329149,3.0086495335,3.8730130496
H,0,3.4224076337,0.7200528192,3.7618765572
H,0,1.8302099626,0.703498365,4.5536057983
H,0,4.5365403148,1.559708713,-1.6376725755
H,0,4.8381305576,0.6646816239,-0.1320133525
H,0,3.9212584429,-0.4403555258,-2.8118716246
H,0,4.7037966922,-1.3175397521,-1.4783730685
H,0,2.0488767331,-3.9736766505,1.5503279556
H,0,2.7307883646,-2.6178636822,0.6003783595
H,0,2.2878438631,-2.3611805348,2.2961564698
H,0,-0.4277867869,-4.1744092132,2.3382258822
H,0,-0.4245022551,-2.590904735,3.1520119194
H,0,-1.7372478792,-2.9992957896,2.0470216635
H,0,-2.6458708045,-1.2178514306,-3.5125818679
H,0,-3.126849252,-0.5530733143,-1.9215729091
H,0,-2.2191454524,0.4565598506,-3.0635976921
H,0,-0.1249926541,-1.6784619435,-4.2560171458
H,0,0.5187322074,-0.0908935312,-3.7322488655
H,0,1.3014843745,-1.5799267802,-3.1713077944
H,0,-0.7103163764,0.4126199791,1.483861029

C,0,-2.2041978354,0.238057043,0.7331565472
C,0,-3.1105786733,-0.8390387305,0.8257018386
C,0,-4.4695220089,-0.6579363789,1.0776459629
C,0,-4.9824325337,0.6287403962,1.2814895553
C,0,-4.1102356756,1.7186255711,1.2254552788
C,0,-2.7499645371,1.5135396466,0.9599991587
H,0,-2.7673116167,-1.8566893019,0.6749235967
H,0,-5.1501740405,-1.503297465,1.1261666349
O,0,-6.3275514351,0.7083704952,1.53125905
H,0,-4.4665865085,2.729455486,1.3918252962
H,0,-2.0996545905,2.3808474221,0.925460183
C,0,-6.8831964745,1.990783616,1.7600867353
H,0,-7.9488688994,1.8334725566,1.9373336643
H,0,-6.4403391309,2.476213215,2.6400308736
H,0,-6.7568928676,2.6511699494,0.8916545191

dmpeBpin2ParaAnisHBpinRotTS
E(RB+HF-LYP) = -2134.28247165

Zero-point correction= 0.555886 (Hartree/Particle)
Thermal correction to Energy= 0.593325
Thermal correction to Enthalpy= 0.594269
Thermal correction to Gibbs Free Energy= 0.485887
Sum of electronic and zero-point Energies= -2133.726585
Sum of electronic and thermal Energies= -2133.689147
Sum of electronic and thermal Enthalpies= -2133.688203
Sum of electronic and thermal Free Energies= -2133.796584

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	372.317	137.111	228.108

C,0,4.0782813136,0.3535866897,1.0163597168
C,0,2.6744892257,0.2826613414,1.0626330957
C,0,1.85596129,0.0032542705,-0.0463967979
C,0,2.5780573961,-0.2048602851,-1.2481634777
C,0,3.9671337718,-0.1415457508,-1.3319004529
C,0,4.734172829,0.1385069803,-0.1951598281
Ir,0,-0.3794600323,-0.0906347437,-0.0441280805
B,0,-0.1672386951,-1.898529663,-1.1036571661
O,0,-0.1484975497,-3.1919895456,-0.5696289127
C,0,-0.0475505974,-4.143110988,-1.6402891174
C,0,0.3123957847,-3.2942700705,-2.875920264
O,0,0.0311381316,-1.948058787,-2.4799126668

B,0,-2.4875175237,-0.3045091103,-0.3070208725
O,0,-3.4866337899,-0.0313969277,0.6517345377
C,0,-4.7731713464,-0.3837491126,0.1181965437
C,0,-4.5114937942,-0.6157423775,-1.3810985298
O,0,-3.0919061629,-0.7621852618,-1.4766593684
P,0,-0.5462306475,1.8239126754,1.4504954384
C,0,0.7138723863,3.1741976599,1.4218317004
P,0,-0.5735910848,-1.3495626782,1.9037088687
C,0,0.8967807397,-2.2973728051,2.4824283413
B,0,-0.5163071331,1.6037261929,-1.5363854745
O,0,-1.73141335,2.1179020811,-1.9549707853
C,0,-1.4821191439,3.312872666,-2.7103764689
C,0,0.0112470211,3.6270503778,-2.4606987455
O,0,0.5350283925,2.4407948724,-1.8503490186
C,0,-0.3818620204,1.1595712312,3.191528007
C,0,-1.0388405847,-0.2191264805,3.3178802834
C,0,-2.1237021323,2.7837524478,1.5214350068
C,0,-1.8899081015,-2.6343660933,2.0107865807
H,0,-0.2618058054,0.2932442617,-1.677614569
H,0,-0.7898087471,-0.6965786049,4.2725672035
H,0,-2.1288772121,-0.123154744,3.2693638326
H,0,-0.8154975754,1.8719412052,3.9028670828
H,0,0.6895873189,1.0969134558,3.4091794199
H,0,0.1506728598,4.4746665133,-1.7776118947
H,0,0.5655242183,3.8351928878,-3.3803275881
H,0,-2.1503056135,4.1086786901,-2.3665163271
H,0,-1.6956447223,3.1137606363,-3.7667527002
H,0,-0.2849637063,-3.5509598907,-3.7563802801
H,0,1.3744374642,-3.3775105007,-3.1387727346
H,0,-1.0108172328,-4.655551546,-1.756654264
H,0,0.7155986982,-4.8890803359,-1.3969203109
H,0,-4.8277550494,0.2402575439,-1.9909875088
H,0,-5.0041444153,-1.5143455986,-1.7664252159
H,0,-5.4865479146,0.424325651,0.3100739732
H,0,-5.1377028284,-1.289885246,0.6210217124
H,0,2.03719729,-0.4317988961,-2.1628871046
H,0,4.4809610008,-0.3069651747,-2.2753246235
O,0,6.09772953,0.1773207094,-0.375061667
H,0,4.6306425025,0.5748294436,1.9241763033
H,0,2.2269054683,0.4634291909,2.0389072066
H,0,-1.6907038138,-3.3873546768,1.247414927
H,0,-1.887796713,-3.0987559319,3.0023725505
H,0,-2.857869631,-2.1681110543,1.8227736323
H,0,1.1150991677,-3.0463885232,1.7178635814

H,0,1.7665605906,-1.6481353047,2.5776399774
H,0,0.6859852898,-2.7920520005,3.4360491924
H,0,-2.2818812647,3.2730816042,0.5569701729
H,0,-2.9506997969,2.0885966158,1.6758327781
H,0,-2.099613873,3.5386874694,2.3142206715
H,0,0.5724343617,3.7779746311,0.5230935472
H,0,0.625814325,3.8157710714,2.3046613146
H,0,1.7110763458,2.7336126517,1.3722632749
C,0,6.9006239578,0.4521574211,0.7540101358
H,0,7.935783996,0.4379664834,0.4058222802
H,0,6.681727273,1.4399120657,1.1838713146
H,0,6.7777233941,-0.3059256909,1.5405530001

dmpe Bpin3 Meta Anisole CH Activation Transition Structure
dmpeBpin3MetaAnisCHactTSParParBackA
E(RB+HF-LYP) = -2134.27447502

Zero-point correction= 0.553169 (Hartree/Particle)
Thermal correction to Energy= 0.591298
Thermal correction to Enthalpy= 0.592242
Thermal correction to Gibbs Free Energy= 0.479907
Sum of electronic and zero-point Energies= -2133.721306
Sum of electronic and thermal Energies= -2133.683177
Sum of electronic and thermal Enthalpies= -2133.682233
Sum of electronic and thermal Free Energies= -2133.794568

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	371.045	138.796	236.430

C,0,2.713461871,1.1913254302,0.3891227466
C,0,1.9790035187,0.0507420332,0.7777685978
C,0,2.6360485012,-0.9018355885,1.5732458151
C,0,3.9897812146,-0.7612675026,1.9064967693
C,0,4.7161780127,0.3417303918,1.4781555427
C,0,4.0660849485,1.3292983224,0.7247304023
Ir,0,-0.1857907159,-0.1755833113,0.0373545434
P,0,0.3250900006,-0.0018739105,-2.3178925168
C,0,0.1026971435,-1.6954245075,-3.0754416376
C,0,0.6824537834,-2.7819683109,-2.1615064244
P,0,0.0361409515,-2.6141425313,-0.4117530617
B,0,-2.2389928438,-0.0285794663,-0.5168581548
O,0,-2.8532003787,1.156605111,-0.9346295781
C,0,-4.2712962722,0.9704711741,-0.9953311412

C,0,-4.45773027,-0.5581486291,-0.9468323007
O,0,-3.1880436,-1.0593619668,-0.5088472145
B,0,-1.2531669776,-0.6604879024,1.8028123164
O,0,-1.0639119162,-1.8821206871,2.4646528837
C,0,-2.0337825898,-1.9941262574,3.5166478449
C,0,-2.6195219205,-0.5737918012,3.647429106
O,0,-2.219923559,0.0927534349,2.4457328374
B,0,-0.4041330805,1.8997824529,0.2297657249
O,0,-0.7758231836,2.5813849218,1.3792177253
C,0,-0.6484341058,3.9891842909,1.1706368362
C,0,-0.4156367589,4.13799683,-0.3463636751
O,0,-0.0686350291,2.8167603041,-0.7825417965
H,0,-4.7348756207,1.4698886746,-0.1360008938
H,0,-4.6655252754,1.421601284,-1.9121303668
H,0,-5.2381181095,-0.870718185,-0.2455468525
H,0,-4.6936694567,-0.9807366768,-1.9325268824
H,0,-2.7948184409,-2.7304715289,3.2278497846
H,0,-1.5443754359,-2.3426275182,4.4315050401
H,0,-3.711340558,-0.5688059215,3.7260235005
H,0,-2.2079671731,-0.033845067,4.5092580832
H,0,-1.3213407917,4.4646490847,-0.8728870199
H,0,0.3953254538,4.8329909426,-0.5902158299
H,0,-1.5562045213,4.4974965208,1.5119284198
H,0,0.1985234624,4.3665312045,1.7586627036
H,0,0.5084253533,0.0793180165,1.4847032767
H,0,2.2186645954,1.9685883362,-0.1785015135
O,0,4.8465352882,2.3980581315,0.3637556566
H,0,2.0828205447,-1.7440171556,1.9710606002
H,0,4.474541168,-1.515554211,2.5221055945
H,0,5.7633299893,0.4759759699,1.729368578
C,0,-0.6811118941,1.0706684399,-3.4282294906
C,0,2.0398544171,0.4465880214,-2.8456300341
C,0,-1.4897173851,-3.6573598369,-0.4415857598
C,0,1.1790565707,-3.7649746441,0.4825786624
H,0,0.4712257084,-3.7840170725,-2.5532400132
H,0,1.7731049248,-2.6821736677,-2.1023316116
H,0,-0.9758842635,-1.8444783888,-3.2063176641
H,0,0.5588360096,-1.7247417526,-4.0723403001
H,0,2.1632576405,0.300708903,-3.9237305052
H,0,2.220833877,1.4960222783,-2.6040782204
H,0,2.7718182205,-0.1533331153,-2.3019802576
H,0,-0.3916574242,0.9343291475,-4.4752952216
H,0,-1.7408312722,0.8453567995,-3.2976441434
H,0,-0.5231686159,2.1061199266,-3.1226297713

H,0,1.144569555,-4.7632028175,0.0334973808
H,0,2.2027972485,-3.38846858,0.4485615439
H,0,0.8642227443,-3.8320097457,1.5267677956
H,0,-1.2754156871,-4.6560162265,-0.8365892137
H,0,-1.859462591,-3.7413080465,0.5829656168
H,0,-2.2650906487,-3.165347932,-1.0284133248
C,0,4.2380573192,3.4690400496,-0.3335535641
H,0,5.0202460814,4.2158368764,-0.4843410399
H,0,3.8504906691,3.1545395085,-1.3119925196
H,0,3.4169403937,3.9169848837,0.2415057696

dmpeBpin3MetaAnisCHactTSParSptBackA
E(RB+HF-LYP) = -2134.27655396

Zero-point correction= 0.553193 (Hartree/Particle)
Thermal correction to Energy= 0.591257
Thermal correction to Enthalpy= 0.592201
Thermal correction to Gibbs Free Energy= 0.481746
Sum of electronic and zero-point Energies= -2133.723361
Sum of electronic and thermal Energies= -2133.685297
Sum of electronic and thermal Enthalpies= -2133.684353
Sum of electronic and thermal Free Energies= -2133.794808

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	371.019	138.951	232.473

C,0,4.0455379452,1.4527487208,0.4006472369
C,0,2.6744200814,1.2759936771,0.1620896593
C,0,1.9649701409,0.1854851784,0.6801074033
C,0,2.6789236489,-0.691820484,1.5242124895
C,0,4.0393071877,-0.514015622,1.7739427326
C,0,4.7457965686,0.5500244612,1.2071148581
Ir,0,-0.2087794231,-0.1427969742,0.0715655326
B,0,-0.5126765357,1.9154079732,-0.1860282409
O,0,-1.1044356869,2.5122005468,-1.3115870012
C,0,-1.2753413267,3.9138736835,-1.0586815276
C,0,-0.4027486043,4.1895448589,0.1826656683
O,0,-0.1219730218,2.8940848484,0.7169859642
H,0,5.8027372128,0.6721531538,1.4125108919
P,0,0.4000313886,-0.4760549391,-2.2520593586
C,0,2.1706486341,-0.2325665335,-2.7257074272
P,0,-0.125462743,-2.61908936,0.1212814542
C,0,0.8048751895,-3.6890682286,1.3150799766

B,0,-2.2513716338,-0.1907419566,-0.5406503021
O,0,-2.7308507591,-0.8563004087,-1.6870381929
C,0,-4.1161006306,-0.5375098598,-1.8848511863
C,0,-4.5503069576,0.1119377334,-0.5577515149
O,0,-3.3236435308,0.4193732922,0.1104441834
B,0,-1.2544650632,-0.1091475401,1.9217546086
O,0,-1.6658972368,1.0003694045,2.6353631103
C,0,-2.5165733747,0.5761688611,3.7021557249
C,0,-2.2332326372,-0.9317919977,3.8390879287
O,0,-1.6177384118,-1.2867924918,2.5911441316
C,0,0.120446941,-2.2761729458,-2.6613562706
C,0,0.5885834746,-3.1828585985,-1.5147055368
C,0,-0.4702329149,0.3935213891,-3.6232605229
C,0,-1.7681892024,-3.4678939838,0.1542404246
H,0,-5.1406751352,-0.5728958035,0.0647662504
H,0,-5.1298027856,1.0291775224,-0.7032188762
H,0,-4.6743312244,-1.4496610613,-2.120213063
H,0,-4.2087965262,0.1532908466,-2.7324066124
H,0,-3.1392554683,-1.5282672563,3.9867943489
H,0,-1.5360010285,-1.1500308741,4.6583142997
H,0,-3.5608161123,0.7736476433,3.4283638592
H,0,-2.2804159954,1.141095939,4.6093280563
H,0,-2.3369876346,4.1165045294,-0.8692106017
H,0,-0.9655862463,4.4888872165,-1.9379258669
H,0,-0.9157571579,4.7951830882,0.9366453187
H,0,0.541295834,4.6876720808,-0.0750859734
H,0,0.4761073623,0.3634741608,1.4492778243
H,0,2.1819842818,2.0296048492,-0.4409030777
O,0,4.6094187785,2.5471751708,-0.2062400322
H,0,2.1604492634,-1.5020506183,2.0219863664
H,0,4.5618249804,-1.2057508218,2.4310836145
H,0,0.3193913094,-4.2285632076,-1.7061563204
H,0,1.6802870835,-3.1430403094,-1.4168294115
H,0,-0.9581923681,-2.3808509278,-2.8138142008
H,0,0.6232425357,-2.5306850126,-3.601980729
H,0,2.3390124863,-0.5804804321,-3.7502275394
H,0,2.4295939554,0.8262054374,-2.6602495553
H,0,2.8247554003,-0.7716156325,-2.0380937251
H,0,-0.0491321437,0.111980155,-4.5937393039
H,0,-1.527392476,0.1294100093,-3.5821668804
H,0,-0.3825864131,1.4700091482,-3.4679947338
H,0,0.6426251355,-4.7485743464,1.0906105206
H,0,1.8743028428,-3.4761495825,1.2700923826
H,0,0.4444862618,-3.4812908799,2.3258808319

H,0,-1.6608146195,-4.5529124816,0.0534687035
H,0,-2.2430587839,-3.2270358939,1.1077680335
H,0,-2.3905440893,-3.0769637508,-0.6524472243
C,0,5.9779966899,2.8118565914,0.0389964164
H,0,6.2155294879,3.7243989029,-0.5113355665
H,0,6.1770932134,2.9744950761,1.1068181078
H,0,6.6237534441,1.9989439451,-0.3207044204

dmpeBpin3MetaAnisCHactTSSptSptBackA
E(RB+HF-LYP) = -2134.27770407

Zero-point correction= 0.553243 (Hartree/Particle)
Thermal correction to Energy= 0.591316
Thermal correction to Enthalpy= 0.592261
Thermal correction to Gibbs Free Energy= 0.482004
Sum of electronic and zero-point Energies= -2133.724461
Sum of electronic and thermal Energies= -2133.686388
Sum of electronic and thermal Enthalpies= -2133.685444
Sum of electronic and thermal Free Energies= -2133.795700

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	371.057	138.917	232.055

C,0,3.1755398497,-0.6961767473,0.7900930997
C,0,2.275751457,0.3678075002,0.6339856849
C,0,2.8169117111,1.6692400848,0.7183239772
C,0,4.1844488093,1.8708165132,0.8981361379
C,0,5.0750597373,0.7996817456,1.0180080474
C,0,4.5539801028,-0.4948869928,0.9668911289
Ir,0,0.0797699321,0.0072154989,0.0788919832
P,0,0.7227799292,-0.7240342544,-2.1309869502
C,0,0.5233824276,-2.5854572396,-2.1998828493
C,0,0.9022847177,-3.2618900216,-0.8719675947
P,0,0.061404722,-2.4056343714,0.5651595365
B,0,-1.9492065338,-0.0453748459,-0.5634837943
O,0,-2.458187879,-0.9192066899,-1.542301675
C,0,-3.8223526728,-0.5783299716,-1.8296904643
C,0,-4.2247815053,0.3736784813,-0.6882414727
O,0,-2.9839742899,0.765144429,-0.0936581927
B,0,-1.008432933,0.3971370273,1.867546524
O,0,-1.5504785294,-0.6423278029,2.6394615988
C,0,-2.1420809166,-0.0779973445,3.8191030342
C,0,-2.1984671488,1.4333910618,3.5251409557

O,0,-1.2789975473,1.6207585729,2.447036225
B,0,-0.1541149946,2.0052442794,-0.5342951119
O,0,0.0638440487,3.1425671863,0.2367661208
C,0,-0.1139623519,4.3168312176,-0.5579695751
C,0,-0.7613456383,3.8064256881,-1.8596724296
O,0,-0.5542536428,2.3889373423,-1.8276907238
H,0,-3.8726270579,-0.0912430009,-2.8118700537
H,0,-4.4300917809,-1.4884466229,-1.8644572944
H,0,-4.760340596,1.2604936714,-1.041637855
H,0,-4.8455407919,-0.1261649657,0.0665200388
H,0,-3.1295224213,-0.5207278825,3.9852494469
H,0,-1.5087673389,-0.308896078,4.6856597499
H,0,-3.1982223469,1.7519267011,3.2038227956
H,0,-1.8950481567,2.0476151597,4.3787363698
H,0,-1.8389037486,4.0124881629,-1.8923884867
H,0,-0.3025794194,4.2278903587,-2.7606197759
H,0,-0.7440107887,5.0323545566,-0.0199656608
H,0,0.8630438971,4.7856418604,-0.7377567722
H,0,0.8203615355,0.4441725095,1.4622006789
H,0,2.852854155,-1.7290777498,0.7606808593
O,0,5.3028025195,-1.6417959249,1.0739421465
H,0,2.1560655609,2.5252599462,0.6632224435
H,0,4.5712574054,2.8857890231,0.9563369058
H,0,6.1338298877,0.9827920072,1.1588980327
C,0,-0.1592359111,-0.1786281346,-3.6543840333
C,0,2.4818258828,-0.4512099056,-2.6252135046
C,0,-1.5920382338,-3.2312188236,0.6003756168
C,0,0.8279234639,-3.1826941959,2.0614356538
H,0,0.6398673286,-4.3265600085,-0.8879470307
H,0,1.9839275649,-3.1971037419,-0.7073947247
H,0,-0.5350203451,-2.7587016073,-2.423192837
H,0,1.1086868872,-2.9937154771,-3.0322675957
H,0,2.6894690361,-0.9165394834,-3.5942505888
H,0,2.6615910226,0.624802789,-2.6956229183
H,0,3.1577566142,-0.8496862695,-1.867371805
H,0,0.2793544686,-0.642209074,-4.5439175774
H,0,-1.2102108195,-0.454676128,-3.5668513625
H,0,-0.0923342695,0.9083860208,-3.7192905833
H,0,0.8025645023,-4.2757891649,2.0003237905
H,0,1.8580752577,-2.8517442884,2.2004539657
H,0,0.2447075984,-2.8582915474,2.9272019673
H,0,-1.494407502,-4.3164040357,0.7118608255
H,0,-2.1449311377,-2.8191206703,1.4473555516
H,0,-2.1344396291,-2.9939308824,-0.3161480769

C,0,6.6973406444,-1.5065275371,1.2771801724
H,0,7.0960453734,-2.5208162817,1.3424884789
H,0,7.1833353969,-0.9834740466,0.4424024486
H,0,6.9236094309,-0.9711565851,2.2090523771

dmpeBpin3MetaAnisCHactTSSptSptFrntA
E(RB+HF-LYP) = -2134.27607120

Zero-point correction= 0.553291 (Hartree/Particle)
Thermal correction to Energy= 0.591369
Thermal correction to Enthalpy= 0.592313
Thermal correction to Gibbs Free Energy= 0.481633
Sum of electronic and zero-point Energies= -2133.722780
Sum of electronic and thermal Energies= -2133.684702
Sum of electronic and thermal Enthalpies= -2133.683758
Sum of electronic and thermal Free Energies= -2133.794438

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	371.090	138.867	232.945

C,0,0.0054220221,-3.4478032636,-0.6156472746
C,0,-1.0841638483,-2.8921187372,-1.5448429875
P,0,-0.7932291614,-1.0838271194,-1.9270450291
Ir,0,-0.0378847631,-0.0277043638,0.0982585519
B,0,-0.1207780571,1.8355839646,-0.8764128365
O,0,-0.2863401085,3.0946381084,-0.3173237298
C,0,-0.1660880727,4.098555621,-1.3265048123
C,0,-0.2448832914,3.3223984205,-2.6557826294
O,0,-0.0440857248,1.9541740954,-2.2803111492
P,0,0.318330974,-2.336396942,0.8659306003
B,0,1.0449474518,0.8353419387,1.725965396
O,0,1.8449392664,0.0709900527,2.5861888673
C,0,2.3447000699,0.9199148452,3.6295445735
C,0,2.0386478004,2.3457471097,3.133331245
O,0,1.0560505698,2.1624773982,2.1114178353
B,0,1.9629427425,0.0390151645,-0.6246173145
O,0,2.6284690098,-1.0172709381,-1.2721572107
C,0,3.9136055669,-0.5708118358,-1.7293706202
C,0,4.1228818529,0.7797526784,-1.0193216681
O,0,2.825195438,1.1330641694,-0.5311093212
C,0,2.0077146294,-2.8860902655,1.3735119859
C,0,-0.6756284814,-3.1102193041,2.2301451946
H,0,-0.2387585122,-4.4644136558,-0.2854949504

H,0,0.9605370482,-3.4995535133,-1.1503110737
C,0,0.2918876861,-1.1257771788,-3.4169207368
C,0,-2.3947141685,-0.5371682749,-2.6573263685
H,0,-1.1391236136,-3.4675055843,-2.4769381182
H,0,-2.0679224429,-2.961175287,-1.0668024932
H,0,0.5241379267,3.6259120847,-3.3740619298
H,0,-1.2262304443,3.4259887147,-3.1379186615
H,0,0.79427374,4.6157031646,-1.2062187649
H,0,-0.9695441374,4.8344460624,-1.2144711994
H,0,2.923092138,2.8281933191,2.6983280618
H,0,1.6380540068,2.9964337395,3.916970017
H,0,3.4138645835,0.7351754091,3.7755852074
H,0,1.8218651307,0.6851778342,4.5659524194
H,0,4.4901188092,1.5622617197,-1.6909475673
H,0,4.8171070389,0.698201795,-0.1731189511
H,0,3.8903145404,-0.4660702181,-2.8217184486
H,0,4.6750645358,-1.3138366307,-1.4709249563
H,0,2.0319629772,-3.9636651194,1.5677302999
H,0,2.7086815267,-2.6344556092,0.576344606
H,0,2.2914776971,-2.3343645002,2.2711795601
H,0,-0.423393486,-4.1692120344,2.3505506071
H,0,-0.4431150525,-2.5834777689,3.1603857503
H,0,-1.7471840511,-3.0138053065,2.051983479
H,0,-2.7035124014,-1.1990285593,-3.4729887272
H,0,-3.1643417282,-0.5165123516,-1.8840584473
H,0,-2.2568587706,0.4755419822,-3.042780158
H,0,-0.1800687432,-1.6871915419,-4.2297917223
H,0,0.4609449903,-0.0920521562,-3.7262135512
H,0,1.2507407334,-1.5723826829,-3.1526809997
H,0,-0.7354408775,0.413797616,1.5012937625
C,0,-2.2153961011,0.2649159044,0.7569753505
C,0,-3.105458404,-0.8140215385,0.8501629746
C,0,-4.4773452424,-0.633394895,1.0918107681
C,0,-4.99602784,0.6501564438,1.2775682526
C,0,-4.1125837278,1.7325362245,1.2184853487
C,0,-2.7529637385,1.5535325584,0.9695397518
H,0,-2.7790431102,-1.8383226431,0.7175277487
O,0,-5.221994368,-1.7869749116,1.1226607764
H,0,-6.0490153534,0.8154984613,1.4729394476
H,0,-4.4987223328,2.7368212221,1.3775554043
H,0,-2.0981360588,2.4161928827,0.9384453243
C,0,-6.6103746184,-1.6738138559,1.3766153735
H,0,-7.0070854466,-2.6908349087,1.3620591861
H,0,-6.810027823,-1.2247808314,2.3588075013

H,0,-7.1196183995,-1.0792003777,0.6061541794

dmpeBpin2MetaAnisHBpinRotTS
E(RB+HF-LYP) = -2134.28483325

Zero-point correction=	0.556138 (Hartree/Particle)
Thermal correction to Energy=	0.593495
Thermal correction to Enthalpy=	0.594439
Thermal correction to Gibbs Free Energy=	0.486545
Sum of electronic and zero-point Energies=	-2133.728696
Sum of electronic and thermal Energies=	-2133.691338
Sum of electronic and thermal Enthalpies=	-2133.690394
Sum of electronic and thermal Free Energies=	-2133.798288

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	372.424	137.015	227.082

C,0,4.1147736561,0.3349048576,0.8472836479
C,0,2.7127528254,0.2658582853,0.9150338727
C,0,1.895988222,-0.0349444289,-0.188043864
C,0,2.5974496909,-0.2721273397,-1.3971911254
C,0,3.9867779779,-0.2072906795,-1.4775325598
C,0,4.7723249979,0.0968290521,-0.3594758139
Ir,0,-0.3335913482,-0.110152303,-0.1392198873
B,0,-0.1458486722,-1.921093444,-1.1969080806
O,0,-0.083783391,-3.2086285095,-0.6508045276
C,0,0.0058640984,-4.1688882382,-1.7141295455
C,0,0.305885295,-3.3250253092,-2.9687873472
O,0,0.0001658379,-1.9824801474,-2.5792940951
B,0,-2.4500781245,-0.3037194367,-0.3660348226
O,0,-3.4269719736,-0.07868712,0.6290073645
C,0,-4.7244271138,-0.4131272131,0.1104519578
C,0,-4.4992386436,-0.5641359886,-1.4045922979
O,0,-3.0823569908,-0.7031128102,-1.5420062094
P,0,-0.4731822478,1.8040097203,1.3671878878
C,0,0.7737257258,3.1657719382,1.3182002336
P,0,-0.5013602467,-1.3723200892,1.81603092
C,0,0.9751179264,-2.3121656321,2.3923077755
B,0,-0.4540551247,1.5931152436,-1.6132407745
O,0,-1.6667028756,2.1663974312,-1.9594931219
C,0,-1.4051949123,3.3420433443,-2.740811866
C,0,0.1122337258,3.5874587932,-2.576169678
O,0,0.6145837098,2.3771209551,-1.9964835261

C,0,-0.27772742,1.1330726212,3.1001835248
C,0,-0.9548434134,-0.2353464654,3.2277786884
C,0,-2.0576662093,2.7484736904,1.4672205126
C,0,-1.815847596,-2.6563286661,1.9376971148
H,0,-0.2648340666,0.268652803,-1.7741029053
H,0,-0.7178033378,-0.7138582637,4.1848663832
H,0,-2.0428039808,-0.1234445281,3.1698267556
H,0,-0.6872246754,1.8481802931,3.8230582306
H,0,0.796515179,1.0521184448,3.2963130848
H,0,0.3279773474,4.4257315146,-1.9014750349
H,0,0.6227122005,3.7728570574,-3.5255735504
H,0,-2.0161653364,4.1712937534,-2.3704111976
H,0,-1.6852887193,3.1438314284,-3.7818173534
H,0,-0.3087909387,-3.608061227,-3.8289980923
H,0,1.3621374261,-3.3824393796,-3.2605499626
H,0,-0.9474741269,-4.706447641,-1.7945718978
H,0,0.7946351816,-4.8932232108,-1.4876165079
H,0,-4.8303945932,0.322948984,-1.9597384387
H,0,-5.0005455613,-1.4416961712,-1.8255621602
H,0,-5.4386388568,0.3773389265,0.3628613296
H,0,-5.0691713666,-1.347802863,0.5735221817
H,0,2.0446433656,-0.5115293178,-2.3008000901
H,0,4.4793191331,-0.3953199537,-2.4298893336
H,0,5.8519671197,0.1423750043,-0.4436725359
O,0,4.7466683391,0.6475468653,2.0315895561
H,0,2.2918357407,0.4683321347,1.8969654401
H,0,-1.6252520848,-3.4066747054,1.1698577487
H,0,-1.8008058434,-3.1231014615,2.9279431025
H,0,-2.7850824046,-2.1881353898,1.7625541738
H,0,1.1737846943,-3.0875667292,1.6493973965
H,0,1.849726941,-1.6646647298,2.4508155792
H,0,0.7794081992,-2.7745564572,3.3651504316
H,0,-2.2421223851,3.2265672332,0.5020334076
H,0,-2.8735586909,2.0463491945,1.6465626813
H,0,-2.021697829,3.5086919454,2.2543852667
H,0,0.6198715549,3.7617534632,0.4159640157
H,0,0.6823388519,3.8129456571,2.1964534174
H,0,1.776043833,2.7369955254,1.2690894585
C,0,6.1571406642,0.7444365345,2.0192488552
H,0,6.4569362828,0.9995315637,3.038158166
H,0,6.6310028843,-0.2049886104,1.733946704
H,0,6.5080214691,1.5298185075,1.3354656629

dmpe Bpin3 Ortho Anisole CH Activation Transition Structure
E(RB+HF-LYP) = -2134.27489358

Zero-point correction= 0.553095 (Hartree/Particle)
Thermal correction to Energy= 0.591067
Thermal correction to Enthalpy= 0.592011
Thermal correction to Gibbs Free Energy= 0.482549
Sum of electronic and zero-point Energies= -2133.721799
Sum of electronic and thermal Energies= -2133.683826
Sum of electronic and thermal Enthalpies= -2133.682882
Sum of electronic and thermal Free Energies= -2133.792344

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	370.900	138.953	230.383

C,0,3.140816,-0.031857,0.383722
C,0,1.986067,-0.812137,0.627899
C,0,2.207463,-2.055464,1.242405
C,0,3.482166,-2.549351,1.543477
C,0,4.596293,-1.771428,1.251144
C,0,4.425357,-0.509685,0.676837
Ir,0,-0.112794,-0.109061,0.048085
P,0,0.441252,0.133469,-2.311068
C,0,-0.522837,-1.158634,-3.249122
C,0,-0.439662,-2.512177,-2.529792
P,0,-0.902799,-2.340102,-0.724014
B,0,-1.999822,0.762176,-0.395817
O,0,-2.835922,1.427516,0.502329
C,0,-4.053518,1.807867,-0.144153
C,0,-3.780894,1.583943,-1.642372
O,0,-2.609813,0.755386,-1.667405
B,0,-1.149639,-0.388338,1.880765
O,0,-1.848649,-1.573129,2.163582
C,0,-2.361618,-1.495470,3.502697
C,0,-2.190614,-0.012920,3.884924
O,0,-1.240476,0.488312,2.944167
B,0,0.319987,1.892204,0.502855
O,0,0.826263,2.341398,1.716810
C,0,1.059995,3.746330,1.650694
C,0,0.352503,4.196942,0.356537
O,0,0.111490,2.980952,-0.361135
H,0,-4.872787,1.176980,0.225067
H,0,-4.288635,2.849880,0.095096

H,0,-4.602991,1.077680,-2.158941
H,0,-3.568347,2.523690,-2.167899
H,0,-3.405098,-1.826472,3.518699
H,0,-1.776388,-2.161131,4.150187
H,0,-3.128335,0.548294,3.782626
H,0,-1.811272,0.126157,4.902231
H,0,-0.605932,4.691064,0.561772
H,0,0.962599,4.873680,-0.252578
H,0,0.657519,4.231800,2.546028
H,0,2.141661,3.936431,1.615973
H,0,0.664301,-0.271005,1.458545
O,0,2.950058,1.208264,-0.184156
H,0,5.300219,0.093743,0.462672
H,0,1.345050,-2.649518,1.524712
H,0,3.592978,-3.521103,2.017182
H,0,5.598304,-2.126171,1.476675
C,0,0.086773,1.680041,-3.244116
C,0,2.167964,-0.247833,-2.854905
C,0,-2.737294,-2.571172,-0.775204
C,0,-0.377348,-3.987760,-0.059807
H,0,-1.079116,-3.259212,-3.015090
H,0,0.586487,-2.898208,-2.560390
H,0,-1.556552,-0.803092,-3.285085
H,0,-0.150260,-1.232532,-4.277928
H,0,2.219572,-0.318277,-3.946427
H,0,2.832205,0.541604,-2.503702
H,0,2.502591,-1.187773,-2.411106
H,0,0.378518,1.580245,-4.294567
H,0,-0.980900,1.887422,-3.169538
H,0,0.626113,2.503081,-2.773347
H,0,-0.839114,-4.801402,-0.629004
H,0,0.708903,-4.087293,-0.108028
H,0,-0.690463,-4.061478,0.984733
H,0,-3.007348,-3.530415,-1.229348
H,0,-3.109453,-2.525422,0.249914
H,0,-3.183070,-1.754361,-1.346054
C,0,4.044298,2.106407,-0.236742
H,0,3.639277,3.051447,-0.603781
H,0,4.488724,2.261138,0.754470
H,0,4.827672,1.764079,-0.927357

dmpeBpin3OrthoAnisCHactTSParSptBackA
E(RB+HF-LYP) = -2134.27489358

Zero-point correction= 0.553095 (Hartree/Particle)
Thermal correction to Energy= 0.591067
Thermal correction to Enthalpy= 0.592011
Thermal correction to Gibbs Free Energy= 0.482549
Sum of electronic and zero-point Energies= -2133.721799
Sum of electronic and thermal Energies= -2133.683826
Sum of electronic and thermal Enthalpies= -2133.682882
Sum of electronic and thermal Free Energies= -2133.792344

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	370.900	138.953	230.383

C,0,3.1408160396,-0.0318570366,0.3837219512
C,0,1.9860670396,-0.8121370366,0.6278989512
C,0,2.2074630396,-2.0554640366,1.2424049512
C,0,3.4821660396,-2.5493510366,1.5434769512
C,0,4.5962930396,-1.7714280366,1.2511439512
C,0,4.4253570396,-0.5096850366,0.6768369512
Ir,0,-0.1127939604,-0.1090610366,0.0480849512
P,0,0.4412520396,0.1334689634,-2.3110680488
C,0,-0.5228369604,-1.1586340366,-3.2491220488
C,0,-0.4396619604,-2.5121770366,-2.5297920488
P,0,-0.9027989604,-2.3401020366,-0.7240140488
B,0,-1.9998219604,0.7621759634,-0.3958170488
O,0,-2.8359219604,1.4275159634,0.5023289512
C,0,-4.0535179604,1.8078669634,-0.1441530488
C,0,-3.7808939604,1.5839429634,-1.6423720488
O,0,-2.6098129604,0.7553859634,-1.6674050488
B,0,-1.1496389604,-0.3883380366,1.8807649512
O,0,-1.8486489604,-1.5731290366,2.1635819512
C,0,-2.3616179604,-1.4954700366,3.5026969512
C,0,-2.1906139604,-0.0129200366,3.8849239512
O,0,-1.2404759604,0.4883119634,2.9441669512
B,0,0.3199870396,1.8922039634,0.5028549512
O,0,0.8262630396,2.3413979634,1.7168099512
C,0,1.0599950396,3.7463299634,1.6506939512
C,0,0.3525030396,4.1969419634,0.3565369512
O,0,0.1114900396,2.9809519634,-0.3611350488
H,0,-4.8727869604,1.1769799634,0.2250669512
H,0,-4.2886349604,2.8498799634,0.0950959512
H,0,-4.6029909604,1.0776799634,-2.1589410488
H,0,-3.5683469604,2.5236899634,-2.1678990488
H,0,-3.4050979604,-1.8264720366,3.5186989512

H,0,-1.7763879604,-2.1611310366,4.1501869512
H,0,-3.1283349604,0.5482939634,3.7826259512
H,0,-1.8112719604,0.1261569634,4.9022309512
H,0,-0.6059319604,4.6910639634,0.5617719512
H,0,0.9625990396,4.8736799634,-0.2525780488
H,0,0.6575190396,4.2317999634,2.5460279512
H,0,2.1416610396,3.9364309634,1.6159729512
H,0,0.6643010396,-0.2710050366,1.4585449512
O,0,2.9500580396,1.2082639634,-0.1841560488
H,0,5.3002190396,0.0937429634,0.4626719512
H,0,1.3450500396,-2.6495180366,1.5247119512
H,0,3.5929780396,-3.5211030366,2.0171819512
H,0,5.5983040396,-2.1261710366,1.4766749512
C,0,0.0867730396,1.6800409634,-3.2441160488
C,0,2.1679640396,-0.2478330366,-2.8549050488
C,0,-2.7372939604,-2.5711720366,-0.7752040488
C,0,-0.3773479604,-3.9877600366,-0.0598070488
H,0,-1.0791159604,-3.2592120366,-3.0150900488
H,0,0.5864870396,-2.8982080366,-2.5603900488
H,0,-1.5565519604,-0.8030920366,-3.2850850488
H,0,-0.1502599604,-1.2325320366,-4.2779280488
H,0,2.2195720396,-0.3182770366,-3.9464270488
H,0,2.8322050396,0.5416039634,-2.5037020488
H,0,2.5025910396,-1.1877730366,-2.4111060488
H,0,0.3785180396,1.5802449634,-4.2945670488
H,0,-0.9808999604,1.8874219634,-3.1695380488
H,0,0.6261130396,2.5030809634,-2.7733470488
H,0,-0.8391139604,-4.8014020366,-0.6290040488
H,0,0.7089030396,-4.0872930366,-0.1080280488
H,0,-0.6904629604,-4.0614780366,0.9847329512
H,0,-3.0073479604,-3.5304150366,-1.2293480488
H,0,-3.1094529604,-2.5254220366,0.2499139512
H,0,-3.1830699604,-1.7543610366,-1.3460540488
C,0,4.0442980396,2.1064069634,-0.2367420488
H,0,3.6392770396,3.0514469634,-0.6037810488
H,0,4.4887240396,2.2611379634,0.7544699512
H,0,0,4.8276720396,1.7640789634,-0.9273570488

dmpeBpin3OrthoAnisCHactTSSptSptBackS
E(RB+HF-LYP) = -2134.27130714

Zero-point correction=	0.552663 (Hartree/Particle)
Thermal correction to Energy=	0.590695
Thermal correction to Enthalpy=	0.591639

Thermal correction to Gibbs Free Energy= 0.482176
Sum of electronic and zero-point Energies= -2133.718644
Sum of electronic and thermal Energies= -2133.680612
Sum of electronic and thermal Enthalpies= -2133.679668
Sum of electronic and thermal Free Energies= -2133.789131

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	370.667	139.012	230.384

C,0,3.19753338,-0.6942817488,0.5976640227
C,0,2.2573495147,0.3473053818,0.625005926
C,0,2.7747454179,1.6316444524,0.9251472697
C,0,4.1473756042,1.8521496567,1.1056340072
C,0,5.0470368912,0.7878185833,1.0261746208
C,0,4.5722596455,-0.4953065056,0.7792642027
Ir,0,0.0551053458,-0.0157943072,0.0439980564
P,0,0.6358161972,-0.7379938864,-2.177111761
C,0,0.3627418302,-2.5875565119,-2.264144731
C,0,0.7491981915,-3.290190668,-0.9517590806
P,0,0.0026390179,-2.4109102437,0.5271621326
B,0,-1.9995041859,-0.066678251,-0.4930286194
O,0,-2.5363525255,-0.84290664,-1.5432764069
C,0,-3.9353325254,-0.5558170971,-1.684358971
C,0,-4.2983377105,0.1955109225,-0.3910930742
O,0,-3.0400616277,0.6037915127,0.1473027064
B,0,-0.9149830384,0.4654892881,1.8879536511
O,0,-1.4752468944,-0.5357252785,2.6962697694
C,0,-2.0076302807,0.0754216788,3.8800591568
C,0,-1.9860203866,1.5840780753,3.5670529965
O,0,-1.0762042561,1.7061069019,2.4719987126
B,0,-0.0675567276,1.9653526346,-0.6734062701
O,0,-0.939742972,2.9801779071,-0.3036264572
C,0,-0.6369306988,4.168523578,-1.0301475681
C,0,0.3242349244,3.713802647,-2.1491711112
O,0,0.7115183631,2.3899730251,-1.7710795586
H,0,-4.0891221432,0.0626002283,-2.5783125675
H,0,-4.4934042664,-1.489278504,-1.8120033395
H,0,-4.926698921,1.0739322027,-0.5695020554
H,0,-4.8100384007,-0.4539387058,0.3316583985
H,0,-3.0150844912,-0.3072790004,4.0733563823
H,0,-1.3698015797,-0.1803100116,4.736666729
H,0,-2.9715375476,1.9515553028,3.2552818398
H,0,-1.6359894488,2.1916850679,4.4078317151

H,0,-0.1687862915,3.6840479834,-3.1310062941
H,0,1.2112860244,4.3513209052,-2.2353194753
H,0,-1.5610721884,4.6121009975,-1.4172551136
H,0,-0.1670369595,4.8995212467,-0.3584803174
H,0,0.8275185298,0.3486210337,1.4361929509
H,0,2.8613346852,-1.7073272312,0.4057887401
H,0,5.2554658968,-1.3390268083,0.7286001019
O,0,1.8578170252,2.6402594692,1.0482342658
H,0,4.5201948416,2.8482142656,1.3155850223
H,0,6.1086178643,0.9699140088,1.1696798664
C,0,-0.2703152659,-0.1259384071,-3.6606738832
C,0,2.3844691437,-0.4971652713,-2.7141359724
C,0,-1.6570625391,-3.2093920734,0.6742826105
C,0,0.8654341051,-3.1836039907,1.9721551218
H,0,0.4407289912,-4.3426046876,-0.9659109212
H,0,1.8377915555,-3.2774541495,-0.821348241
H,0,-0.7072477988,-2.7164839265,-2.4586042904
H,0,0.9085662728,-3.0131304302,-3.1146387291
H,0,2.5442910322,-0.9097849251,-3.7156292628
H,0,2.5751664409,0.5785566546,-2.7204032572
H,0,3.0772349455,-0.956920026,-2.0084717779
H,0,0.0756456537,-0.6316440062,-4.5680320273
H,0,-1.3365017211,-0.3006318901,-3.5172720355
H,0,-0.084562073,0.9465677776,-3.7448672164
H,0,0.8334525274,-4.2774843796,1.9287098811
H,0,1.9040003764,-2.8519116391,2.0261950486
H,0,0.3532188565,-2.8463603943,2.8771700394
H,0,-1.5731299648,-4.2936405692,0.802856607
H,0,-2.1562561511,-2.7694589257,1.5406720406
H,0,-2.2446500729,-2.9834506954,-0.2174259637
C,0,2.2771062619,3.9068308815,1.5179381231
H,0,1.3653638311,4.494459397,1.6343216776
H,0,2.7840768738,3.8312938759,2.4889198087
H,0,2.9464495958,4.4091232431,0.8058431488

dmpeBpin2OrthoAnisHBpinRotTS
E(RB+HF-LYP) = -2134.28193795

Zero-point correction= 0.556049 (Hartree/Particle)
Thermal correction to Energy= 0.593057
Thermal correction to Enthalpy= 0.594001
Thermal correction to Gibbs Free Energy= 0.488122
Sum of electronic and zero-point Energies= -2133.725889
Sum of electronic and thermal Energies= -2133.688881

Sum of electronic and thermal Enthalpies= -2133.687937
Sum of electronic and thermal Free Energies= -2133.793816

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	372.149	136.967	222.842

C,0,4.2465340955,0.4781333172,1.2774849193
C,0,2.8467708647,0.3783820532,1.2528411594
C,0,2.0875338357,0.0578227107,0.1145681497
C,0,2.8683726347,-0.1683219448,-1.0464603668
C,0,4.2660879379,-0.0739155415,-1.060337903
C,0,4.9601721441,0.2511250277,0.1085148873
Ir,0,-0.1508802594,-0.0439702208,0.0823611112
B,0,-0.0253377902,-1.859493528,-0.9850715843
O,0,0.4422796788,-3.0655800141,-0.4403986184
C,0,0.3014878808,-4.105728128,-1.4178654843
C,0,-0.0074963519,-3.355316119,-2.7278870796
O,0,-0.400141725,-2.0482798755,-2.3088696083
B,0,-2.2677676836,-0.2144650087,-0.1185950124
O,0,-3.2013071006,-0.04908471,0.9362013475
C,0,-4.522275259,-0.339054142,0.4518627345
C,0,-4.3627609394,-0.3708306116,-1.0782136355
O,0,-2.9572651588,-0.51797595,-1.2859899315
P,0,-0.3332423746,1.8618910376,1.6119399204
C,0,0.9191237008,3.2202271379,1.6403104883
P,0,-0.3227562536,-1.3295677154,2.0253265887
C,0,1.166984825,-2.209795875,2.6567733533
B,0,-0.2807648347,1.643862224,-1.4013425864
O,0,-1.4861992658,2.1571507662,-1.846437792
C,0,-1.2231175853,3.3509877532,-2.5968581897
C,0,0.2605151031,3.6745248719,-2.3063463586
O,0,0.775378116,2.4893523263,-1.6874592005
C,0,-0.238969964,1.1668055213,3.3472536203
C,0,-0.8895542989,-0.2200933522,3.416447035
C,0,-1.908045819,2.8298447947,1.6408490824
C,0,-1.5755852485,-2.6807885975,2.0920874124
H,0,-0.0038660388,0.3252673381,-1.5460049839
H,0,-0.7046740284,-0.7021897187,4.3834070279
H,0,-1.9721774104,-0.1326105851,3.2796902003
H,0,-0.7147992832,1.8607555001,4.0498262803
H,0,0.8208695512,1.1106620343,3.6186319446
H,0,0.3757226691,4.5207414297,-1.6166567714
H,0,0.8365658004,3.8914026119,-3.2107666843

H,0,-1.9056113453,4.1440510563,-2.2751195313
H,0,-1.4054649609,3.1483180271,-3.6586047336
H,0,-0.8151734526,-3.8178463317,-3.3045148292
H,0,0.8786165262,-3.2804417487,-3.3722508535
H,0,-0.5185731666,-4.7734585412,-1.1209108547
H,0,1.2242697268,-4.6925151176,-1.4655113908
H,0,-4.7024864477,0.5623474726,-1.546559353
H,0,-4.8965872408,-1.204502358,-1.5459995937
H,0,-5.2214498658,0.4291870067,0.7981064146
H,0,-4.851036421,-1.3076367275,0.8533797872
O,0,2.1656287894,-0.4994702374,-2.1889107286
H,0,4.8259918907,-0.2522763655,-1.9717190222
H,0,6.0446851309,0.3213473524,0.0911227898
H,0,4.7608814361,0.7321363926,2.2016299551
H,0,2.3311668753,0.5677272637,2.1921757678
H,0,-1.2934661912,-3.4471428721,1.3686370238
H,0,-1.6058766999,-3.118913987,3.0951112621
H,0,-2.5551005086,-2.2748100329,1.8373151842
H,0,1.4678981127,-2.9196725667,1.883413813
H,0,1.9930186401,-1.5192984111,2.8230043997
H,0,0.9290153088,-2.7429266163,3.5829897689
H,0,-2.0384780149,3.317587323,0.6713721484
H,0,-2.7434047501,2.1423592744,1.781795963
H,0,-1.8958345758,3.587145389,2.4316203857
H,0,0.8041446457,3.825056642,0.7381519701
H,0,0.7897898189,3.8585419131,2.520453282
H,0,1.9229284061,2.7939096187,1.6273350201
C,0,2.8648318548,-0.6961839143,-3.3989706419
H,0,2.1067822787,-0.9319259041,-4.1488956178
H,0,3.4104610114,0.2058067721,-3.7090455819
H,0,3.5777203698,-1.5306920197,-3.3337707109

dmpe Bpin3 Para Chlorobenzene CH Activation Transition Structure
E(RB+HF-LYP) = -2479.34400826

Zero-point correction= 0.510604 (Hartree/Particle)
Thermal correction to Energy= 0.547560
Thermal correction to Enthalpy= 0.548505
Thermal correction to Gibbs Free Energy= 0.439155
Sum of electronic and zero-point Energies= -2478.833405
Sum of electronic and thermal Energies= -2478.796448
Sum of electronic and thermal Enthalpies= -2478.795504
Sum of electronic and thermal Free Energies= -2478.904854

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	343.599	133.843	230.146

C,0,2.635652488,1.2867682781,0.3174180378
C,0,1.8691941435,0.1704478753,0.7084899427
C,0,2.5155156334,-0.7709849422,1.5310146516
C,0,3.8646826866,-0.6615253235,1.8831023013
C,0,4.5962754261,0.4288442235,1.4228408124
C,0,3.9866720214,1.4147425025,0.6495540022
Ir,0,-0.2818346212,-0.0485018294,-0.0632560769
P,0,0.2356273421,0.1498535503,-2.4174991724
C,0,-0.0510102046,-1.5238800295,-3.1940369576
C,0,0.5219053564,-2.6393917728,-2.311194088
P,0,-0.0549343192,-2.4798485367,-0.5349730359
B,0,-2.329900991,0.0819042061,-0.6394308632
O,0,-2.9563132346,1.2711480138,-1.02377814
C,0,-4.3698481994,1.0634397245,-1.1172677479
C,0,-4.528454844,-0.4687454949,-1.1374503956
O,0,-3.2587719443,-0.9652804264,-0.6932187203
B,0,-1.3489640503,-0.5264348252,1.7062883274
O,0,-1.0816924305,-1.6866709969,2.445475648
C,0,-2.069698564,-1.8154990028,3.479570662
C,0,-2.7725829237,-0.4435449651,3.5082092175
O,0,-2.3937482939,0.1798118865,2.2763348209
B,0,-0.5089661525,2.0257378138,0.139472232
O,0,-0.8727894941,2.6968383598,1.2974633038
C,0,-0.7532597524,4.1077819915,1.0968972008
C,0,-0.5187479902,4.2670371098,-0.4191792876
O,0,-0.1779486743,2.947439925,-0.8665296227
H,0,-4.8566474104,1.5174193203,-0.245766938
H,0,-4.7565312745,1.5464814583,-2.0208158677
H,0,-5.3170981922,-0.8252399904,-0.4672525671
H,0,-4.7344011261,-0.8526700574,-2.1453700152
H,0,-2.7591850173,-2.6285187948,3.2183997626
H,0,-1.5798172154,-2.0672403556,4.4251893871
H,0,-3.8629387645,-0.5241423145,3.5600247366
H,0,-2.4313723313,0.1799117372,4.3437911678
H,0,-1.4228170016,4.6010671283,-0.9435234108
H,0,0.2960816535,4.9589987174,-0.657004522
H,0,-1.6654669477,4.6074906271,1.4387304509
H,0,0.0896196274,4.4864121303,1.6892455066
H,0,0.401804426,0.2173368236,1.3848163996
H,0,2.1762400189,2.0812733342,-0.2615124308

H,0,4.5580553007,2.2759222085,0.31756602
H,0,1.9487982721,-1.6006960558,1.9390778361
H,0,4.3341896151,-1.4057129258,2.5185136216
Cl,0,6.3022543683,0.5808557201,1.8469611799
C,0,-0.7359298239,1.2731773183,-3.5064817049
C,0,1.9650762684,0.5479608878,-2.9405033644
C,0,-1.5608720213,-3.5504271402,-0.4867593061
C,0,1.1494590096,-3.6039619926,0.3118904081
H,0,0.267120587,-3.6294382199,-2.7070393845
H,0,1.6165035978,-2.5733976544,-2.2898950948
H,0,-1.1363728861,-1.6385527483,-3.2977580503
H,0,0.3786819247,-1.5527608605,-4.2025580452
H,0,2.0707737556,0.4557721015,-4.0263446418
H,0,2.1983620614,1.5734427154,-2.6461845899
H,0,2.6783824119,-0.1136468468,-2.4448149821
H,0,-0.4619699758,1.1350137007,-4.5572086977
H,0,-1.80178119,1.0873071704,-3.3665573772
H,0,-0.5353180204,2.298100339,-3.1909924159
H,0,1.1314081311,-4.5990615231,-0.1450528322
H,0,2.1607746159,-3.1981819542,0.250231533
H,0,0.8707727969,-3.691609999,1.3650202066
H,0,-1.3432270666,-4.5531209165,-0.869287577
H,0,-1.8894635168,-3.6209805928,0.5531043204
H,0,-2.3655183439,-3.0827248347,-1.0536236209

dmpeBpin3ParaClPhHCHactTSParSptBack
E(RB+HF-LYP) = -2479.34638830

Zero-point correction= 0.510729 (Hartree/Particle)
Thermal correction to Energy= 0.547642
Thermal correction to Enthalpy= 0.548586
Thermal correction to Gibbs Free Energy= 0.439853
Sum of electronic and zero-point Energies= -2478.835659
Sum of electronic and thermal Energies= -2478.798747
Sum of electronic and thermal Enthalpies= -2478.797803
Sum of electronic and thermal Free Energies= -2478.906535

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	343.650	133.827	228.847

C,0,4.3138150429,1.6614282579,0.4209591165
C,0,2.946256453,1.4814164089,0.2014950175
C,0,2.2505162654,0.348812877,0.6672278591

C,0,2.9956609793,-0.5566119336,1.44393424
C,0,4.3646407599,-0.3979946146,1.6851394024
C,0,5.0182982788,0.709337523,1.154633216
Ir,0,0.0764916223,-0.0064073172,0.0597917673
B,0,-0.2573284189,2.0480160236,-0.2099710652
O,0,-0.933809626,2.6207560876,-1.2980549768
C,0,-1.1107600956,4.0229188125,-1.0530769853
C,0,-0.1662924139,4.3297761128,0.1273559768
O,0,0.1853561914,3.045466121,0.6490943997
Cl,0,6.7470209656,0.924871743,1.4368782487
P,0,0.6899131982,-0.3552017733,-2.2520286818
C,0,2.4755068494,-0.1747438932,-2.6951114843
P,0,0.1351147984,-2.480405594,0.1233752968
C,0,1.080385332,-3.5509241445,1.3062179187
B,0,-1.9653295552,-0.0698575407,-0.5473629817
O,0,-2.4311650572,-0.6658421486,-1.7355859412
C,0,-3.8242455947,-0.3649294498,-1.9077794348
C,0,-4.2723041712,0.149261605,-0.5280480284
O,0,-3.0518467776,0.4531203985,0.1538596061
B,0,-0.9432411806,0.0530400062,1.9286055515
O,0,-1.3944910773,1.1714238416,2.601244936
C,0,-2.2356936714,0.7513932813,3.678115255
C,0,-1.8904340462,-0.7372594731,3.8730517132
O,0,-1.2514935941,-1.1127663041,2.6415505503
C,0,0.3568609939,-2.143552063,-2.6684333445
C,0,0.8052377859,-3.0655931963,-1.5251573749
C,0,-0.1299232069,0.5549204121,-3.6262326575
C,0,-1.5157201062,-3.3102778982,0.2015072554
H,0,-4.8234583014,-0.6130009461,0.0379489431
H,0,-4.8934800447,1.0482873686,-0.5896084204
H,0,-4.3595474411,-1.2649033591,-2.227337675
H,0,-3.932780754,0.3989920693,-2.6878468263
H,0,-2.772130645,-1.3648795402,4.0367837104
H,0,-1.1905936475,-0.8963309085,4.7032990554
H,0,-3.2840916173,0.8936205857,3.3874222472
H,0,-2.0314307298,1.3593606495,4.5647352468
H,0,-2.1613411311,4.2126688477,-0.8004149352
H,0,-0.8659841243,4.5898474655,-1.9576633599
H,0,-0.6448777172,4.9254329683,0.9109691558
H,0,0.7444664398,4.8527372541,-0.1936644066
H,0,0.7728009374,0.4852372595,1.4430850187
H,0,2.4124488311,2.254294393,-0.3391594955
H,0,4.8249768893,2.5376699256,0.0349887803
H,0,2.4982800442,-1.4031329717,1.9020622511

H,0,4.9094624815,-1.1181202739,2.2873286901
H,0,0.4994709048,-4.1016089109,-1.7129034714
H,0,1.8988303447,-3.063928939,-1.4413823004
H,0,-0.7242209368,-2.2170625424,-2.8208000548
H,0,0.8519399251,-2.410832079,-3.6096807827
H,0,2.6438044313,-0.4800254513,-3.732892259
H,0,2.7847833475,0.8652181778,-2.5726701366
H,0,3.0931079439,-0.7805430374,-2.0290338349
H,0,0.2440624091,0.2147964822,-4.59730248
H,0,-1.2042339337,0.3858672088,-3.5540997027
H,0,0.0549685971,1.6235944065,-3.5054320806
H,0,0.8771964698,-4.6101023792,1.1170512865
H,0,2.1540420136,-3.3768867149,1.2120993022
H,0,0.7700143882,-3.3054747955,2.3252107934
H,0,-1.422205021,-4.3953149535,0.0879509516
H,0,-1.9604833234,-3.0763858786,1.170961863
H,0,-2.1579419532,-2.909345549,-0.5845644441

dmpeBpin3ParaClPhHCHactTSSptSptBack
E(RB+HF-LYP) = -2479.34686349

Zero-point correction= 0.511073 (Hartree/Particle)
Thermal correction to Energy= 0.547752
Thermal correction to Enthalpy= 0.548696
Thermal correction to Gibbs Free Energy= 0.440999
Sum of electronic and zero-point Energies= -2478.835790
Sum of electronic and thermal Energies= -2478.799111
Sum of electronic and thermal Enthalpies= -2478.798167
Sum of electronic and thermal Free Energies= -2478.905864

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	343.720	133.644	226.668

C,0,3.1871492815,-0.6999062885,0.8158054872
C,0,2.2746309282,0.3570803018,0.6316751555
C,0,2.8204922608,1.6553017042,0.6795086173
C,0,4.1895411238,1.8869070069,0.8414551502
C,0,5.0551552286,0.8059136967,0.9798002902
C,0,4.5614588167,-0.4952407347,0.9752179435
Ir,0,0.0752981809,-0.0137138205,0.0904945679
P,0,0.6939664136,-0.8433708936,-2.0951031404
C,0,0.4940836466,-2.7059066273,-2.0774093716
C,0,0.8695502924,-3.3237991149,-0.7207291883

P,0,0.0325400788,-2.398962181,0.6773006941
B,0,-1.9576336793,-0.0670661035,-0.5377469825
O,0,-2.4884429434,-0.9904395065,-1.4571728135
C,0,-3.8507784682,-0.6466691292,-1.7525146136
C,0,-4.2257733795,0.3843162474,-0.6718186213
O,0,-2.9724056463,0.7910862343,-0.1137644178
B,0,-1.0030336899,0.473959702,1.8622741068
O,0,-1.5651761935,-0.5183031102,2.6789483185
C,0,-2.1439372945,0.1109455085,3.83274907
C,0,-2.16717025,1.6088101905,3.4720561037
O,0,-1.2445030982,1.7277003109,2.3863042292
B,0,-0.1277124848,1.9588933658,-0.6166394096
O,0,0.1077233444,3.1303227933,0.0954682175
C,0,-0.0519363843,4.2653353427,-0.7603440517
C,0,-0.7057640504,3.697345523,-2.0342147159
O,0,-0.5146865877,2.280405396,-1.929993677
H,0,-3.9042280077,-0.2245799913,-2.7640422345
H,0,-4.4725991299,-1.5471875646,-1.7209502183
H,0,-4.748731007,1.2561276395,-1.0772132353
H,0,-4.8477079456,-0.0541142835,0.1191075578
H,0,-3.1406450525,-0.3023159783,4.0174739461
H,0,-1.51534612,-0.0955432108,4.7086607534
H,0,-3.1595062543,1.9349251624,3.1362061542
H,0,-1.8491855592,2.2535797654,4.2971443541
H,0,-1.7809248414,3.9129151285,-2.0769525517
H,0,-0.2427359296,4.0669890033,-2.9552727296
H,0,-0.6713953075,5.0166693471,-0.2606970991
H,0,0.9322833062,4.7087801998,-0.962493015
H,0,0.8300061767,0.4638068489,1.4529403327
H,0,2.8423383455,-1.7269550269,0.8190719921
H,0,5.2364871997,-1.3366155386,1.0966239168
H,0,2.1589526555,2.5104004319,0.6029570196
H,0,4.5761190035,2.9008006024,0.8686212929
Cl,0,6.7860595783,1.0838286991,1.1796995401
C,0,-0.2112960674,-0.3744050791,-3.629640254
C,0,2.4453657795,-0.5908721914,-2.6261762397
C,0,-1.6226185666,-3.2157767711,0.7570886151
C,0,0.7996397307,-3.1017765179,2.2096533425
H,0,0.6040983427,-4.3873309486,-0.6900286989
H,0,1.9517855561,-3.25759167,-0.5610064215
H,0,-0.5637027114,-2.8893186843,-2.2952761761
H,0,1.0796712829,-3.151794391,-2.8900072651
H,0,2.6425632619,-1.1070999218,-3.5712645499
H,0,2.6185198811,0.4802044223,-2.7604317122

H,0,3.1371950311,-0.9445259664,-1.8604241322
H,0,0.2119570688,-0.8857436939,-4.5001856625
H,0,-1.2607193315,-0.6442824276,-3.5094861558
H,0,-0.1441636958,0.7073955382,-3.7527941617
H,0,0.7631238477,-4.1962039853,2.2118885763
H,0,1.8335617962,-2.7736436236,2.3269392407
H,0,0.2244848565,-2.7220621686,3.0581537079
H,0,-1.5270958317,-4.2948545213,0.9169496735
H,0,-2.1701677417,-2.764324869,1.5872937921
H,0,-2.1684690458,-3.0165075785,-0.1659322425

dmpeBpin3ParaClPhHCHactTSSptSptFrnt
E(RB+HF-LYP) = -2479.34507493

Zero-point correction= 0.511058 (Hartree/Particle)
Thermal correction to Energy= 0.547797
Thermal correction to Enthalpy= 0.548741
Thermal correction to Gibbs Free Energy= 0.440853
Sum of electronic and zero-point Energies= -2478.834017
Sum of electronic and thermal Energies= -2478.797278
Sum of electronic and thermal Enthalpies= -2478.796334
Sum of electronic and thermal Free Energies= -2478.904222

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	343.748	133.654	227.070

C,0,0.3351068865,-3.5152407194,-0.6947319552
C,0,-0.7391873014,-2.9491073402,-1.6348514026
P,0,-0.4406988187,-1.140800309,-2.012913244
Ir,0,0.2894146118,-0.0879725862,0.0232670416
B,0,0.1815847164,1.7770986399,-0.9486685833
O,0,-0.0305365163,3.0299629925,-0.3921769307
C,0,0.0831166247,4.0376841317,-1.4002566012
C,0,0.048696878,3.2596991648,-2.7302324988
O,0,0.28063746,1.8965869023,-2.3506538081
P,0,0.6747419411,-2.3978108866,0.7789150885
B,0,1.3607663447,0.7755343586,1.6581573542
O,0,2.1895660357,0.0174994037,2.4954360363
C,0,2.6871821141,0.8632941573,3.5434781326
C,0,2.3185023607,2.2887875461,3.0874747921
O,0,1.3337320115,2.0940274957,2.0689063288
B,0,2.2918180823,0.0199348648,-0.6885684629
O,0,2.9778807774,-1.0163634069,-1.3447354294

C,0,4.2581850888,-0.5428579839,-1.7891827788
C,0,4.4376587739,0.807278213,-1.0690020245
O,0,3.132752005,1.127849034,-0.5764203227
C,0,2.3783960867,-2.935533106,1.2480903042
C,0,-0.278110673,-3.1702298757,2.1738137465
H,0,0.0695769624,-4.5230670354,-0.3548026123
H,0,1.2886333799,-3.5949064124,-1.2283076675
C,0,0.6596497748,-1.1833359796,-3.4910717668
C,0,-2.0359604274,-0.5969387822,-2.7601163898
H,0,-0.7860427109,-3.5229768115,-2.5682555614
H,0,-1.7297002836,-3.0129915946,-1.1720891241
H,0,0.8212432714,3.5841691708,-3.4351165697
H,0,-0.9265559667,3.3357596164,-3.2293306223
H,0,1.0280210976,4.5776440525,-1.2616829687
H,0,-0.7403828002,4.7528393647,-1.3027019163
H,0,3.1776588313,2.818923051,2.6580585704
H,0,1.8989750324,2.9012921934,3.8915753784
H,0,3.7659014968,0.714371527,3.6555136027
H,0,2.2002537966,0.5892296322,4.4882463852
H,0,4.7852987863,1.6027526546,-1.7356990154
H,0,5.1345530063,0.7363610069,-0.2242720237
H,0,4.2406956257,-0.4320372686,-2.8808627227
H,0,5.0309463646,-1.2735274525,-1.5294167895
H,0,2.4151029691,-4.0136061394,1.4370863657
H,0,3.0601049711,-2.6743221901,0.4375425921
H,0,2.6759403994,-2.3851087055,2.1421438236
H,0,-0.0358565621,-4.233023638,2.2787868129
H,0,-0.0007640206,-2.6521765657,3.0966605145
H,0,-1.3549408522,-3.0583265872,2.04111562
H,0,-2.3270402934,-1.2498308105,-3.5893617649
H,0,-2.8214227282,-0.5914076078,-2.0024475147
H,0,-1.900299121,0.4211741118,-3.1317938683
H,0,0.1934952029,-1.7430137166,-4.3083179987
H,0,0.8334378552,-0.1500351287,-3.7988845502
H,0,1.6158760001,-1.6311897004,-3.2186989697
H,0,-0.4202899542,0.3385513223,1.4248768542
C,0,-1.890789553,0.1690999866,0.6874889268
C,0,-2.7706497682,-0.9243751393,0.7937020631
C,0,-4.1404185691,-0.7704262423,1.0312381135
C,0,-4.657069839,0.5110149281,1.1995790285
C,0,-3.8212107958,1.6227521117,1.1372918023
C,0,-2.4573906225,1.4437261494,0.8892059784
H,0,-2.3992211156,-1.934664603,0.6686065854
H,0,-4.7941172267,-1.6351857309,1.0875683441

Cl,0,-6.3814929411,0.7236688646,1.506465193
H,0,-4.2272902529,2.6182287839,1.286109682
H,0,-1.8193252471,2.3197015786,0.8476996185

dmpeBpin2ParaClHBpinRotTS
E(RB+HF-LYP) = -2479.35526755

Zero-point correction= 0.514092 (Hartree/Particle)
Thermal correction to Energy= 0.550096
Thermal correction to Enthalpy= 0.551040
Thermal correction to Gibbs Free Energy= 0.445733
Sum of electronic and zero-point Energies= -2478.841175
Sum of electronic and thermal Energies= -2478.805172
Sum of electronic and thermal Enthalpies= -2478.804228
Sum of electronic and thermal Free Energies= -2478.909534

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	345.190	131.765	221.636

C,0,4.4284745757,0.3571629502,1.0039214458
C,0,3.0305640071,0.2808181578,1.0673697752
C,0,2.2022057833,0.0171816097,-0.04442317
C,0,2.9073862176,-0.170019965,-1.2561935016
C,0,4.2998300136,-0.1002109365,-1.3599088711
C,0,5.0553687258,0.1647147108,-0.2211318031
Ir,0,-0.0323191153,-0.0719995413,-0.0230706844
B,0,0.1619363626,-1.879866028,-1.0896605917
O,0,0.1492239851,-3.174171242,-0.5607216546
C,0,0.2475554506,-4.1241672872,-1.6333071083
C,0,0.6292274529,-3.2772354678,-2.8642612536
O,0,0.3779278368,-1.9259351715,-2.4627099537
B,0,-2.1417670549,-0.2861976691,-0.2754403645
O,0,-3.1377401102,0.0022793811,0.6805639701
C,0,-4.4254417045,-0.3596026175,0.1552567091
C,0,-4.1667440336,-0.6139429311,-1.3409587136
O,0,-2.7467901672,-0.761600105,-1.4367406824
P,0,-0.182881368,1.8459721059,1.4724032048
C,0,1.081171741,3.1919276063,1.44010355
P,0,-0.2331607112,-1.3305902585,1.927914465
C,0,1.226115484,-2.2993988166,2.4987554239
B,0,-0.1863701919,1.6210490983,-1.5152464821
O,0,-1.4051774013,2.1243175872,-1.932692636
C,0,-1.1667411624,3.3202283475,-2.6909634139

C,0,0.3268145011,3.6427345451,-2.4514035832
O,0,0.8590595442,2.4630597016,-1.8335865656
C,0,-0.010343737,1.1794405134,3.2115667084
C,0,-0.677634187,-0.1930383856,3.3435487239
C,0,-1.7569518339,2.8095363312,1.5476075816
C,0,-1.5658374093,-2.5967397843,2.0408986895
H,0,0.0744643316,0.3103605415,-1.6564697223
H,0,-0.4263425685,-0.671424436,4.2971327493
H,0,-1.7670625307,-0.0872704369,3.3035426742
H,0,-0.4313258757,1.8954454332,3.9267457423
H,0,1.06231365,1.1077593086,3.4206058967
H,0,0.4667036521,4.4960332104,-1.7760035388
H,0,0.8757674117,3.8447985233,-3.3754420648
H,0,-1.8367997823,4.1125566166,-2.3431033404
H,0,-1.3866937125,3.1187031143,-3.7454252074
H,0,0.0276701366,-3.5156271435,-3.7468416806
H,0,1.6893601165,-3.3830972746,-3.1259389662
H,0,-0.7208660577,-4.6241595349,-1.7582756425
H,0,0.9994051877,-4.8797142432,-1.3847638758
H,0,-4.4834178679,0.2327855112,-1.9631377478
H,0,-4.6594755059,-1.518401678,-1.7118139845
H,0,-5.1390672123,0.4503463341,0.3370361813
H,0,-4.7869556039,-1.258638544,0.6725838757
H,0,2.3563055471,-0.3858296398,-2.1672613161
H,0,4.7916326942,-0.2500364714,-2.3164340242
Cl,0,6.8193597188,0.255360399,-0.3319856768
H,0,5.016339388,0.5638620456,1.8933943194
H,0,2.5917877174,0.443396874,2.050207711
H,0,-1.387703942,-3.3440220904,1.2672004084
H,0,-1.5561658625,-3.0711640573,3.0275663929
H,0,-2.5293814748,-2.1148239969,1.8711819625
H,0,1.4133276846,-3.0692445616,1.7466903867
H,0,2.1124181873,-1.6697101905,2.5678639741
H,0,1.0214133953,-2.7707719947,3.4652892243
H,0,-1.9156705582,3.2997964483,0.5837078061
H,0,-2.58564045,2.1166851365,1.7026611074
H,0,-1.7289042156,3.5639367642,2.3406268067
H,0,0.943341757,3.7937725153,0.5395953452
H,0,0.9915751752,3.8350051883,2.3214499347
H,0,2.0782399754,2.7509208904,1.3951850753

dmpe Bpin3 Meta Chlorobenzene CH Activation Transition Structure
dmpeBpin3MetaClPhHCHactTSParParBackA
E(RB+HF-LYP) = -2479.34487672

Zero-point correction= 0.510950 (Hartree/Particle)
Thermal correction to Energy= 0.547819
Thermal correction to Enthalpy= 0.548763
Thermal correction to Gibbs Free Energy= 0.439557
Sum of electronic and zero-point Energies= -2478.833927
Sum of electronic and thermal Energies= -2478.797058
Sum of electronic and thermal Enthalpies= -2478.796114
Sum of electronic and thermal Free Energies= -2478.905320

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	343.761	133.569	229.843

C,0,2.6688428651,1.2154745,0.3979426539
C,0,1.9468449809,0.0689519215,0.7840973093
C,0,2.6294790986,-0.882179979,1.565164607
C,0,3.9826165117,-0.7385794185,1.8857586317
C,0,4.7023952391,0.3743844308,1.4529091744
C,0,4.019622726,1.3413212393,0.717536734
Ir,0,-0.2115799772,-0.1657413354,0.029593702
P,0,0.3284310783,0.0296712156,-2.3216219929
C,0,0.1069810417,-1.6572252262,-3.0955673474
C,0,0.6653479156,-2.7569012366,-2.1832868363
P,0,0.0061410338,-2.5957575105,-0.4369960731
B,0,-2.2604204994,-0.0282353525,-0.5331747732
O,0,-2.8617629008,1.1377184218,-1.0173971889
C,0,-4.2816259854,0.9618900091,-1.0773596169
C,0,-4.4870470069,-0.557868695,-0.9212800914
O,0,-3.2185638118,-1.0468580164,-0.4665893936
B,0,-1.2793167477,-0.6575646077,1.7950125902
O,0,-1.0877298482,-1.8826214105,2.4500856021
C,0,-2.0594960101,-2.001873874,3.5003947949
C,0,-2.6468417029,-0.5828311878,3.6385676629
O,0,-2.2438228551,0.0922502377,2.4425772276
B,0,-0.4454146754,1.9128052942,0.2216005027
O,0,-0.8609126826,2.5911163274,1.3559880347
C,0,-0.7264508266,4.0009906536,1.1547709587
C,0,-0.4014257648,4.1540767034,-0.3459654543
O,0,-0.0668823035,2.8260582133,-0.7748653286
H,0,-4.7467349986,1.5278006142,-0.2614157294
H,0,-4.6625053449,1.3499098256,-2.0280600783
H,0,-5.2609178998,-0.8098341996,-0.1891021275
H,0,-4.7432891952,-1.044573037,-1.8714987427

H,0,-2.8191302913,-2.736979311,3.2053340588
H,0,-1.5711466042,-2.3555794029,4.4137666676
H,0,-3.7388611926,-0.5793841761,3.7131973299
H,0,-2.2389491663,-0.0479873551,4.5052258537
H,0,-1.2644805574,4.5104402513,-0.922049848
H,0,0.4430691812,4.8247662389,-0.5352624034
H,0,-1.6566976404,4.5035220575,1.4394359429
H,0,0.0800646734,4.3805692339,1.7946123421
H,0,0.4931216599,0.0944385326,1.473215577
H,0,2.1821430356,2.0096548959,-0.15503433
Cl,0,4.8968808711,2.7802041557,0.1754298176
H,0,2.0883198739,-1.7357156789,1.9566358996
H,0,4.4790273097,-1.4936621862,2.4904327871
H,0,5.7519336927,0.5017738775,1.6935175791
C,0,-0.6530408183,1.1185683305,-3.4363725587
C,0,2.0560512705,0.4663259438,-2.813277119
C,0,-1.5246352007,-3.6302139703,-0.4848705624
C,0,1.1369613379,-3.7557041275,0.4619018927
H,0,0.4455072101,-3.753509815,-2.5839934189
H,0,1.7567501421,-2.6715387302,-2.1158235844
H,0,-0.9699741296,-1.7986666083,-3.2470743213
H,0,0.5797777883,-1.6810059663,-4.0847965141
H,0,2.1861710372,0.3591251001,-3.8950693097
H,0,2.2609710286,1.5009112534,-2.5305944184
H,0,2.7712326298,-0.1720506261,-2.2908628504
H,0,-0.3606878837,0.9748995304,-4.4815290801
H,0,-1.716897316,0.9130139235,-3.3077441948
H,0,-0.4764215606,2.1513012275,-3.1319049213
H,0,1.0998835144,-4.753018369,0.011157838
H,0,2.1641901238,-3.3877469973,0.4320658222
H,0,0.8165424173,-3.8229254617,1.5043804183
H,0,-1.3093667728,-4.6321065714,-0.8710090365
H,0,-1.9124748293,-3.7054537613,0.5335261079
H,0,-2.2883913764,-3.1384546646,-1.0874025012

dmpeBpin3MetaClPhHCHactTSParSptBack
E(RB+HF-LYP) = -2479.34706746

Zero-point correction= 0.511026 (Hartree/Particle)
Thermal correction to Energy= 0.547750
Thermal correction to Enthalpy= 0.548694
Thermal correction to Gibbs Free Energy= 0.440586
Sum of electronic and zero-point Energies= -2478.836042
Sum of electronic and thermal Energies= -2478.799318

Sum of electronic and thermal Enthalpies= -2478.798373
Sum of electronic and thermal Free Energies= -2478.906482

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	343.718	133.713	227.533

C,0,4.319459488,1.5717451287,0.3949788711
C,0,2.956493713,1.4201815131,0.1479036964
C,0,2.243570884,0.3302363055,0.6829600161
C,0,2.9583126066,-0.5308724674,1.5368314206
C,0,4.323423619,-0.3624907545,1.7881730773
C,0,5.029549689,0.6889098785,1.2059468577
Ir,0,0.0712211851,-0.0029549903,0.0647304907
B,0,-0.2472497117,2.0526351635,-0.2028123198
O,0,-0.91604832,2.6324045909,-1.2911326438
C,0,-1.0737675359,4.0373281661,-1.0447664451
C,0,-0.1172626078,4.331969717,0.1286851375
O,0,0.2093238571,3.0427423802,0.6560560838
H,0,6.0882831895,0.83446184,1.3888650958
P,0,0.6678831238,-0.3376342073,-2.2644667983
C,0,2.4390947017,-0.106695478,-2.7428870002
P,0,0.1586347941,-2.4790177245,0.1136350835
C,0,1.111137296,-3.5346811623,1.3021673261
B,0,-1.9736234501,-0.0622185793,-0.5345861355
O,0,-2.4488331533,-0.7172025887,-1.68775921
C,0,-3.8406546918,-0.417126192,-1.8717531778
C,0,-4.2758409865,0.2065421032,-0.5323479717
O,0,-3.0493675471,0.5188587142,0.1347100694
B,0,-0.9672430635,0.0348297564,1.9188175599
O,0,-1.3732791614,1.1505712153,2.6253902947
C,0,-2.2220664312,0.735339706,3.6981552151
C,0,-1.943150828,-0.7729019315,3.8431041315
O,0,-1.3270929183,-1.1371024048,2.5972252864
C,0,0.3742755634,-2.1348823996,-2.670929698
C,0,0.8538069374,-3.0433307184,-1.53014516
C,0,-0.1985187829,0.5415091184,-3.631693732
C,0,-1.4811907892,-3.3312713808,0.1720352885
H,0,-4.8544515113,-0.4946172774,0.0827841944
H,0,-4.8666904539,1.1189013445,-0.6609747985
H,0,-4.3858563501,-1.3346283776,-2.1162535449
H,0,-3.9495027242,0.2839955995,-2.7086158509
H,0,-2.8511207735,-1.3657651865,3.9923555173
H,0,-1.2474215883,-0.9895268362,4.6638234293

H,0,-3.2661426442,0.9349646556,3.4261505617
H,0,-1.9805327654,1.3049229555,4.6008221583
H,0,-2.1202573631,4.238847632,-0.7842465928
H,0,-0.8284890838,4.6011633816,-1.9509968056
H,0,-0.5795222374,4.9417506809,0.911228737
H,0,0.802999435,4.8324951411,-0.1995745157
H,0,0.7693436868,0.5211586243,1.4301631932
H,0,2.4536300188,2.1626113515,-0.4580026952
Cl,0,5.1764269257,2.9346055384,-0.3416111728
H,0,2.4374993653,-1.3342255945,2.0442847466
H,0,4.840248531,-1.0496321284,2.4538472656
H,0,0.5806821795,-4.0883484329,-1.7191484965
H,0,1.9467065908,-3.0060308035,-1.4445860927
H,0,-0.7068433173,-2.233647893,-2.8077387345
H,0,0.86346352,-2.3919945211,-3.6178977695
H,0,2.6014758182,-0.451098984,-3.7693834829
H,0,2.7073627541,0.9497488986,-2.6765122257
H,0,3.0931591486,-0.6547534964,-2.0621758383
H,0,0.2011765216,0.2369190002,-4.6042763729
H,0,-1.2616608209,0.3076902733,-3.5724313865
H,0,-0.0788113404,1.6175488201,-3.4946404347
H,0,0.9568198437,-4.5970591207,1.0865988293
H,0,2.1783928664,-3.3129887718,1.2444979651
H,0,0.760307837,-3.3237460647,2.3158238259
H,0,-1.3721010804,-4.4172380855,0.0846386587
H,0,-1.9491311744,-3.0785631571,1.1259638621
H,0,-2.1112374827,-2.9537244836,-0.6352568438

dmpeBpin3MetaClPhHCHactTSSptSptBackA
E(RB+HF-LYP) = -2479.34811590

Zero-point correction= 0.511216 (Hartree/Particle)
Thermal correction to Energy= 0.547887
Thermal correction to Enthalpy= 0.548831
Thermal correction to Gibbs Free Energy= 0.441665
Sum of electronic and zero-point Energies= -2478.836900
Sum of electronic and thermal Energies= -2478.800229
Sum of electronic and thermal Enthalpies= -2478.799285
Sum of electronic and thermal Free Energies= -2478.906451

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	343.804	133.613	225.549

C,0,3.1776275189,-0.6980090913,0.7932446795
C,0,2.274359219,0.3698717472,0.6295483791
C,0,2.8163326022,1.6684012851,0.7056139544
C,0,4.1854542088,1.8842041166,0.8822480381
C,0,5.0748898393,0.8166087608,1.0076960347
C,0,4.5434130509,-0.468164925,0.9638490932
Ir,0,0.076566125,-0.008730716,0.076438804
P,0,0.6949687618,-0.84904029,-2.1014933274
C,0,0.4661736637,-2.7077710004,-2.0826647194
C,0,0.8441607212,-3.3311704664,-0.7293154066
P,0,0.0315939514,-2.3967193806,0.6753240075
B,0,-1.9551160528,-0.0728356503,-0.549233154
O,0,-2.4805678498,-0.9958444888,-1.470835411
C,0,-3.8469246651,-0.6635601119,-1.7601984637
C,0,-4.2262036645,0.3658264142,-0.6788110648
O,0,-2.9752410338,0.7749609881,-0.1173252503
B,0,-0.9933523913,0.4840425332,1.8535036624
O,0,-1.5535339724,-0.5096395153,2.6702957263
C,0,-2.1247868267,0.1170479102,3.8290745837
C,0,-2.1424973521,1.6169045053,3.4760752596
O,0,-1.2289773258,1.7366497653,2.3821734047
B,0,-0.1368446839,1.9633441839,-0.6280653424
O,0,0.1063010966,3.1323042762,0.0857177772
C,0,-0.0690615882,4.2711335571,-0.7607419661
C,0,-0.7315606748,3.7072224726,-2.0327453195
O,0,-0.5432489551,2.2897074549,-1.9338796767
H,0,-3.9088029115,-0.2438481798,-2.772176803
H,0,-4.4608881012,-1.5693390374,-1.7244840785
H,0,-4.7498885645,1.2368268154,-1.0851472907
H,0,-4.8494192058,-0.0741909105,0.1101020225
H,0,-3.1228110633,-0.2921998312,4.0156897934
H,0,-1.4937481591,-0.0967541521,4.701405555
H,0,-3.1358421851,1.9511168767,3.1514592653
H,0,-1.8128290228,2.2553513493,4.301538814
H,0,-1.8063809544,3.92554646,-2.0693578295
H,0,-0.2727619762,4.0782870368,-2.955436564
H,0,-0.6892644876,5.0148185797,-0.25044188
H,0,0.9098145404,4.7235595423,-0.969048573
H,0,0.8363342994,0.4602321449,1.4409293612
H,0,2.8425477965,-1.7258804542,0.7709424554
Cl,0,5.6288689151,-1.8589331964,1.127218219
H,0,2.1514602759,2.5210982332,0.6398440432
H,0,4.5660961544,2.9015195042,0.9319211253
H,0,6.1388768283,0.9725858709,1.1465924896

C,0,-0.189433347,-0.3643407595,-3.6435872623
C,0,2.4545715305,-0.6245638212,-2.6186367032
C,0,-1.6290558472,-3.1993347753,0.7782288024
C,0,0.8180372279,-3.1005578807,2.1972143908
H,0,0.5617400657,-4.3901961592,-0.6958192174
H,0,1.9287327247,-3.2832689806,-0.5774642735
H,0,-0.5967308324,-2.8724200602,-2.2899170692
H,0,1.0375954626,-3.1624228482,-2.9004381993
H,0,2.6473100302,-1.1333239134,-3.5685813737
H,0,2.6501166371,0.4445421723,-2.7368413096
H,0,3.1342000261,-1.0023790805,-1.8535357257
H,0,0.2314788997,-0.8842597526,-4.5102173713
H,0,-1.2448357334,-0.6141779206,-3.5334209937
H,0,-0.1009638047,0.715747264,-3.7680344107
H,0,0.7832833923,-4.1949734982,2.1946123185
H,0,1.8536059549,-2.773272482,2.3017749949
H,0,0.2539067023,-2.7263930294,3.0555675582
H,0,-1.5407603915,-4.2767659068,0.9526972737
H,0,-2.166823449,-2.7307113125,1.6050778723
H,0,-2.17870615,-3.0103672419,-0.144988729

dmpeBpin3MetaClPhHCHactTSSptSptBackS
E(RB+HF-LYP) = -2479.34749715

Zero-point correction= 0.511514 (Hartree/Particle)
Thermal correction to Energy= 0.547983
Thermal correction to Enthalpy= 0.548927
Thermal correction to Gibbs Free Energy= 0.442409
Sum of electronic and zero-point Energies= -2478.835983
Sum of electronic and thermal Energies= -2478.799514
Sum of electronic and thermal Enthalpies= -2478.798570
Sum of electronic and thermal Free Energies= -2478.905088

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	343.864	133.432	224.186

C,0,3.0231817342,0.0095220643,0.4548179083
C,0,1.8896092014,0.8460482024,0.4586469087
C,0,2.1275139681,2.2283586207,0.5879030689
C,0,3.4301701306,2.7230164946,0.6516060519
C,0,4.5460505942,1.8912166652,0.6143840826
C,0,4.3232992271,0.5180963097,0.5196157164
Ir,0,-0.2201093253,0.0226165546,0.0568040787

P,0,0.3416701226,-0.4226177287,-2.2501655921
C,0,0.5739837427,-2.2698446181,-2.4459940892
C,0,1.2163120911,-2.9169751796,-1.2076714643
P,0,0.3430601094,-2.3561177261,0.3529573214
B,0,-2.2452700654,-0.4443177186,-0.3938662105
O,0,-2.6603987757,-1.3408547217,-1.3951023977
C,0,-4.0897689879,-1.291385135,-1.5212152462
C,0,-4.5561997355,-0.5365869654,-0.2628414471
O,0,-3.3692257494,0.0793082168,0.2460575923
B,0,-1.1724241918,0.0698122856,1.9632123958
O,0,-1.3829452808,-1.0997320421,2.7076502426
C,0,-1.9691365223,-0.7400901326,3.9686752691
C,0,-2.3887561178,0.7312191047,3.7833073021
O,0,-1.6470859612,1.1721506073,2.6432950136
B,0,-0.9429877569,1.9477548798,-0.3859042913
O,0,-0.8685718186,3.0692724554,0.4321263465
C,0,-1.3597899,4.2181913158,-0.2652082103
C,0,-2.0437875459,3.6413741879,-1.5192590797
O,0,-1.5582374671,2.2942468482,-1.6013928012
H,0,-4.350828805,-0.7581087068,-2.4440034241
H,0,-4.4893861925,-2.3086337371,-1.5852100795
H,0,-5.3053709355,0.2313208771,-0.4795206599
H,0,-4.966118969,-1.2142543546,0.4970204476
H,0,-2.812748982,-1.4031294676,4.1855593325
H,0,-1.2197297584,-0.8616482544,4.7614355464
H,0,-3.4609418415,0.8289749012,3.5720683186
H,0,-2.1445978323,1.3588364474,4.6459195826
H,0,-3.1367525438,3.6240155173,-1.422548851
H,0,-1.7867703141,4.1834682791,-2.4354405786
H,0,-2.0479542393,4.7719509276,0.3808189165
H,0,-0.5173155839,4.8754690676,-0.517145757
H,0,0.5545669189,0.5386456946,1.3961182914
H,0,2.9060867715,-1.0641404765,0.3774319308
H,0,5.1718609516,-0.1617277191,0.4974438762
H,0,1.2946307228,2.9173024156,0.6536320917
Cl,0,3.676612448,4.4695124233,0.7919264635
H,0,5.5476138649,2.3027851205,0.6684737839
C,0,-0.8010311429,-0.0242511429,-3.6388153216
C,0,1.9261284044,0.2933940103,-2.8740967344
C,0,-1.0750869687,-3.5372188549,0.4519469568
C,0,1.3944510904,-3.0197151979,1.7261029171
H,0,1.1960759235,-4.0105967614,-1.2854003083
H,0,2.2677774526,-2.6189350006,-1.1257901107
H,0,-0.4305566948,-2.6768309044,-2.6035200514

H,0,1.1588123594,-2.47818662,-3.3495406166
H,0,2.1401240004,-0.0596066988,-3.8880724213
H,0,1.8352034751,1.3827474173,-2.884480617
H,0,2.7524120972,0.0377876686,-2.2094042553
H,0,-0.3654309677,-0.3178185695,-4.5993425136
H,0,-1.7413770719,-0.5512335567,-3.474967424
H,0,-0.9994479068,1.0484253775,-3.6216374494
H,0,1.6002834414,-4.0870363813,1.5942654657
H,0,2.3366285241,-2.4755412733,1.8073415176
H,0,0.8359854226,-2.8730021029,2.6542764843
H,0,-0.7294384308,-4.5762881827,0.4462935182
H,0,-1.6121331431,-3.3325246803,1.3808036162
H,0,-1.7521982645,-3.3597773467,-0.3848733535

dmpeBpin3MetaClPhHCHactTSSptSptFrntA
E(RB+HF-LYP) = -2479.34623238

Zero-point correction= 0.511150 (Hartree/Particle)
Thermal correction to Energy= 0.547884
Thermal correction to Enthalpy= 0.548828
Thermal correction to Gibbs Free Energy= 0.440672
Sum of electronic and zero-point Energies= -2478.835082
Sum of electronic and thermal Energies= -2478.798349
Sum of electronic and thermal Enthalpies= -2478.797405
Sum of electronic and thermal Free Energies= -2478.905561

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	343.802	133.639	227.634

C,0,-0.0001133377,-3.4838665412,-0.6231532743
C,0,-1.0860060532,-2.9191148702,-1.551626317
P,0,-0.7862159635,-1.1125429877,-1.9351061665
Ir,0,-0.0407196668,-0.0543539472,0.0944830118
B,0,-0.1307220081,1.8120023053,-0.8734278375
O,0,-0.373915864,3.0597269926,-0.3166600071
C,0,-0.2277456457,4.0766381513,-1.3106320581
C,0,-0.1937806318,3.3093953456,-2.6473651757
O,0,0.0215979979,1.9437407207,-2.2688226251
P,0,0.3446596764,-2.3661126262,0.8482195847
B,0,1.0256202355,0.8144631581,1.732570851
O,0,1.8391744479,0.0592589343,2.5855513297
C,0,2.3243214057,0.9109210854,3.6346805577
C,0,1.9885583645,2.3341639136,3.1501403722

O,0,1.009084457,2.138729419,2.1263577707
B,0,1.9587739417,0.0517587523,-0.6227767346
O,0,2.6412830769,-0.9775264171,-1.2932441687
C,0,3.9195351767,-0.4994550626,-1.7389004915
C,0,4.1040187467,0.8415399472,-1.0032698678
O,0,2.8022143286,1.1569420001,-0.5001849893
C,0,2.0537149628,-2.8944839048,1.3099243734
C,0,-0.5958901536,-3.1509240777,2.2447450204
H,0,-0.2612161553,-4.4920624327,-0.2811314332
H,0,0.9490609964,-3.5620158872,-1.164568091
C,0,0.304916352,-1.1498185291,-3.4191813971
C,0,-2.3851730264,-0.5593267724,-2.6663694699
H,0,-1.1458450689,-3.4946604945,-2.4831398895
H,0,-2.0702740531,-2.9812248595,-1.0739825294
H,0,0.613108571,3.6408672008,-3.3093229645
H,0,-1.1422569772,3.3887004106,-3.195137104
H,0,0.7030440077,4.6270311259,-1.125744912
H,0,-1.0635999783,4.7811834674,-1.2445427763
H,0,2.8620355124,2.8385346686,2.718302414
H,0,1.5742457271,2.9699548957,3.9386820797
H,0,3.3972182632,0.7465822247,3.7763646079
H,0,1.8085130416,0.6581951703,4.5700727461
H,0,4.4489192588,1.6448215927,-1.6620580037
H,0,4.8056880752,0.759651055,-0.1634659287
H,0,3.8959954401,-0.3750403127,-2.8289389928
H,0,4.6931524333,-1.2337796008,-1.492330294
H,0,2.0966853498,-3.9728902372,1.4956579287
H,0,2.7315053666,-2.6275355894,0.4979352228
H,0,2.3506877165,-2.3466402206,2.2060230595
H,0,-0.3071084025,-4.199635139,2.3716367076
H,0,-0.3570252563,-2.605635965,3.162543559
H,0,-1.6747365862,-3.095093302,2.0949287455
H,0,-2.6912342632,-1.2146087675,-3.4881134502
H,0,-3.1600292399,-0.544426411,-1.8981292154
H,0,-2.2475611681,0.4563649573,-3.0445386848
H,0,-0.1627653852,-1.7079186064,-4.2366781962
H,0,0.475382489,-0.1143305632,-3.7217513016
H,0,1.2633483443,-1.5953788629,-3.1517774193
H,0,-0.7498801236,0.3805335032,1.4949434393
C,0,-2.2217201666,0.2031499499,0.7623081045
C,0,-3.0803655852,-0.9044608096,0.8936818123
C,0,-4.4454426141,-0.7328529319,1.1288733408
C,0,-5.0149882528,0.528001017,1.2745474269
C,0,-4.1670480728,1.6325655576,1.1813949024

C,0,-2.8005036457,1.476485061,0.9365488744
H,0,-2.7087832342,-1.9155273863,0.7981132608
Cl,0,-5.4779717756,-2.1673674428,1.2462200806
H,0,-6.0769833124,0.6381021654,1.4637092587
H,0,-4.5789612636,2.6308143765,1.307736863
H,0,-2.1700668318,2.3560064334,0.8772004605

dmpeBpin2MetaClHBpinRotTS
E(RB+HF-LYP) = -2479.35701584

Zero-point correction= 0.513991 (Hartree/Particle)
Thermal correction to Energy= 0.550032
Thermal correction to Enthalpy= 0.550976
Thermal correction to Gibbs Free Energy= 0.445651
Sum of electronic and zero-point Energies= -2478.843025
Sum of electronic and thermal Energies= -2478.806984
Sum of electronic and thermal Enthalpies= -2478.806040
Sum of electronic and thermal Free Energies= -2478.911365

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	345.150	131.824	221.675

C,0,4.3882267554,0.3683900119,0.9521811218
C,0,2.9959710598,0.2982481332,1.0423140788
C,0,2.1826075469,0.0106489547,-0.0742744717
C,0,2.8906966192,-0.2015266981,-1.2806035426
C,0,4.2826916793,-0.1303553048,-1.3672345962
C,0,5.0617060266,0.1580425102,-0.2442160553
Ir,0,-0.0480702368,-0.0735777098,-0.0333540161
B,0,0.1552881432,-1.8846169511,-1.09000715
O,0,0.2047608525,-3.1712510415,-0.5436186088
C,0,0.3172885141,-4.1322836272,-1.6048409325
C,0,0.6295272207,-3.2882637086,-2.857209023
O,0,0.3307280131,-1.9431898974,-2.46835641
B,0,-2.1596003861,-0.2755351586,-0.2763695052
O,0,-3.1466753149,-0.0389702323,0.7032290509
C,0,-4.4382544381,-0.3806718022,0.1737312793
C,0,-4.1944901472,-0.557507385,-1.3359910893
O,0,-2.7749127969,-0.691700112,-1.4547527263
P,0,-0.2025346755,1.8418689171,1.4735252608
C,0,1.0472601778,3.200956203,1.4325045898
P,0,-0.2333164456,-1.337129221,1.9223870497
C,0,1.2372933731,-2.27690237,2.5144420894

B,0,-0.1680308688,1.6277585554,-1.5116351036
O,0,-1.3794412321,2.2028751816,-1.8545723481
C,0,-1.1172519221,3.3780840763,-2.6376937737
C,0,0.4030198849,3.6155995794,-2.4848722329
O,0,0.9025266707,2.4055198135,-1.9000283463
C,0,-0.0233349941,1.1688986501,3.2082074032
C,0,-0.7018014586,-0.1997717091,3.3279760959
C,0,-1.7850380237,2.7900279161,1.5599681788
C,0,-1.5475262243,-2.6223084707,2.0298747815
H,0,0.0151533384,0.301357545,-1.6688920466
H,0,-0.4756593304,-0.6779112202,4.2878125669
H,0,-1.788999269,-0.0876004249,3.2581696482
H,0,-0.4405130564,1.8830534602,3.9274164602
H,0,1.0487481545,1.0894531951,3.4172587866
H,0,0.6292123984,4.4567269124,-1.8176151422
H,0,0.9080204765,3.7905210345,-3.4390448151
H,0,-1.7207969957,4.2100757447,-2.261657101
H,0,-1.4070537451,3.1815626805,-3.6761570527
H,0,0.0167585102,-3.56575784,-3.7204605266
H,0,1.6863319101,-3.3522128591,-3.1449277226
H,0,-0.6303539869,-4.6773144752,-1.6974810445
H,0,1.1083714949,-4.8497545481,-1.365358948
H,0,-4.5230626863,0.3175212894,-1.9110397591
H,0,-4.6859947582,-1.4452561412,-1.7467535484
H,0,-5.1538772542,0.4151385954,0.4037611349
H,0,-4.7898835132,-1.3065689668,0.6486864883
H,0,2.3393617557,-0.4314788082,-2.187526485
H,0,4.7735855523,-0.3004495795,-2.3233105868
H,0,6.1431442729,0.2171115762,-0.2954780725
Cl,0,5.3241198737,0.7423785588,2.4175842842
H,0,2.5617607685,0.4802882299,2.0204267662
H,0,-1.3492340951,-3.3729632186,1.264342619
H,0,-1.5415921909,-3.0885274288,3.0204046987
H,0,-2.5155476203,-2.1551024678,1.8457618028
H,0,1.447433701,-3.0504701187,1.772777283
H,0,2.1122017041,-1.6319225212,2.591540922
H,0,1.0283233988,-2.7427177271,3.4827242095
H,0,-1.9559985201,3.2782584789,0.5974258986
H,0,-2.6056480868,2.0896857773,1.7235390535
H,0,-1.7561843711,3.5432272215,2.3540301026
H,0,0.911496853,3.7845163543,0.5193146086
H,0,0.9392107314,3.8595595313,2.3000924536
H,0,2.051994213,2.7759830569,1.4090160154

dmpeBpin3MetaBr2PhHCHactTSSptSptBack
E(RB+HF-LYP) = -7161.36208279

Zero-point correction= 0.500325 (Hartree/Particle)
Thermal correction to Energy= 0.538029
Thermal correction to Enthalpy= 0.538973
Thermal correction to Gibbs Free Energy= 0.428857
Sum of electronic and zero-point Energies= -7160.861758
Sum of electronic and thermal Energies= -7160.824054
Sum of electronic and thermal Enthalpies= -7160.823110
Sum of electronic and thermal Free Energies= -7160.933226

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	337.618	136.306	231.759

C,0,2.2032267017,-0.8744206449,0.6384472503
C,0,1.3125867207,0.2036088104,0.4797174369
C,0,1.8576053729,1.5007154226,0.5498675699
C,0,3.2287946486,1.6842713466,0.7147348033
C,0,4.1189470972,0.6201443332,0.8397525125
C,0,3.5702914907,-0.6576398731,0.8024695732
Ir,0,-0.8812055694,-0.1564735809,-0.1081788641
P,0,-0.2299463476,-0.8852386728,-2.3204371774
C,0,-0.4313679376,-2.7451389419,-2.3974852531
C,0,-0.0736248387,-3.4285752007,-1.0671174088
P,0,-0.9255188964,-2.5736822473,0.3656759495
B,0,-2.9038678794,-0.1834653018,-0.7586406278
O,0,-3.4130592304,-1.0453076844,-1.7455694191
C,0,-4.7770943001,-0.6975503426,-2.0298649233
C,0,-5.1740676798,0.2540458437,-0.8854961599
O,0,-3.9313056445,0.6300624845,-0.283410289
B,0,-1.9693066812,0.238136717,1.6835749824
O,0,-2.5142685942,-0.7972127255,2.4562170521
C,0,-3.1062422369,-0.2251926645,3.6339536058
C,0,-3.1561500088,1.2851119172,3.3340843676
O,0,-2.2318560248,1.4646868561,2.2572980873
B,0,-1.0941807938,1.8464837852,-0.7196787147
O,0,-0.8345528481,2.9782011836,0.044655219
C,0,-0.9950111066,4.1560232944,-0.753366491
C,0,-1.6745708532,3.6560551845,-2.0425713986
O,0,-1.5016397714,2.2324714574,-2.0075318356
H,0,-4.8266774543,-0.2092521551,-3.0111520555
H,0,-5.3880558277,-1.6052950458,-2.0643801567

H,0,-5.6980379713,1.1482448653,-1.2371108077
H,0,-5.8026922172,-0.2417809529,-0.1349679923
H,0,-4.0954066897,-0.6636578557,3.7993682873
H,0,-2.4747885434,-0.4557653928,4.5015948973
H,0,-4.1528172323,1.6059745498,3.0064700861
H,0,-2.8529440409,1.9021115476,4.1853892747
H,0,-2.7471134031,3.887013426,-2.0603013914
H,0,-1.2189625091,4.0612330102,-2.9521585226
H,0,-1.5993027531,4.8871351025,-0.2077238902
H,0,-0.0090626825,4.5978166023,-0.9473936436
H,0,-0.1193383166,0.2703754906,1.2712865086
H,0,1.8483295054,-1.8939936687,0.6155337018
Br,0,4.739565977,-2.1722048832,0.9739654652
H,0,1.2049723353,2.3616749944,0.488546082
Br,0,3.9313198459,3.4693952805,0.7775564186
H,0,5.1811401877,0.7790598366,0.9690427763
C,0,-1.100010277,-0.3316922155,-3.8465120034
C,0,1.5351078744,-0.6192523187,-2.7970705231
C,0,-2.5877094842,-3.3782605374,0.3808752078
C,0,-0.1813912391,-3.3642782198,1.8664395581
H,0,-0.3409056762,-4.4917241157,-1.0922811876
H,0,1.0068644979,-3.3742365462,-0.8899853431
H,0,-1.4852046626,-2.9192659371,-2.6397742593
H,0,0.1673005892,-3.1507869661,-3.2214511649
H,0,1.7433838523,-1.0633366922,-3.7756497654
H,0,1.7302271969,0.4554005213,-2.8413204285
H,0,2.2049306184,-1.0479671023,-2.0501328564
H,0,-0.6660396846,-0.8063206812,-4.7323461513
H,0,-2.1548040781,-0.5928648372,-3.7590599574
H,0,-1.0173675767,0.7538529467,-3.9180041263
H,0,-0.2364461643,-4.456283454,1.8089288872
H,0,0.8584578068,-3.0659681532,2.009412106
H,0,-0.7569380626,-3.0208064497,2.7299757856
H,0,-2.5038072143,-4.4638078974,0.4962775909
H,0,-3.1464683156,-2.9574669968,1.21949598
H,0,-3.1143078017,-3.1355361043,-0.5428983055

dmpeBpin2Br2PhHBinRotTS
E(RB+HF-LYP) = -7161.37356865

Zero-point correction= 0.503439 (Hartree/Particle)
Thermal correction to Energy= 0.541450
Thermal correction to Enthalpy= 0.542394
Thermal correction to Gibbs Free Energy= 0.430658

Sum of electronic and zero-point Energies= -7160.870130
Sum of electronic and thermal Energies= -7160.832119
Sum of electronic and thermal Enthalpies= -7160.831174
Sum of electronic and thermal Free Energies= -7160.942911

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	339.765	136.393	235.169

C,0,3.4527456987,0.3174388359,1.021543794
C,0,2.062130754,0.2507664337,1.1068130697
C,0,1.2545807838,-0.0220473003,-0.0167288937
C,0,1.9550478411,-0.2273140573,-1.2282349242
C,0,3.344317471,-0.1558910174,-1.2880366525
C,0,4.1340732119,0.1176856138,-0.1728330763
Ir,0,-0.9788781606,-0.1000562712,0.0130145445
B,0,-0.7983986289,-1.9054699761,-1.0616308868
O,0,-0.8089893306,-3.2004520209,-0.5380958177
C,0,-0.7007169483,-4.1459825028,-1.6150386926
C,0,-0.3299869335,-3.2913048348,-2.8447012981
O,0,-0.5811180418,-1.9418079615,-2.4334166835
B,0,-3.0857320762,-0.3092285254,-0.2320285144
O,0,-4.0755478837,-0.0132827566,0.7266923182
C,0,-5.366406028,-0.3735773646,0.2068012226
C,0,-5.1134055593,-0.6305892266,-1.2896249234
O,0,-3.6944977981,-0.7900297567,-1.3878331719
P,0,-1.113812918,1.8227828194,1.51881268
C,0,0.1594172058,3.1598219396,1.4988240846
P,0,-1.1853637083,-1.3562270137,1.9684155364
C,0,0.2812328806,-2.3061938941,2.5526013226
B,0,-1.1599943608,1.588976154,-1.4812161912
O,0,-2.3799725273,2.0517378578,-1.9352941032
C,0,-2.1560244135,3.2564110792,-2.6855409224
C,0,-0.6821768566,3.627446161,-2.3987108955
O,0,-0.131474481,2.4641879515,-1.7630199984
C,0,-0.9667256656,1.1483375133,3.2577565934
C,0,-1.6476441543,-0.2192119851,3.3763145917
C,0,-2.6813658717,2.7978764852,1.5767103813
C,0,-2.5065637562,-2.6344904369,2.0708426443
H,0,-0.8617199255,0.2864327691,-1.6186827774
H,0,-1.4163565829,-0.7006281698,4.3333565451
H,0,-2.735424664,-0.1050790985,3.3157685437
H,0,-1.3913377781,1.8648982045,3.9700846451
H,0,0.1023613487,1.068598936,3.4830637494

H,0,-0.5914882975,4.4839225863,-1.719009238
H,0,-0.1104877954,3.8466879443,-3.3046152796
H,0,-2.8623573607,4.0257537652,-2.3589771813
H,0,-2.3352187402,3.0481962357,-3.7462097818
H,0,-0.9390996979,-3.525034233,-3.7231539253
H,0,0.7277048707,-3.3914036619,-3.1162490109
H,0,-1.6631723995,-4.6570648652,-1.7394001617
H,0,0.0605499847,-4.8926879107,-1.3690701509
H,0,-5.4228096344,0.2191679796,-1.9110907979
H,0,-5.6140103968,-1.5308739306,-1.6596137421
H,0,-6.0773835724,0.4381891635,0.3901101907
H,0,-5.7270340608,-1.27107521,0.727117137
H,0,1.413902399,-0.4547464158,-2.1393804689
Br,0,4.228654493,-0.4504164343,-2.9732153555
H,0,5.2126375687,0.1696579048,-0.2337811183
Br,0,4.4690956084,0.7031532262,2.613864307
H,0,1.6179499981,0.4208580379,2.0812680618
H,0,-2.3160013159,-3.381767284,1.2999122851
H,0,-2.5005330013,-3.1054113168,3.0590455128
H,0,-3.4731587904,-2.1615364781,1.8931859901
H,0,0.5130384698,-3.0459468974,1.7832225902
H,0,1.1490961746,-1.6589567073,2.6766362162
H,0,0.0575653616,-2.8132819803,3.4963996617
H,0,-2.8162870311,3.3078340955,0.6192461034
H,0,-3.5184215908,2.1094463529,1.7035156994
H,0,-2.6627777723,3.5382385038,2.3830079026
H,0,0.0825908469,3.7106767565,0.5595181935
H,0,0.0186250362,3.8470338852,2.3391134581
H,0,1.1573204365,2.7208056992,1.5419777345

dmpeBpin3MetaXyleneHCHactTSSptSptBack
E(RB+HF-LYP) = -2098.39259645

Zero-point correction= 0.575435 (Hartree/Particle)
Thermal correction to Energy= 0.614683
Thermal correction to Enthalpy= 0.615627
Thermal correction to Gibbs Free Energy= 0.500928
Sum of electronic and zero-point Energies= -2097.817161
Sum of electronic and thermal Energies= -2097.777914
Sum of electronic and thermal Enthalpies= -2097.776969
Sum of electronic and thermal Free Energies= -2097.891668

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	385.719	141.806	241.404

C,0,3.1788883104,-0.7302499198,0.7077118435
C,0,2.2581994406,0.3368661673,0.6626214089
C,0,2.7775570083,1.6203441131,0.8964085955
C,0,4.1458281049,1.8467514797,1.1242012539
C,0,5.0228403766,0.7613078,1.1267197629
C,0,4.549496458,-0.5406487122,0.9213960168
Ir,0,0.0632495366,-0.0118654285,0.0728948957
P,0,0.6960028948,-0.7524135921,-2.1407398804
C,0,0.4660578934,-2.6092103602,-2.1994502428
C,0,0.8496969709,-3.2917064109,-0.8768483677
P,0,0.0374583281,-2.4204680196,0.5696647048
B,0,-1.9617043966,-0.0574920311,-0.5831956434
O,0,-2.482704254,-0.9777127623,-1.5136460174
C,0,-3.8389779812,-0.6276798292,-1.8279435419
C,0,-4.2268977388,0.3995568209,-0.7483946254
O,0,-2.9805913654,0.8034495496,-0.1735847975
B,0,-1.0417910145,0.4111587223,1.8426893009
O,0,-1.6328745455,-0.6083784186,2.604420496
C,0,-2.2235261361,-0.0244274996,3.7750137456
C,0,-2.2222560516,1.4881801249,3.4817762422
O,0,-1.2792236533,1.6434359253,2.419392902
B,0,-0.1125492178,1.9888122849,-0.5479214179
O,0,0.0900563631,3.1247767496,0.2296872488
C,0,-0.0101887822,4.297589982,-0.5802107526
C,0,-0.6202452062,3.7983035022,-1.902859235
O,0,-0.4407611547,2.3774273286,-1.8605465604
H,0,-3.875805891,-0.1999493004,-2.8381159015
H,0,-4.4649147662,-1.5257760418,-1.8108340184
H,0,-4.7447436345,1.2730210868,-1.1570629994
H,0,-4.8589516529,-0.0419035871,0.0329173117
H,0,-3.2283261476,-0.4325531336,3.9247576111
H,0,-1.6128638934,-0.2775500735,4.6515721292
H,0,-3.2047501629,1.8418474399,3.1443393595
H,0,-1.911709994,2.0912389917,4.3407866015
H,0,-1.6921354827,4.0240176317,-1.9727770839
H,0,-0.1223632876,4.2094834101,-2.787607528
H,0,-0.6343218507,5.0416723988,-0.0750785813
H,0,0.9908132146,4.7273306131,-0.7233839896
H,0,0.7895089308,0.3843115723,1.4739773777
H,0,2.8403912491,-1.7471472361,0.542958405
C,0,5.5059783404,-1.7127859284,0.9227856321
H,0,2.1005971535,2.4679153288,0.91335578

C,0,4.647357311,3.2475396203,1.396445941
H,0,6.0851303959,0.9265009453,1.2999667205
C,0,-0.2001324514,-0.2070079617,-3.6561513623
C,0,2.4502117564,-0.4990692049,-2.6621617171
C,0,-1.6050632824,-3.2648037094,0.6608887829
C,0,0.8534657845,-3.1593051017,2.0587454536
H,0,0.5691024315,-4.3517474216,-0.8896724922
H,0,1.9341825979,-3.2484205947,-0.7264789427
H,0,-0.5996485383,-2.757827559,-2.4035104962
H,0,1.0280617012,-3.0312745085,-3.0410731134
H,0,2.644326437,-0.9858238288,-3.6235582719
H,0,2.6316345367,0.5746653098,-2.7603010377
H,0,3.1356129185,-0.881873162,-1.9050251067
H,0,0.2174528545,-0.6858074123,-4.5477917287
H,0,-1.2535194691,-0.4677876694,-3.5506860829
H,0,-0.1179786167,0.8780468496,-3.7308760079
H,0,0.8587765353,-4.2535216008,2.0154440106
H,0,1.8749764025,-2.7919974731,2.1687276758
H,0,0.2801511218,-2.8395705342,2.9330562798
H,0,-1.4891308356,-4.34687213,0.7842963485
H,0,-2.1419941908,-2.8493169672,1.5164437829
H,0,-2.1758171783,-3.0487898424,-0.2436586203
H,0,6.226531683,-1.646365692,0.0982723326
H,0,6.0880528869,-1.7544822087,1.8508076212
H,0,4.9745926621,-2.6643284851,0.8214406226
H,0,5.732142521,3.3179978867,1.2695163419
H,0,4.1791512005,3.9775780956,0.7280307757
H,0,4.415271512,3.5592126216,2.4226958492

dmpeBpin2MetaXyleneHBinRotTS
E(RB+HF-LYP) = -2098.39908753

Zero-point correction= 0.578508 (Hartree/Particle)
Thermal correction to Energy= 0.617824
Thermal correction to Enthalpy= 0.618768
Thermal correction to Gibbs Free Energy= 0.504494
Sum of electronic and zero-point Energies= -2097.820579
Sum of electronic and thermal Energies= -2097.781264
Sum of electronic and thermal Enthalpies= -2097.780320
Sum of electronic and thermal Free Energies= -2097.894594

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	387.690	141.891	240.511

C,0,4.1675964349,0.334111745,1.0241401024
C,0,2.7661737276,0.2618610182,1.0764528669
C,0,1.9469775827,0.0088868618,-0.0441158973
C,0,2.6502118649,-0.176607658,-1.2540873238
C,0,4.0476958234,-0.1173034505,-1.3552584903
C,0,4.8014967164,0.1411043473,-0.2057475577
Ir,0,-0.2846404182,-0.0771361538,-0.0197827154
B,0,-0.0836310069,-1.8808240687,-1.084995552
O,0,-0.0435583623,-3.1706370217,-0.5426415813
C,0,0.0392493798,-4.1276431383,-1.6093232625
C,0,0.3673361341,-3.283892837,-2.8572210486
O,0,0.0833339692,-1.9374720569,-2.4647166357
B,0,-2.3973047887,-0.2867271202,-0.2704317659
O,0,-3.3898029666,0.0061313933,0.6888699789
C,0,-4.6809541586,-0.3497459666,0.1691869614
C,0,-4.4280531163,-0.6155941035,-1.3260638884
O,0,-3.0092918496,-0.7668365085,-1.4267672374
P,0,-0.4270305186,1.8356141297,1.4895337251
C,0,0.8391224701,3.1801077473,1.4682576195
P,0,-0.4913818963,-1.3419039136,1.9299298302
C,0,0.9674778505,-2.3044659849,2.5159799008
B,0,-0.4549589597,1.6150787521,-1.4947233184
O,0,-1.6799435252,2.1067863222,-1.9137692915
C,0,-1.4519586007,3.2948596305,-2.6864811643
C,0,0.0314195717,3.6446234814,-2.4305051583
O,0,0.58039435,2.469350259,-1.8208856203
C,0,-0.2689332058,1.160517915,3.2259761887
C,0,-0.9501866312,-0.2068737131,3.3422050773
C,0,-2.0002421906,2.8023819012,1.5593786858
C,0,-1.8193426099,-2.6143618624,2.0404309206
H,0,-0.1667855943,0.3063609137,-1.6488694101
H,0,-0.7185463972,-0.690994561,4.2979011591
H,0,-2.0379015164,-0.0915558176,3.2831130972
H,0,-0.6893940815,1.875859874,3.9424041533
H,0,0.8018187329,1.0773497372,3.44110482
H,0,0.1466232318,4.4934542092,-1.7441694763
H,0,0.5843204503,3.8686075877,-3.3471998939
H,0,-2.1401685049,4.0811831504,-2.3610552882
H,0,-1.6522821376,3.0738944084,-3.7412806198
H,0,-0.2451299152,-3.5513913681,-3.7239998148
H,0,1.4246712493,-3.3607789002,-3.1403459262
H,0,-0.923392085,-4.6462371207,-1.7021199333
H,0,0.8117274259,-4.8680277862,-1.3784685428

H,0,-4.7463622178,0.2271281485,-1.9530189312
H,0,-4.924192115,-1.521774689,-1.6885684807
H,0,-5.3886175644,0.4665715224,0.3468174665
H,0,-5.0488188949,-1.2423158355,0.6934762875
H,0,2.094756885,-0.3800073562,-2.166760325
C,0,4.7350216052,-0.3531202006,-2.6825600563
H,0,5.8879392516,0.1922281733,-0.2691341201
C,0,4.9794602787,0.6291744744,2.2669702256
H,0,2.3135177538,0.4199401487,2.0552668014
H,0,-1.623806386,-3.3792147641,1.2880938831
H,0,-1.8266185621,-3.0674784269,3.0371858967
H,0,-2.7825069258,-2.1421204883,1.8434677396
H,0,1.1496892211,-3.0889960259,1.7781823858
H,0,1.8545399708,-1.6735115914,2.566954458
H,0,0.7650973558,-2.7558483114,3.4927269158
H,0,-2.1618154876,3.2787831885,0.5891273156
H,0,-2.8297128976,2.1128179649,1.7252745906
H,0,-1.9676041075,3.5662426321,2.3430504483
H,0,0.7413913015,3.7495138224,0.5417075149
H,0,0.7140159175,3.8524777205,2.3232952694
H,0,1.8367435408,2.7378078743,1.4803292645
H,0,5.7748069291,-0.1109101481,2.4146795811
H,0,5.4669882539,1.6107437563,2.2090456542
H,0,4.353388884,0.6266461428,3.1654932529
H,0,5.5377878317,0.3726304917,-2.8561058802
H,0,5.1920032194,-1.3504959406,-2.7272770564
H,0,4.0283336985,-0.2790898914,-3.5146604255

Ir(bpy)(BPin)$_3$
E(RB+HF-LYP) = -1361.88604005

Zero-point correction= 0.371266 (Hartree/Particle)
Thermal correction to Energy= 0.398025
Thermal correction to Enthalpy= 0.398970
Thermal correction to Gibbs Free Energy= 0.308975
Sum of electronic and zero-point Energies= -1361.514774
Sum of electronic and thermal Energies= -1361.488015
Sum of electronic and thermal Enthalpies= -1361.487070
Sum of electronic and thermal Free Energies= -1361.577065

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	249.765	96.398	189.409

Ir,0,0.1635529963,-0.0019094733,-0.3550644187
N,0,-1.6842220373,-1.3242024742,-0.3021789652
C,0,-1.6256370623,-2.6645757355,-0.3534373128
C,0,-2.7634429459,-3.4671133061,-0.3567002198
C,0,-4.0120662192,-2.850196709,-0.3178834255
C,0,-4.0771453459,-1.460367922,-0.2837350353
C,0,-2.8927170904,-0.7133997067,-0.2741108335
C,0,-2.8769697537,0.7727534562,-0.2485551209
C,0,-4.0399715543,1.5393847251,-0.1068660274
C,0,-3.9501671081,2.9283665343,-0.0957830814
C,0,-2.6970568276,3.5234925114,-0.220905321
C,0,-1.577029354,2.7050171787,-0.350527355
N,0,-1.6619781442,1.3631004046,-0.3661778484
H,0,-0.6272553316,-3.0831748911,-0.4117908427
H,0,-2.6644566116,-4.5465073703,-0.3943192874
H,0,-4.9243368776,-3.4388223782,-0.3231714212
H,0,-5.0417444668,-0.9677926489,-0.2744218921
H,0,-5.0060173682,1.0622849603,0.0048971541
H,0,-4.8459147062,3.5319721479,0.0146066334
H,0,-2.5781267236,4.6016437793,-0.2128689361
H,0,-0.5689868252,3.1020477523,-0.429607818
B,0,1.6178556436,-1.421365855,-0.4417094845
O,0,1.5694137791,-2.409250205,-1.4468809594
C,0,2.655211665,-3.3264759146,-1.2670842422
C,0,3.5114341307,-2.704496194,-0.1410901345
O,0,2.7010996382,-1.6632724251,0.4036356553
H,0,3.7678717277,-3.4257634036,0.6432478285
H,0,4.4434804406,-2.2720535592,-0.5269004419
H,0,3.2067247901,-3.4364883299,-2.2070309954
H,0,2.2560693642,-4.3119243577,-0.9898754063
H,0,2.5546383656,-0.1494755472,3.7241725914
H,0,1.7241588098,1.3376963939,4.2393296195
C,0,0.3660479798,-0.360954298,3.8267241368
H,0,0.5421253971,-1.270617768,4.410605262
H,0,-0.410655612,0.2283672293,4.3337189737
O,0,-0.0833650325,-0.7068422912,2.5122959171
B,0,0.6163648935,0.0787194677,1.5840153612
O,0,1.5629434267,0.8714867851,2.2239470178
B,0,1.6601240438,1.349395882,-0.6708013671
O,0,2.9000269003,1.1053276589,-1.2698762643
C,0,3.6766342648,2.3031729144,-1.2779826212
C,0,2.6664399321,3.4230846142,-0.9548401305
O,0,1.5254329132,2.7345559308,-0.4363748757
H,0,4.4640426897,2.2296571702,-0.5162487195

H,0,4.1557006179,2.4313683395,-2.2550353844
H,0,3.0419319346,4.1335178567,-0.2102943564
H,0,2.3766735708,3.9880415964,-1.8521626357
C,0,1.6510621992,0.4591371613,3.5894623135

Ir(bpy)(BPin)$_3$(^{2}-PhH)
E(RB+HF-LYP) = -1594.14747822

Zero-point correction= 0.472651 (Hartree/Particle)
Thermal correction to Energy= 0.504986
Thermal correction to Enthalpy= 0.505930
Thermal correction to Gibbs Free Energy= 0.402049
Sum of electronic and zero-point Energies= -1593.674827
Sum of electronic and thermal Energies= -1593.642492
Sum of electronic and thermal Enthalpies= -1593.641548
Sum of electronic and thermal Free Energies= -1593.745429

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	316.883	117.313	218.636

Ir,0,-0.3281355405,-0.009959939,-0.0074661745
N,0,1.2735572334,-1.5861961954,0.2173081074
C,0,1.1123179409,-2.6990356973,0.9503029795
C,0,2.0841102484,-3.6902095659,1.0439101569
C,0,3.2781520335,-3.516669888,0.3464675287
C,0,3.4532503376,-2.362419736,-0.4094330788
C,0,2.4321681558,-1.4042844939,-0.4590357637
C,0,2.5411186639,-0.1525147582,-1.2521005658
N,0,1.4604516954,0.664797847,-1.2366490529
C,0,1.4815527933,1.7975524184,-1.959568744
C,0,2.5828329713,2.1791778322,-2.7217381944
C,0,3.705825775,1.3546769509,-2.7340732413
C,0,3.6828547641,0.176885414,-1.9941711102
B,0,-1.7804268193,-0.7427877012,1.2191071778
O,0,-1.6063624067,-0.7886971467,2.6192559623
C,0,-2.7414592413,-1.4174787909,3.2238985071
C,0,-3.7617230123,-1.5677893262,2.0749131034
O,0,-3.0110452139,-1.3181570481,0.8872417167
B,0,-1.6131728418,1.5539551811,-0.2991169095
O,0,-2.6442856207,1.9690690898,0.5564010401
C,0,-3.3596947313,3.0526688901,-0.0394813338
C,0,-2.4502225488,3.5313150928,-1.1901617308
O,0,-1.5052950466,2.4725023893,-1.363407164

B,0,-1.3122066995,-0.9790294288,-1.4565314603
O,0,-2.3891580079,-0.5246815618,-2.2124954424
C,0,-2.8923249328,-1.612144819,-2.9901796096
C,0,-1.7546698336,-2.6532906651,-2.9730160107
O,0,-0.9393733503,-2.2710419797,-1.8607276887
C,0,1.3426062865,2.8009514938,1.7214264005
C,0,0.6165992643,1.7624331245,2.3191014399
C,0,1.2948755695,0.7277681893,2.9752120381
C,0,2.6917833969,0.7376833003,3.0380478153
C,0,3.4116225879,1.7762158784,2.4429511191
C,0,2.7366535141,2.8081929865,1.7822106545
H,0,0.8152580229,3.6017457108,1.2111142864
H,0,0.1689231856,-2.7775078221,1.4774591802
H,0,4.375671267,-2.2151025443,-0.9574598376
H,0,1.9016695986,-4.5723587594,1.6480412871
H,0,4.0622668363,-4.266404645,0.3886728519
H,0,4.5468420728,-0.4762631535,-1.9984951669
H,0,4.5855290188,1.6182987381,-3.3134271415
H,0,2.5505186822,3.1017915931,-3.2914625998
H,0,0.5689319822,2.3844701633,-1.9207497824
H,0,-2.4404087325,-2.3884954033,3.6413638497
H,0,-3.1162692943,-0.7968263232,4.045146744
H,0,-4.2073204039,-2.5680614892,2.0314266939
H,0,-4.5740622094,-0.8334422507,2.1512468822
H,0,3.297917332,3.6171917309,1.3224311209
H,0,4.4971330808,1.7872955048,2.4987008043
H,0,3.2178922238,-0.0595504759,3.5565723938
H,0,-0.4681987686,1.7671923859,2.2986817858
H,0,0.7176867905,-0.070730167,3.4290498606
H,0,-1.1533713115,-2.6212651736,-3.8922470259
H,0,-2.1159906972,-3.6779712541,-2.8348063649
H,0,-3.1399266413,-1.2656143619,-3.9992889895
H,0,-3.8063716186,-1.9987069725,-2.5207085299
H,0,-1.9184796153,4.4594640593,-0.936876199
H,0,-2.9980983864,3.6963254231,-2.1241972781
H,0,-3.548047434,3.8321478154,0.7072396511
H,0,-4.3275119082,2.688338228,-0.4074820091

Ir(bpy)(BPin)$_3$(Ph-H) C-H Activation TS
E(RB+HF-LYP) = -1594.10718476

Zero-point correction=	0.468878 (Hartree/Particle)
Thermal correction to Energy=	0.500951
Thermal correction to Enthalpy=	0.501896

Thermal correction to Gibbs Free Energy= 0.401240
Sum of electronic and zero-point Energies= -1593.638306
Sum of electronic and thermal Energies= -1593.606233
Sum of electronic and thermal Enthalpies= -1593.605289
Sum of electronic and thermal Free Energies= -1593.705944

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	314.352	118.627	211.847

C,0,-3.1488959587,3.0024722008,-2.6260586062
C,0,-2.3480037554,3.5389683806,-1.6160863832
C,0,-1.3401889858,2.768909144,-1.0283888314
C,0,-1.1209579837,1.432658029,-1.4116503175
C,0,-1.9217123737,0.9217277399,-2.4484893358
C,0,-2.9261751663,1.6900488548,-3.044818907
Ir,0,0.2261427672,0.1380044766,-0.1778117126
N,0,-1.242776276,-1.5986742643,-0.4876133999
C,0,-2.2728811956,-1.6760772232,0.384446917
C,0,-3.2249212868,-2.7009870847,0.290367618
C,0,-3.1119338244,-3.6526130077,-0.7165265914
C,0,-2.0458511843,-3.5627336789,-1.6085800733
C,0,-1.1341061112,-2.5216951479,-1.4563289667
C,0,-2.3216235924,-0.6354449741,1.4390374084
N,0,-1.3107312616,0.268604591,1.4511937031
C,0,-1.288703656,1.2193363967,2.4025150771
C,0,-2.2752424935,1.3233249279,3.3785458513
C,0,-3.3259176944,0.4094792961,3.371305914
C,0,-3.3458066751,-0.5784385261,2.3935516679
B,0,1.3483984575,-1.0422182173,1.2055543175
O,0,1.3274923845,-2.43973934,1.2259065046
C,0,2.0779808414,-2.9072587986,2.3545229381
C,0,2.7810371991,-1.6472946948,2.9022339125
O,0,2.1230984264,-0.554813676,2.2506506593
B,0,1.7928176349,-0.6679371611,-1.2768925149
O,0,3.1470813853,-0.6855771368,-0.9694285559
C,0,3.8727651748,-1.2720162611,-2.0525224081
C,0,2.7947728107,-1.9696891993,-2.9031369838
O,0,1.5673692119,-1.3627576365,-2.4778397744
B,0,1.4459151553,1.7141537658,0.3030835297
O,0,1.2734042805,2.5231674366,1.4397262099
C,0,2.1741190307,3.6348962142,1.3767412255
C,0,3.1396962035,3.2758513669,0.2298533396
O,0,2.4792884373,2.2267367833,-0.4783374996

H,0,0.3990761114,0.8017565506,-1.6348834681
H,0,-0.2803017765,-2.4018284297,-2.114788313
H,0,-4.0455958862,-2.7610373646,0.9942322719
H,0,-1.9138671768,-4.2824862649,-2.4093401278
H,0,-3.8440124818,-4.4501443878,-0.7991605351
H,0,-4.1552354099,-1.2969726914,2.3728784919
H,0,-4.1170665913,0.4604817714,4.1130924232
H,0,-2.2108718583,2.1094183014,4.1230667215
H,0,-0.4442983701,1.898325419,2.3607196091
H,0,2.7511055005,-3.0497174461,-2.7096309889
H,0,2.9273499307,-1.814488161,-3.9783956369
H,0,4.6234331426,-1.9664981728,-1.6616968462
H,0,4.3896171364,-0.4803524588,-2.6098567591
H,0,-0.7281025644,3.2122379404,-0.2477276784
H,0,-2.5024618292,4.564010079,-1.2862611959
H,0,-3.9272173276,3.6035088449,-3.0886952254
H,0,-1.7558834075,-0.0911825463,-2.8054510837
H,0,-3.5289588904,1.2626905232,-3.8430852301
H,0,1.3902726393,-3.3512702769,3.0861794694
H,0,2.7820968814,-3.6823096418,2.0337539432
H,0,2.6837352699,-1.5422679451,3.9880295761
H,0,3.8480614098,-1.6260056595,2.6480246366
H,0,1.6046803421,4.5503574623,1.1667609878
H,0,2.6797398668,3.7556755328,2.3403111745
H,0,3.3305898835,4.1169563479,-0.4449271614
H,0,4.1034499582,2.9086185741,0.6059368903

bpyBpin2PhHBpinRotTS
E(RB+HF-LYP) = -1594.09606502

Zero-point correction= 0.471260 (Hartree/Particle)
Thermal correction to Energy= 0.502948
Thermal correction to Enthalpy= 0.503892
Thermal correction to Gibbs Free Energy= 0.403993
Sum of electronic and zero-point Energies= -1593.624805
Sum of electronic and thermal Energies= -1593.593117
Sum of electronic and thermal Enthalpies= -1593.592173
Sum of electronic and thermal Free Energies= -1593.692072

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	315.605	117.518	210.256

C,0,-3.0963950744,0.6526592537,-2.613015284

C,0,-2.1552316372,0.147266271,-1.7075057213
N,0,-0.9879022488,0.8027135517,-1.4616929813
C,0,-0.7519456307,1.9539701677,-2.1274521111
C,0,-1.6455454146,2.4943330573,-3.0428853268
C,0,-2.8476449373,1.8370089768,-3.2908139667
C,0,-2.3608006018,-1.1138660848,-0.981804821
N,0,-1.3909985328,-1.4471744345,-0.1000750627
C,0,-1.4981076229,-2.6194844467,0.5511818929
C,0,-2.5696801084,-3.4875837247,0.388846021
C,0,-3.5837254777,-3.1392325858,-0.5026780151
C,0,-3.4698302454,-1.9451480928,-1.1992312072
Ir,0,0.3065232653,0.0673338887,0.0834606153
B,0,1.840824445,1.451997147,-0.1058564653
O,0,1.9492893093,2.4353115599,-1.0924015442
C,0,3.2066822754,3.1128203713,-0.9608803135
C,0,3.7666454806,2.63050438,0.3950794918
O,0,2.9303714113,1.5311870607,0.7590740421
C,0,-0.9059267906,1.3330579224,1.4331314718
C,0,-1.8396548117,0.8058533826,2.3484739299
C,0,-2.6720298501,1.6167722141,3.1273912922
C,0,-2.5990598643,3.0068077856,3.023416228
C,0,-1.6837803012,3.5660233071,2.131324945
C,0,-0.860761588,2.7404048945,1.3561774593
B,0,1.0107180098,-1.1508669412,1.7306921927
O,0,0.7338589965,-0.94376562,3.0650813288
C,0,1.033665118,-2.141202416,3.7911264837
C,0,1.809486442,-3.0204069952,2.7847180968
O,0,1.568343014,-2.4018721184,1.5100710235
B,0,1.4543906849,-1.0873880955,-1.303451449
O,0,0.8611912933,-1.8558525546,-2.3130227253
C,0,1.8845348351,-2.4131257772,-3.1501138116
C,0,3.1960768798,-2.1489263193,-2.3837168123
O,0,2.8425748259,-1.1819007814,-1.3878548759
H,0,1.5002986356,0.0103987029,1.1715843665
H,0,-4.2337192829,-1.6650604709,-1.9131161298
H,0,-4.438630861,-3.7889955162,-0.6609226563
H,0,-2.5972702121,-4.4172994502,0.9467087709
H,0,-0.6736041125,-2.8775609884,1.2011406364
H,0,-4.0250553881,0.1224827949,-2.7799867333
H,0,-3.5743176787,2.2348092798,-3.9919489478
H,0,-1.3903574958,3.4223631874,-3.5426753315
H,0,0.1906347529,2.4375858109,-1.9142425681
H,0,3.5755278188,-3.0527058329,-1.8896624851
H,0,3.9904413758,-1.7486458204,-3.0226559905

H,0,1.8663282568,-1.9111940233,-4.1264451225
H,0,1.6911651767,-3.4791609967,-3.3102406271
H,0,-0.1628223435,3.2197293625,0.6704528786
H,0,-1.9174363387,-0.2721492184,2.4772199529
H,0,-3.3763781029,1.1598187567,3.8207300125
H,0,-3.2411017016,3.6418104686,3.6289978549
H,0,-1.6059383692,4.6479365654,2.0376421149
H,0,0.0944448936,-2.6062943103,4.1162377946
H,0,1.6180536164,-1.8898285033,4.6808503528
H,0,1.4612090108,-4.0579093721,2.760347178
H,0,2.8887009681,-3.0214257436,2.9753791235
H,0,3.7027575671,3.4044513574,1.169620909
H,0,4.8061850115,2.2944727074,0.3256610686
H,0,3.8515537211,2.8309584178,-1.8015225191
H,0,3.0427631328,4.194753078,-0.9951848117

Ir(bpy)(BPin)$_3$(Ph)(H)
E(RB+HF-LYP) = -1594.12080695

Zero-point correction= 0.471227 (Hartree/Particle)
Thermal correction to Energy= 0.503172
Thermal correction to Enthalpy= 0.504117
Thermal correction to Gibbs Free Energy= 0.404809
Sum of electronic and zero-point Energies= -1593.649580
Sum of electronic and thermal Energies= -1593.617635
Sum of electronic and thermal Enthalpies= -1593.616690
Sum of electronic and thermal Free Energies= -1593.715998

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	315.745	119.135	209.011

C,0,-2.8055939266,-1.5654994903,2.4395703342
C,0,-1.9674507461,-1.2412593949,1.3654448844
N,0,-1.1043043185,-0.1949118581,1.4528452027
C,0,-1.0599186721,0.5306890804,2.5870491932
C,0,-1.8719332165,0.2546096338,3.6819767746
C,0,-2.7609885167,-0.8144420679,3.6079648709
C,0,-1.9599648627,-2.0134074594,0.1019760715
N,0,-1.0932292629,-1.5940520281,-0.8458858954
C,0,-1.0348776378,-2.2482634842,-2.0149770712
C,0,-1.8287369307,-3.3567343177,-2.2967121671
C,0,-2.7172683722,-3.805785948,-1.3225407446
C,0,-2.784809909,-3.126206337,-0.1115433821

Ir,0,0.1699583868,0.2300914453,-0.2755238175
B,0,1.1002911323,1.9612372229,0.3079599847
O,0,1.9255583611,2.7434093229,-0.4918603698
C,0,2.4448802825,3.8260592638,0.2817699474
C,0,1.5561291062,3.8606249752,1.5404433207
O,0,0.9238100162,2.5744368002,1.5569689499
C,0,-1.4333741744,1.5034759703,-0.9770183579
C,0,-2.0567817002,2.4819363796,-0.178630972
C,0,-3.1056100229,3.2778654964,-0.6536656539
C,0,-3.5675627196,3.1276376222,-1.9612204114
C,0,-2.9648851428,2.1728172694,-2.7822178582
C,0,-1.9205345062,1.3808204499,-2.294874265
B,0,1.4967721579,-0.9875930755,0.9318836037
O,0,2.1931867735,-0.4835235952,2.0182372354
C,0,2.8181123705,-1.5655706549,2.718810281
C,0,2.1618798432,-2.834893184,2.135730671
O,0,1.5002829515,-2.3818519365,0.9455381669
B,0,1.9246193461,-0.4804029163,-1.1802005825
O,0,1.8624519557,-1.4393151938,-2.2037310442
C,0,3.198676525,-1.7933283541,-2.5720873132
C,0,4.0539862527,-0.6421727623,-2.0143312777
O,0,3.2408990321,-0.0696487982,-0.985904356
H,0,0.8178391,0.6951343233,-1.661930176
H,0,-0.3008759923,-1.8805688281,-2.7202501894
H,0,-3.4698513802,-3.4648981112,0.6555315759
H,0,-1.739170917,-3.8547322535,-3.2561016801
H,0,-3.3467888802,-4.6726322766,-1.498452787
H,0,-3.488807091,-2.4017745454,2.3647009845
H,0,-3.4082038589,-1.0634517369,4.443260231
H,0,-1.7972611403,0.8723948842,4.5701554199
H,0,-0.3449834724,1.3456717922,2.5900841949
H,0,3.4573877893,-2.7569061966,-2.1131292913
H,0,3.2681452577,-1.8947065534,-3.6598168152
H,0,5.0045610179,-0.9785263018,-1.5887904029
H,0,4.2630749682,0.1208541082,-2.7753924568
H,0,-1.7079413166,2.6485169381,0.8382715492
H,0,-3.5544524246,4.023690986,-0.0001942852
H,0,-4.3767795579,3.7485957337,-2.3371358154
H,0,-1.4705004944,0.6547561257,-2.9694042339
H,0,-3.3034666416,2.0461324437,-3.8087294842
H,0,1.4175017618,-3.268905596,2.8155805134
H,0,2.8865628535,-3.6140866148,1.8789741318
H,0,2.6497685924,-1.4533134301,3.7946996358
H,0,3.8988034908,-1.5350106172,2.5331294094

H,0,0.7853134962,4.6400369823,1.480239655
H,0,2.1255555311,4.003912433,2.464511364
H,0,2.3966343269,4.7531122895,-0.2985746593
H,0,3.4957084233,3.6243148649,0.5276774728

Irbpy_Bpin2_H2_Ph_gsIr5
E(RB+HF-LYP) = -1340.69986438

Zero-point correction= 0.409372 (Hartree/Particle)
Thermal correction to Energy= 0.436194
Thermal correction to Enthalpy= 0.437138
Thermal correction to Gibbs Free Energy= 0.348960
Sum of electronic and zero-point Energies= -1340.290493
Sum of electronic and thermal Energies= -1340.263670
Sum of electronic and thermal Enthalpies= -1340.262726
Sum of electronic and thermal Free Energies= -1340.350904

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	273.716	101.497	185.587

C,0,-2.3391409725,-2.1948086579,0.0660636947
C,0,-1.7328985507,-1.3280592701,-0.864715578
C,0,-2.4422942341,-1.111687116,-2.062146617
C,0,-3.6858510566,-1.7020744409,-2.3103180162
C,0,-4.2631772095,-2.5502893739,-1.3637598929
C,0,-3.5791585784,-2.7981287506,-0.1732650409
Ir,0,0.1746661529,-0.3746437316,-0.4866656487
B,0,2.0526074424,-1.2671981866,-0.2401161632
O,0,3.031920601,-1.4626744793,-1.2133333962
C,0,4.0790570709,-2.2594835044,-0.6514209184
C,0,3.840546921,-2.1858803273,0.8686436575
O,0,2.4644006556,-1.8120761938,0.9859427236
N,0,-0.9747055796,1.4237955651,-0.4249162212
C,0,-1.5644844749,1.7501654913,0.7551737499
C,0,-2.4218452251,2.8542592329,0.8384685091
C,0,-2.6673505725,3.6265154978,-0.2903977634
C,0,-2.041010775,3.2869214773,-1.4897926483
C,0,-1.2028270766,2.1800311049,-1.5150453181
C,0,-1.2225140267,0.8932223412,1.9085370815
N,0,-0.3609407514,-0.1240432825,1.6527981862
C,0,0.03195186,-0.9166405099,2.6652265232
C,0,-0.4291825898,-0.7518663263,3.9672937549
C,0,-1.3282283036,0.2790870383,4.2380359833

C,0,-1.7221409633,1.1131821343,3.1985689019
B,0,1.844767335,0.9930809534,-0.4843783881
O,0,2.6480451639,1.3809778594,0.5852739004
C,0,3.4142203881,2.5337949803,0.2064166634
C,0,3.1786819572,2.6755270378,-1.3127203406
O,0,2.0766071879,1.8022175471,-1.5901967787
H,0,0.4083470043,-0.4288098212,-2.0434196225
H,0,0.6482182404,-1.9130029201,-0.5916639396
H,0,0.7544293763,-1.6795526949,2.4016540702
H,0,-2.4121439455,1.9257250763,3.3908456807
H,0,-0.0837579125,-1.4213084135,4.7476652418
H,0,-1.7118671134,0.4359765799,5.2412647696
H,0,-2.8954385087,3.1070424114,1.7788611347
H,0,-3.3341282155,4.4810374621,-0.233395299
H,0,-2.1962102948,3.8633061743,-2.3949882975
H,0,-0.6797228285,1.8715892565,-2.4103758553
H,0,4.4653571844,-1.4188758806,1.3444901196
H,0,4.0094981573,-3.1404873154,1.3771965136
H,0,5.0517296318,-1.8579673361,-0.9528295979
H,0,3.9960520648,-3.2865793319,-1.0308189889
H,0,-2.0115311654,-0.4725073669,-2.8305273309
H,0,-4.1990281146,-1.5060313986,-3.2497674957
H,0,-5.2266170532,-3.0162207044,-1.5546593558
H,0,-1.8338747915,-2.4186251463,1.0038491212
H,0,-4.0081409149,-3.4647122605,0.5725464265
H,0,3.0528345592,3.4043893095,0.768121923
H,0,4.4669102993,2.37539847,0.4623379089
H,0,2.9237375995,3.6979713491,-1.610774321
H,0,4.0467930016,2.3518457988,-1.8996287616

bpyBpin3HPhPrecursorRedElimSak
E(RB+HF-LYP) = -1594.11786833

Zero-point correction= 0.471480 (Hartree/Particle)
Thermal correction to Energy= 0.503443
Thermal correction to Enthalpy= 0.504387
Thermal correction to Gibbs Free Energy= 0.404760
Sum of electronic and zero-point Energies= -1593.646389
Sum of electronic and thermal Energies= -1593.614425
Sum of electronic and thermal Enthalpies= -1593.613481
Sum of electronic and thermal Free Energies= -1593.713109

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	315.915	119.033	209.684

C,0,-3.9341268455,-1.3763598785,0.2605743499
C,0,-2.5964776463,-0.9736060608,0.3723492551
N,0,-1.8801093445,-0.6612502016,-0.7338391037
C,0,-2.4553918603,-0.7358560536,-1.945004945
C,0,-3.7747510276,-1.1349091726,-2.1218508158
C,0,-4.5270129295,-1.4611200562,-0.9935249796
C,0,-1.8938265989,-0.8436913681,1.6691674792
N,0,-0.6308197491,-0.354258386,1.619383624
C,0,0.0514150909,-0.179521613,2.762787074
C,0,-0.484971202,-0.4927676792,4.0081518634
C,0,-1.7757987117,-1.0138716896,4.0716455074
C,0,-2.4869133122,-1.1893932206,2.8897954269
Ir,0,0.1783354414,0.0511358046,-0.415258946
B,0,2.1084277032,-0.6634444493,-0.0028484288
O,0,3.2350194167,-0.5632016396,-0.8149606691
C,0,4.3262867358,-1.2207299628,-0.1706769203
C,0,3.879206839,-1.3418991846,1.29704768
O,0,2.4535940287,-1.2312732073,1.2338924588
C,0,-0.7926237261,2.0010173576,-0.4721149106
C,0,-1.2870531646,2.6520290304,0.6747558794
C,0,-2.0523474063,3.8213317234,0.5946494509
C,0,-2.3494284488,4.3831422829,-0.6469118951
C,0,-1.858075983,3.7700874402,-1.8018353615
C,0,-1.0864004853,2.6087279125,-1.710198956
B,0,1.5801851076,1.5773515902,-0.130435926
O,0,2.1663060845,2.3445133828,-1.1218064002
C,0,3.0853966958,3.2543709918,-0.5155453604
C,0,2.729866707,3.2182278119,0.9843105161
O,0,1.9940942826,1.9967561681,1.1397614958
B,0,0.5698900689,-2.0391608719,-0.8103832078
O,0,-0.0445989858,-3.0258834655,-0.0407485607
C,0,0.0743843691,-4.2896040316,-0.7066675736
C,0,1.0292050204,-4.0172958449,-1.8913613277
O,0,1.1591636566,-2.5917655087,-1.9358658796
H,0,0.6052079542,0.2648127357,-1.9146506609
H,0,-3.4906682506,-1.5949915612,2.9200048236
H,0,-2.2244033558,-1.2786323367,5.0241510556
H,0,0.1061041319,-0.3321889477,4.9032632154
H,0,1.0509202731,0.2197131593,2.6507513531
H,0,-4.5113980383,-1.6126608988,1.145674745
H,0,-5.5629372869,-1.7716780576,-1.0874708475
H,0,-4.1961397484,-1.1815619432,-3.1198948059

H,0,-1.8205452249,-0.4638434515,-2.779669962
H,0,2.0198858558,-4.4631603366,-1.739616605
H,0,0.6365763545,-4.3783850466,-2.8475551954
H,0,-0.9185034562,-4.6181652529,-1.0391868306
H,0,0.4650012347,-5.0363388605,-0.0075528607
H,0,-0.6868883718,2.1730200259,-2.6218361126
H,0,-1.0623747875,2.252498495,1.6599243241
H,0,-2.4131208289,4.2928588581,1.5067181453
H,0,-2.9445432974,5.2903681167,-0.7142192746
H,0,-2.0651720748,4.2039769703,-2.7779195513
H,0,2.9670481108,4.2495047719,-0.9559102725
H,0,4.1111339101,2.9103277414,-0.7041588302
H,0,2.0891416815,4.0605276847,1.2746971566
H,0,3.6085154842,3.2065152787,1.6376129719
H,0,4.2780451504,-0.5256922942,1.9146443469
H,0,4.1566257555,-2.2951626144,1.7584085556
H,0,4.481338729,-2.2042460501,-0.6350099415
H,0,5.2413098407,-0.6330626188,-0.296162112

bpyBpin3HPhTStoPrecRedElimSak
E(RB+HF-LYP) = -1594.11405597

Zero-point correction= 0.471423 (Hartree/Particle)
Thermal correction to Energy= 0.502488
Thermal correction to Enthalpy= 0.503433
Thermal correction to Gibbs Free Energy= 0.407062
Sum of electronic and zero-point Energies= -1593.642633
Sum of electronic and thermal Energies= -1593.611568
Sum of electronic and thermal Enthalpies= -1593.610623
Sum of electronic and thermal Free Energies= -1593.706994

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	315.316	117.028	202.829

C,0,-1.6640744175,1.4288680207,-2.3547252187
C,0,-1.446458345,1.3825607722,-0.9614300184
C,0,-2.3449112994,2.1277924353,-0.1727055952
C,0,-3.4033621779,2.8539760447,-0.7309361407
C,0,-3.6033706558,2.8621200349,-2.1109972544
C,0,-2.7224819527,2.1443192061,-2.9219365572
Ir,0,0.1714262276,0.2063016579,-0.1591847549
B,0,1.8121403734,-1.0503582069,-0.6754922448
O,0,2.902006871,-0.6748809572,-1.4534580153

C,0,3.6824173627,-1.8344362686,-1.7436745488
C,0,2.7342412315,-3.0118842861,-1.4489645672
O,0,1.7297849974,-2.4460857167,-0.5974143615
N,0,-1.1620255827,-0.2538495435,1.5675515459
C,0,-2.0267257546,-1.287198337,1.4337763693
C,0,-2.8896947847,-1.6449802067,2.4791194205
C,0,-2.8770854227,-0.9175453481,3.6623007112
C,0,-2.0024799618,0.1616682794,3.7763242617
C,0,-1.1607422957,0.4555327156,2.7097840979
C,0,-2.0166364391,-1.9894213511,0.1318581858
N,0,-1.1020006853,-1.5625078519,-0.7671173561
C,0,-1.0648823664,-2.1280568789,-1.982961704
C,0,-1.9229118679,-3.1514708227,-2.3666156708
C,0,-2.8634752327,-3.6091578466,-1.4442422653
C,0,-2.9117641131,-3.0211849218,-0.1866303133
B,0,0.9478205005,2.0672274946,0.2863415508
O,0,0.6926865159,2.7145884491,1.5058701381
C,0,1.1696840632,4.064894029,1.4147169611
C,0,2.0596494811,4.0670800204,0.1549876226
O,0,1.684789986,2.8830001928,-0.5525132614
B,0,1.7699875444,-0.2000836681,1.2281676978
O,0,1.4987461853,-0.9103859693,2.3991999203
C,0,2.5311637625,-0.6564014387,3.3568671394
C,0,3.6404113368,0.05570388,2.5531528089
O,0,3.0204171725,0.4083995019,1.3143204034
H,0,0.8820095116,0.640737808,-1.4916793756
H,0,-0.3168451087,-1.7365530397,-2.6622382502
H,0,-3.6465893023,-3.355406585,0.5350155382
H,0,-1.85218995,-3.5733442318,-3.3632155483
H,0,-3.553584791,-4.4064815276,-1.7019437034
H,0,-3.5659523218,-2.4834733916,2.3696117096
H,0,-3.5424276755,-1.1861146749,4.4770447048
H,0,-1.9640906062,0.7686743341,4.6743735689
H,0,-0.4679220397,1.2888009655,2.7392966891
H,0,3.2233931262,-3.8458768484,-0.9361496299
H,0,2.2595298425,-3.3997357915,-2.3611658676
H,0,4.5680752629,-1.8486035321,-1.0940717986
H,0,4.0196695949,-1.8023794214,-2.7843912166
H,0,-2.2197123238,2.1628350822,0.906479518
H,0,-4.0708708535,3.4160812469,-0.0805248931
H,0,-4.4245048064,3.4244911532,-2.548047766
H,0,-0.9844888652,0.9028605353,-3.0212152149
H,0,-2.8507935379,2.1484027921,-4.0024621997
H,0,2.1313364836,-0.0242164612,4.1604021137

H,0,2.8617904706,-1.6027746455,3.7971879516
H,0,4.0114338722,0.959388832,3.0474402145
H,0,4.4964849142,-0.6007572446,2.3521392192
H,0,0.3117343583,4.741920462,1.3161551302
H,0,1.7162004649,4.3262993337,2.3269693886
H,0,1.8945945586,4.9437966231,-0.4792239325
H,0,3.126941465,4.0142881123,0.4050866631

Ir(bpy)(BPin)$_2$(H)(Ph-BPin) Reductive Elimination TS
E(RB+HF-LYP) = -1594.11735189

Zero-point correction= 0.471078 (Hartree/Particle)
Thermal correction to Energy= 0.502294
Thermal correction to Enthalpy= 0.503238
Thermal correction to Gibbs Free Energy= 0.405871
Sum of electronic and zero-point Energies= -1593.646274
Sum of electronic and thermal Energies= -1593.615058
Sum of electronic and thermal Enthalpies= -1593.614114
Sum of electronic and thermal Free Energies= -1593.711481

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	315.194	117.195	204.927

C,0,-2.0811960685,4.4835345582,-0.4897087005
C,0,-1.7873462351,3.8871556079,0.7367239464
C,0,-1.0295743084,2.7120786771,0.7844633094
C,0,-0.54360042,2.0915651761,-0.3822082038
C,0,-0.8285698083,2.7353067712,-1.6042775128
C,0,-1.5920958816,3.902829746,-1.6628218578
Ir,0,0.1769637368,-0.0011115368,-0.430942081
B,0,1.5630947504,1.5462634146,-0.1251068733
O,0,2.032882679,1.8852514555,1.1553257441
C,0,2.8852105333,3.0285541299,1.0168009422
C,0,3.2641683428,3.031103243,-0.476420667
O,0,2.232796002,2.2709852764,-1.1031838639
N,0,-0.6386438253,-0.3924981726,1.6005597922
C,0,-1.9486178638,-0.7369728298,1.658693475
C,0,-2.5573112652,-1.0559882675,2.8787725385
C,0,-1.8118198056,-1.0066065,4.0514825615
C,0,-0.470332329,-0.6369952277,3.9797015519
C,0,0.0781013514,-0.3408136375,2.7352934125
C,0,-2.682418393,-0.7414993705,0.37217193
N,0,-1.956934982,-0.4563702988,-0.7350493027

C,0,-2.5562938726,-0.427820154,-1.9358814425
C,0,-3.9114949036,-0.6879653712,-2.1014860734
C,0,-4.6736172012,-0.9829525791,-0.9713808245
C,0,-4.0548506761,-1.0067632488,0.2727410264
B,0,0.3793483727,-2.0974754904,-0.8313528836
O,0,1.1361467888,-2.7333305649,-1.8063241461
C,0,0.9241343285,-4.1474484865,-1.727189457
C,0,-0.2791149603,-4.3104902274,-0.774524401
O,0,-0.4328826515,-3.020617105,-0.1682599915
B,0,2.1065284689,-0.7115006045,-0.0766818381
O,0,2.4481625011,-1.3830808495,1.1093758542
C,0,3.8630832078,-1.6047724712,1.1104155904
C,0,4.2715773394,-1.3979443451,-0.3588485519
O,0,3.2152846841,-0.6093673712,-0.9072964308
H,0,0.606123123,0.193933388,-1.9346737006
H,0,-3.6009571665,-1.3429084405,2.9159864098
H,0,-2.2729043564,-1.2519453608,5.0032335926
H,0,0.1504225988,-0.5798027811,4.867280595
H,0,1.1164157303,-0.0607227064,2.6161946393
H,0,-4.6379662443,-1.2236080484,1.1590329241
H,0,-5.7363426245,-1.1876366188,-1.056092689
H,0,-4.3516926841,-0.6545349573,-3.0919278552
H,0,-1.9111584314,-0.1880775621,-2.7726794275
H,0,1.8306144028,-4.6251852377,-1.3345496081
H,0,0.7343098628,-4.5460499863,-2.7289874186
H,0,-1.2011958387,-4.5704188005,-1.3103993834
H,0,-0.1100105342,-5.0636780564,0.0019179063
H,0,-0.4257217038,2.3215452891,-2.524129995
H,0,-0.7977912396,2.2849713536,1.7558521686
H,0,-2.1433326193,4.3375135814,1.6609967615
H,0,-2.67021855,5.3962060016,-0.5312548552
H,0,-1.7951774408,4.3673200767,-2.6253164514
H,0,3.2991165156,4.0378962886,-0.9054801902
H,0,4.2320130967,2.5423552416,-0.6532809131
H,0,2.3276095853,3.9319601062,1.2982713642
H,0,3.7485636831,2.9296331734,1.6830567142
H,0,4.3432289695,-0.8755327327,1.7770581457
H,0,4.0799928038,-2.6110367864,1.4833845835
H,0,4.3310720701,-2.349114513,-0.904425868
H,0,5.2257262522,-0.8731487652,-0.4715655439

Ir(bpy)(BPin)$_2$(H)(^{2}-PhBPin)
E(RB+HF-LYP) = -1594.14737468

Zero-point correction= 0.471648 (Hartree/Particle)
Thermal correction to Energy= 0.502621
Thermal correction to Enthalpy= 0.503565
Thermal correction to Gibbs Free Energy= 0.402685
Sum of electronic and zero-point Energies= -1593.675727
Sum of electronic and thermal Energies= -1593.644754
Sum of electronic and thermal Enthalpies= -1593.643810
Sum of electronic and thermal Free Energies= -1593.744690

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	315.399	114.775	212.320

C,0,-4.0314077315,-0.3326262773,-1.1035713589
C,0,-2.7499499808,-0.3898210287,-0.5404793193
N,0,-1.6535553045,-0.1051217554,-1.2818788641
C,0,-1.8000116296,0.2405784629,-2.5706686105
C,0,-3.0424288045,0.3166657813,-3.1925491241
C,0,-4.1791018317,0.0224792944,-2.4405029234
C,0,-2.4990878542,-0.7699101764,0.8722701408
N,0,-1.1985393629,-0.8233346632,1.2616137794
C,0,-0.9087387698,-1.1840830337,2.5254824491
C,0,-1.8920597246,-1.4997238318,3.459196168
C,0,-3.2293215734,-1.4393980004,3.0733480714
C,0,-3.5326282192,-1.0716278365,1.7666808103
Ir,0,0.3271123647,-0.3548196529,-0.2675441851
B,0,2.087295613,-0.6098217545,0.7401570633
O,0,3.3767740833,-0.279496774,0.3045529029
C,0,4.3419634268,-0.7418131146,1.2482213677
C,0,3.5234589008,-1.0826874008,2.5088200637
O,0,2.1745046988,-1.1598510618,2.0410868103
C,0,-0.0204391747,3.038691829,0.2950795498
C,0,-0.0620934192,2.8070228723,1.6831092779
C,0,-1.2586790604,2.909215519,2.3950848365
C,0,-2.4387257193,3.2486409555,1.7292509637
C,0,-2.4194067162,3.4846292658,0.350811351
C,0,-1.2221713786,3.3765394094,-0.3559994352
B,0,1.3263028769,2.9610970422,-0.4867837383
O,0,1.4079650215,3.0325016065,-1.8571919529
C,0,2.7717902357,2.7469141043,-2.2161725754
C,0,3.5539499048,2.774787181,-0.8780964498
O,0,2.5398901047,2.8552338555,0.1380129523
B,0,0.6341393721,-2.2357214918,-0.8424100399
O,0,-0.4277796806,-3.1531591813,-0.918986051

C,0,0.0589315913,-4.3697688122,-1.4943799801
C,0,1.5943011571,-4.2414184855,-1.4185997098
O,0,1.8295665087,-2.8460759979,-1.222155857
H,0,1.3060001288,0.0218225466,-1.4609339328
H,0,-4.5668226885,-1.0219532431,1.4487341079
H,0,-4.0245649867,-1.6768067131,3.7733815382
H,0,-1.6045896322,-1.7879169416,4.4647485128
H,0,0.1498297631,-1.2262292425,2.7617819988
H,0,-4.9072002825,-0.5672347652,-0.5110477631
H,0,-5.1677870335,0.0668451013,-2.8869549598
H,0,-3.1100612321,0.5983798075,-4.2377908693
H,0,-0.8787627067,0.458179455,-3.0991674799
H,0,2.0104147031,-4.803948561,-0.5716205105
H,0,2.0963241557,-4.5778298097,-2.3320364257
H,0,-0.2958663004,-4.4498069939,-2.531051175
H,0,-0.3269765877,-5.2274837085,-0.9330972216
H,0,-1.2068778253,3.5629276951,-1.4262669526
H,0,0.8575084644,2.5535412924,2.202213835
H,0,-1.2708629108,2.7297522655,3.4667578037
H,0,-3.3697437384,3.3377044919,2.2832782636
H,0,-3.335402713,3.7573230321,-0.1667983272
H,0,3.1203490609,3.4960600409,-2.9344684365
H,0,2.8055820988,1.7574053737,-2.6825875151
H,0,4.2078892594,3.6506049225,-0.7907993901
H,0,4.1296908291,1.8614789664,-0.7184023369
H,0,3.6013806311,-0.299124643,3.2752119326
H,0,3.8165958554,-2.0356738328,2.9633047398
H,0,4.8535852632,-1.6244834015,0.8414081347
H,0,5.092462044,0.0360664541,1.4295800355

IrbpyBpin2H
E(RB+HF-LYP) = -1108.46367666

Zero-point correction= 0.309360 (Hartree/Particle)
Thermal correction to Energy= 0.330815
Thermal correction to Enthalpy= 0.331759
Thermal correction to Gibbs Free Energy= 0.254547
Sum of electronic and zero-point Energies= -1108.154317
Sum of electronic and thermal Energies= -1108.132862
Sum of electronic and thermal Enthalpies= -1108.131917
Sum of electronic and thermal Free Energies= -1108.209130

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	207.590	78.944	162.508

C,0,-2.8544778367,2.3976242721,0.8857578303
C,0,-2.1061216051,1.3748867969,0.2923856407
N,0,-0.7493926476,1.4400843936,0.2386570308
C,0,-0.1246241751,2.5131527297,0.7575392513
C,0,-0.81319916,3.5603694872,1.3636871824
C,0,-2.203349749,3.5000150509,1.4316121531
C,0,-2.7286368615,0.166785244,-0.308610476
N,0,-1.8722898713,-0.7278321687,-0.8604122532
C,0,-2.3571712275,-1.8515451121,-1.4134439095
C,0,-3.7177994669,-2.1426693057,-1.4527186971
C,0,-4.608606066,-1.2290710976,-0.8910566105
C,0,-4.1096855585,-0.0654144129,-0.3125787673
Ir,0,0.3190687325,-0.2540409197,-0.7007646773
B,0,2.2548592512,0.3621718181,-0.5896948054
O,0,2.6134855816,1.7256885365,-0.7037095747
C,0,4.0415248705,1.8376593259,-0.7190638297
C,0,4.5376022817,0.4569595815,-0.2453209638
O,0,3.4088568989,-0.4031435714,-0.3983296699
B,0,0.7831828888,-1.2743009833,0.9433023015
O,0,1.1831618559,-0.6837921035,2.1484460736
C,0,1.5315256052,-1.7238764153,3.0670775441
C,0,0.9283801149,-3.0026090641,2.4482165382
O,0,0.6735744911,-2.6575401998,1.0841044519
H,0,0.9258059963,-1.5077815815,-1.4651615155
H,0,0.9547779713,2.5128013463,0.654797635
H,0,-0.2619992567,4.4019568443,1.7690900717
H,0,-2.7749163301,4.2971826535,1.8967601276
H,0,-3.9354490901,2.3385628696,0.9233819815
H,0,-4.7922972889,0.6484046121,0.1322907839
H,0,-5.6775475758,-1.4184460336,-0.8992789172
H,0,-4.0623259733,-3.063491747,-1.9105499918
H,0,-1.6120528147,-2.5241501162,-1.8228256828
H,0,5.3767547765,0.0803124927,-0.8404425251
H,0,4.8467574365,0.4722403324,0.8090212551
H,0,4.35878502,2.6551602905,-0.0620134658
H,0,4.3762701715,2.0690839812,-1.7390583091
H,0,2.6248697281,-1.7846031913,3.1465371901
H,0,1.1261080992,-1.4964415593,4.0589882354
H,0,1.6096771255,-3.8587912621,2.4925920349
H,0,-0.0147410807,-3.2892726418,2.9340127538

Irbpy_Bpin2_H
E(RB+HF-LYP) = -1108.46355912

Zero-point correction= 0.309266 (Hartree/Particle)
Thermal correction to Energy= 0.329830
Thermal correction to Enthalpy= 0.330775
Thermal correction to Gibbs Free Energy= 0.256534
Sum of electronic and zero-point Energies= -1108.154294
Sum of electronic and thermal Energies= -1108.133729
Sum of electronic and thermal Enthalpies= -1108.132785
Sum of electronic and thermal Free Energies= -1108.207025

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	206.972	76.977	156.252

N,0,-1.9315469977,-0.6083347111,-0.7318981071
C,0,-2.7095240145,0.2929890111,-0.0839937834
C,0,-4.0850400455,0.0781716907,0.0664407652
C,0,-4.6608344002,-1.0744368323,-0.4606996044
C,0,-3.8502642725,-1.9946465194,-1.12370627
C,0,-2.489469863,-1.7221367783,-1.2333774638
C,0,-2.0065686238,1.4856332276,0.4550444889
N,0,-0.6546879098,1.501592719,0.3109159869
C,0,0.0409668632,2.5556250384,0.7771876241
C,0,-0.5690291554,3.6329702322,1.4139672837
C,0,-1.9535443816,3.6258998238,1.5686777751
C,0,-2.6778663056,2.5427831468,1.0795166897
Ir,0,0.2809940415,-0.2074553437,-0.7382789495
B,0,0.7262134886,-1.3843121801,0.8030038
O,0,0.4153433383,-2.7438391085,0.8750899606
C,0,0.7229440139,-3.2151315709,2.1904071211
C,0,1.5734725088,-2.0897555813,2.815345855
O,0,1.3087339749,-0.946480007,1.9967496396
B,0,2.2513361219,0.3037540152,-0.6936709261
O,0,3.3661511749,-0.5351967935,-0.6129744464
C,0,4.5483250635,0.2492512078,-0.4559441126
C,0,4.1149805435,1.6818537781,-0.8229454222
O,0,2.6850365992,1.6501801934,-0.741636554
H,0,0.7870212537,-1.4412069518,-1.6013030585
H,0,1.111158297,2.5129642405,0.6058900007
H,0,0.0372016942,4.4571861728,1.7739765184
H,0,-2.4650660398,4.449928762,2.056412129
H,0,-3.7563554837,2.5267982984,1.179997932

H,0,-4.7026286251,0.7936498847,0.5958382045
H,0,-5.7261419837,-1.2513470843,-0.3492540391
H,0,-4.2560760806,-2.9078669281,-1.5451268969
H,0,-1.8027164484,-2.4028471805,-1.7230988648
H,0,5.3404247455,-0.135178843,-1.1078430723
H,0,4.8980473226,0.1813226968,0.583541212
H,0,4.5114241284,2.4385656526,-0.1367604229
H,0,4.4140697548,1.9550432317,-1.8437588058
H,0,2.6463858969,-2.3198243614,2.7785337404
H,0,1.3021418848,-1.8749269796,3.8545820906
H,0,1.2576430999,-4.1686301789,2.1267646235
H,0,-0.2105865966,-3.3813177197,2.7459438125

Ir(bpy)(BPin)$_2$(^{2}-BPinH)
E(RB+HF-LYP) = -1363.08167363

Zero-point correction= 0.389493 (Hartree/Particle)
Thermal correction to Energy= 0.416284
Thermal correction to Enthalpy= 0.417228
Thermal correction to Gibbs Free Energy= 0.328929
Sum of electronic and zero-point Energies= -1362.692180
Sum of electronic and thermal Energies= -1362.665390
Sum of electronic and thermal Enthalpies= -1362.664446
Sum of electronic and thermal Free Energies= -1362.752744

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	261.222	98.729	185.841

C,0,-4.0413554853,-1.7854336315,-0.498514921
C,0,-2.9010051062,-0.9828003987,-0.3530849666
N,0,-1.6622951296,-1.5311173158,-0.3859885388
C,0,-1.5319925341,-2.8610082265,-0.5337853196
C,0,-2.6233659872,-3.710300369,-0.6808276224
C,0,-3.9028800815,-3.1577995606,-0.6702739328
C,0,-2.9725258834,0.4827986982,-0.1309068639
N,0,-1.7946795891,1.1154650911,0.078213801
C,0,-1.7916961061,2.43736391,0.3090348574
C,0,-2.9601006612,3.1949771107,0.3376189203
C,0,-4.1780352601,2.5574897132,0.112948828
C,0,-4.1841742798,1.1871298356,-0.1245443405
Ir,0,0.0978479928,-0.1558736976,-0.2075616663
B,0,0.9144809553,0.3815189278,1.7504933658
O,0,0.2261462493,1.3063428999,2.5410929142

C,0,1.1963708629,2.0120500611,3.3203009402
C,0,2.4320147855,1.0914964652,3.3051998283
O,0,2.2408839797,0.2610852467,2.1563547478
B,0,1.5307374782,1.3086541241,-0.5104515429
O,0,2.7914884505,1.181376306,-1.0735898536
C,0,3.4620256549,2.4399683009,-1.0392737158
C,0,2.349023434,3.4607080538,-0.7363910265
O,0,1.2822537769,2.6644497838,-0.207038325
B,0,1.525886204,-1.5194288359,-0.7384969547
O,0,2.2115687376,-1.6074762646,-1.9453573213
C,0,2.9535388631,-2.8257584374,-1.9915238379
C,0,2.8647697963,-3.3938268825,-0.5593376327
O,0,1.8049563743,-2.6503620934,0.0528807777
H,0,-0.5136602996,-3.2334290282,-0.5113087077
H,0,-2.4654080014,-4.7769187029,-0.7970542999
H,0,-4.7816089171,-3.7851875147,-0.7837851685
H,0,-5.030326555,-1.3455811954,-0.4689989209
H,0,-5.1225559404,0.6776520107,-0.3060776645
H,0,-5.109841653,3.114760588,0.1202880037
H,0,-2.9059061139,4.2615991351,0.5276832271
H,0,-0.8131502097,2.8789897795,0.4552265078
H,0,2.631295553,-4.4642812728,-0.5351098388
H,0,3.7909252032,-3.232918185,0.0068720947
H,0,3.9837249553,-2.6218716269,-2.3031893811
H,0,2.5015029487,-3.4997411051,-2.7325682711
H,0,2.4861965129,0.4602150565,4.2023174012
H,0,3.3744151826,1.6409104378,3.2126992981
H,0,0.8033195642,2.1918999077,4.3260721749
H,0,1.4052327378,2.9792667765,2.844304252
H,0,4.2276952555,2.4223840154,-0.251816017
H,0,3.9592373209,2.6227892166,-1.9976195457
H,0,2.6464839915,4.2190716316,-0.0040073742
H,0,2.0032463307,3.9747323975,-1.6432160079
H,0,0.2559980867,-0.7342131313,1.4533848809
H,0,0.0001358258,0.1823351308,-1.7797282016

bpyBpin2Hn2HBPinaxPrecConfInt
E(RB+HF-LYP) = -1363.08374806

Zero-point correction= 0.389898 (Hartree/Particle)
Thermal correction to Energy= 0.416773
Thermal correction to Enthalpy= 0.417717
Thermal correction to Gibbs Free Energy= 0.328781
Sum of electronic and zero-point Energies= -1362.693851

Sum of electronic and thermal Energies= -1362.666975
Sum of electronic and thermal Enthalpies= -1362.666031
Sum of electronic and thermal Free Energies= -1362.754967

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	261.529	98.620	187.181

H,0,-0.4196167865,-1.7632175518,-1.0267265858
Ir,0,-0.1201012572,-0.0381336575,-0.5202151843
B,0,0.3332480961,1.9412559767,-0.1071358988
O,0,-0.4676341803,3.0689232439,-0.2724935046
C,0,0.2081070957,4.2104337591,0.2613355923
C,0,1.6648689497,3.7436528545,0.4528774582
O,0,1.5908563066,2.3139866028,0.3896763051
N,0,0.8727887047,-0.8474540214,1.3037662372
C,0,2.2010651973,-1.1071508813,1.2051675079
C,0,2.9143636525,-1.6331462019,2.2893268431
C,0,2.2555240381,-1.8902317289,3.4870646305
C,0,0.8931462849,-1.6138772687,3.5766601876
C,0,0.2396614388,-1.0927941968,2.4632788759
C,0,2.8344748522,-0.8170967045,-0.1050790662
N,0,2.0089515254,-0.3830651347,-1.0860632631
C,0,2.5089024894,-0.1114152545,-2.3014774804
C,0,3.8576489295,-0.2571613833,-2.6078107732
C,0,4.7214383929,-0.6974307384,-1.6055220666
C,0,4.205592738,-0.9795972799,-0.3456124944
B,0,-1.7015224623,-1.5836452591,-0.9383921197
O,0,-2.3877974988,-2.2128946489,0.1050442862
C,0,-3.6232660401,-2.7107747113,-0.4250596724
C,0,-3.749999271,-2.0327391258,-1.8049571253
O,0,-2.4150459353,-1.6312463843,-2.1244120225
B,0,-1.8936513932,0.6453301494,0.2817474716
O,0,-2.0677841088,0.8393698155,1.6650283862
C,0,-3.4189482284,1.2394695641,1.9132901029
C,0,-3.9549202113,1.6346006158,0.5248536173
O,0,-3.0604532384,1.0043002531,-0.3933828449
H,0,-0.65626671,0.5562773494,-1.8833308753
H,0,1.7875936817,0.2341908696,-3.0330128489
H,0,4.8674218856,-1.3165288815,0.4426104441
H,0,4.2148653666,-0.0264817367,-3.6054689573
H,0,5.7825774272,-0.8185977552,-1.8001818606
H,0,3.9726673651,-1.8459830631,2.2014120548
H,0,2.7994095294,-2.2988171043,4.3331830969

H,0,0.3367249555,-1.7941100631,4.4900881956
H,0,-0.8127479207,-0.8350524166,2.4774585685
H,0,2.0900811701,4.0507872993,1.4141995428
H,0,2.3239963132,4.1085148491,-0.3463053523
H,0,-0.2597261714,4.4973865027,1.2126263199
H,0,0.1168101265,5.0525276658,-0.4327068757
H,0,-3.9753880369,0.3962248977,2.345651984
H,0,-3.4360533909,2.0666640572,2.6309711748
H,0,-4.9793356582,1.2892593982,0.3471411079
H,0,-3.9249660786,2.7207829599,0.3694005746
H,0,-3.5648842746,-3.8048031756,-0.5032221386
H,0,-4.4458271373,-2.4573018505,0.2517351566
H,0,-4.1287388046,-2.705376157,-2.5811239753
H,0,-4.3863871659,-1.1411264063,-1.7614768355

bpyBpin2Hn2HBPinax2ndBest
E(RB+HF-LYP) = -1363.08574187

Zero-point correction= 0.389134 (Hartree/Particle)
Thermal correction to Energy= 0.416356
Thermal correction to Enthalpy= 0.417300
Thermal correction to Gibbs Free Energy= 0.326749
Sum of electronic and zero-point Energies= -1362.696608
Sum of electronic and thermal Energies= -1362.669386
Sum of electronic and thermal Enthalpies= -1362.668442
Sum of electronic and thermal Free Energies= -1362.758993

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	261.267	98.868	190.581

N,0,-1.7529815228,1.2325729741,-0.0855802061
C,0,-2.8708638976,0.4956813401,-0.2864122602
C,0,-4.1302853331,1.1059498902,-0.3583982415
C,0,-4.232144958,2.4851610681,-0.2076319694
C,0,-3.0754855571,3.2278036053,0.0254704612
C,0,-1.855546331,2.5598088583,0.0795101315
C,0,-2.6680654732,-0.9686785635,-0.4164541819
N,0,-1.3857171189,-1.4103640162,-0.3499847592
C,0,-1.1383631627,-2.7298711615,-0.4298308991
C,0,-2.1506445299,-3.6706223575,-0.5932808732
C,0,-3.4690237086,-3.230192484,-0.6825201033
C,0,-3.7282266849,-1.8671860824,-0.5877638925
Ir,0,0.205268239,0.1130694435,-0.3068768286

B,0,1.2155796049,0.9955974437,1.462047143
O,0,2.5375034268,0.7416886496,1.8092620015
C,0,3.0357390343,1.8577121403,2.5488485178
C,0,1.9510319374,2.9466517369,2.3934342515
O,0,0.7895385142,2.2378207272,1.9494051898
B,0,1.8490678326,-1.0455251131,-0.6783096037
O,0,2.9732253988,-0.702668527,-1.4281029861
C,0,3.8388157691,-1.8322315783,-1.545378959
C,0,3.2685625243,-2.8717432073,-0.5560299727
O,0,1.9707651398,-2.3700097262,-0.2182757049
B,0,0.1297870421,0.2394688418,-2.3715128613
O,0,-0.1999273926,-0.833294122,-3.2074623898
C,0,-0.0932591989,-0.4147298473,-4.5729336609
C,0,0.0553926078,1.1208290335,-4.4988231678
O,0,0.3232032901,1.396192655,-3.120776226
H,0,-0.0924843501,-3.0097935931,-0.3618932308
H,0,-1.8986043166,-4.7237203175,-0.6545411994
H,0,-4.2845875167,-3.9333202012,-0.8209223955
H,0,-4.748175002,-1.5079461324,-0.6470794383
H,0,-5.0220017373,0.5167902008,-0.5344761921
H,0,-5.2017305139,2.9699416116,-0.2677507949
H,0,-3.1100047628,4.3034307755,0.1601091885
H,0,-0.9219815241,3.0746003956,0.2724893614
H,0,-0.984175665,-0.7306772379,-5.126852549
H,0,0.7818542409,-0.8937206204,-5.0298480483
H,0,0.8772975627,1.4971672248,-5.1168475577
H,0,-0.8641035519,1.6404593996,-4.8001296041
H,0,3.1775085995,1.5625731387,3.5970278824
H,0,4.005013002,2.1678887067,2.1445755391
H,0,1.728714629,3.4678472362,3.3304140122
H,0,2.2323905262,3.6941479196,1.6394320811
H,0,3.8725759862,-2.9493565309,0.3567534281
H,0,3.177966351,-3.871957008,-0.9942929959
H,0,4.866151148,-1.5387624492,-1.3036792307
H,0,3.8226115049,-2.1973221153,-2.5810691871
H,0,0.3797326395,-0.0051063216,1.5251615373
H,0,1.2037552583,1.3170092971,-0.5736495554

bpyBpin3HHprecrsrToH2comp
E(RB+HF-LYP) = -1363.07220511

Zero-point correction=	0.388306 (Hartree/Particle)
Thermal correction to Energy=	0.414989
Thermal correction to Enthalpy=	0.415934

Thermal correction to Gibbs Free Energy= 0.329129
Sum of electronic and zero-point Energies= -1362.683899
Sum of electronic and thermal Energies= -1362.657216
Sum of electronic and thermal Enthalpies= -1362.656272
Sum of electronic and thermal Free Energies= -1362.743076

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	260.410	99.543	182.695

H,0,-1.5284671466,1.3422366632,-1.0376503061
Ir,0,-0.3108264869,0.3598675448,-0.4719215585
B,0,0.9754711194,-0.893768566,-1.5564823093
O,0,2.1199822739,-0.5307174507,-2.2532635309
C,0,2.7478003271,-1.7132299098,-2.7427042279
C,0,1.6334249142,-2.7748543448,-2.7059914085
O,0,0.6960001928,-2.2589147348,-1.7521336446
N,0,-1.0824775167,0.9690698087,1.4629798795
C,0,-2.0901357718,0.228155376,1.9951976031
C,0,-2.6637755272,0.5821501946,3.2237939587
C,0,-2.2016511935,1.6957704378,3.9124095938
C,0,-1.1635150255,2.4411457288,3.3568538508
C,0,-0.6321175595,2.046841837,2.1349319222
C,0,-2.5372601222,-0.9488703594,1.2199412856
N,0,-1.869751854,-1.1894866138,0.0682548298
C,0,-2.2093202206,-2.2532656856,-0.6767962111
C,0,-3.241544082,-3.1168265939,-0.3253719288
C,0,-3.9482110474,-2.8703970195,0.8509637118
C,0,-3.5895814413,-1.7787863422,1.632426515
B,0,0.8851477764,1.969694707,-0.9000007783
O,0,1.4714230374,2.8072019772,0.0682474049
C,0,2.0940635012,3.9172705972,-0.5900800608
C,0,2.1489749086,3.4920636859,-2.0696159422
O,0,1.1895688533,2.4407446224,-2.1726190309
B,0,1.2410299721,-0.6075212669,0.7195078299
O,0,0.8394135006,-1.3533426348,1.8302111222
C,0,2.0010714762,-1.8442800579,2.5135141627
C,0,3.1707914283,-1.0586589655,1.8885839979
O,0,2.6231281052,-0.4876232323,0.6938807885
H,0,-0.2338638965,0.155788518,-2.0591950455
H,0,-1.6053630888,-2.4114479644,-1.5617625688
H,0,-4.1262637355,-1.5775653986,2.5511906637
H,0,-3.4788107614,-3.961620056,-0.9629893632
H,0,-4.7627839268,-3.5188491007,1.1585695753

H,0,-3.4659026555,-0.0128477701,3.6415269284
H,0,-2.6430469175,1.9732533616,4.8646479076
H,0,-0.7629112792,3.3174464977,3.8547344476
H,0,0.178917959,2.5839977492,1.655076611
H,0,1.9838087127,-3.7604581041,-2.3828548502
H,0,1.1383893365,-2.8842578325,-3.6807243894
H,0,3.585370578,-1.9795591224,-2.083598234
H,0,3.1395112861,-1.536914395,-3.7495739739
H,0,1.8967047332,-1.672951044,3.5899588233
H,0,2.0873355757,-2.9250216128,2.3431403168
H,0,3.524237469,-0.2504070444,2.5412862321
H,0,4.0262168513,-1.6929341405,1.634472381
H,0,1.4829721866,4.8184440431,-0.4420372447
H,0,3.0836029493,4.095653747,-0.1567232407
H,0,1.8875082373,4.3042478441,-2.7562805938
H,0,3.1395669951,3.108586422,-2.347630901

Irbpy_B2_H_n2BH_rotTS
E(RB+HF-LYP) = -1363.04753146

Zero-point correction= 0.388242 (Hartree/Particle)
Thermal correction to Energy= 0.414601
Thermal correction to Enthalpy= 0.415545
Thermal correction to Gibbs Free Energy= 0.328143
Sum of electronic and zero-point Energies= -1362.659289
Sum of electronic and thermal Energies= -1362.632930
Sum of electronic and thermal Enthalpies= -1362.631986
Sum of electronic and thermal Free Energies= -1362.719388

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	260.166	97.807	183.953

C,0,-4.1015873507,-0.1759820811,-0.2945060932
C,0,-2.7164491057,-0.3922437038,-0.3720250998
N,0,-1.8484052837,0.6372279562,-0.5180898649
C,0,-2.3519359051,1.8801935882,-0.6488218542
C,0,-3.7080493775,2.1635610674,-0.5877019952
C,0,-4.6050048589,1.1118251354,-0.3901964265
C,0,-2.1101507847,-1.7265712384,-0.353204935
N,0,-0.7542399409,-1.7719602584,-0.485355279
C,0,-0.1617698275,-2.9883471313,-0.533009206
C,0,-0.8695600421,-4.1770241742,-0.4389250001
C,0,-2.2554152036,-4.1386958896,-0.2856138239

C,0,-2.8720960239,-2.898680543,-0.2476976925
Ir,0,0.3426151042,0.0657577193,-0.4712873186
B,0,0.3758726686,-0.0696952956,1.6791142619
O,0,1.4715785715,0.1233925307,2.5155418324
C,0,1.0435853883,0.0673754859,3.8808730751
C,0,-0.379642805,-0.522524114,3.8178210394
O,0,-0.752549237,-0.4088041352,2.4366509993
B,0,2.2603529228,-0.709939483,-0.64356236
O,0,2.6029329883,-2.0593447464,-0.7857219546
C,0,4.0293421705,-2.1941881392,-0.7649641762
C,0,4.5487969151,-0.7554443373,-0.9526811165
O,0,3.41889921,0.0690115649,-0.6661567712
B,0,0.6828154862,2.1875584379,-0.3250845768
O,0,0.6810031224,3.0466041021,-1.4120241901
C,0,0.771989483,4.3934557735,-0.92559213
C,0,0.4885863482,4.2769878759,0.5892420207
O,0,0.6228382292,2.8792191987,0.8724962129
H,0,-1.6325002775,2.6647614761,-0.8383817184
H,0,-4.0484987704,3.1873547273,-0.6986518932
H,0,-5.6736519847,1.2913755389,-0.3282897588
H,0,-4.779406296,-1.0101149062,-0.1646268312
H,0,-3.9471413505,-2.8345424335,-0.13874375
H,0,-2.8396339956,-5.0496891515,-0.2034849005
H,0,-0.3285018942,-5.1159031417,-0.4854142158
H,0,0.9136199942,-2.9818274288,-0.6459497868
H,0,-0.4045041558,-1.5798252987,4.1137915003
H,0,-1.0964674121,0.0234517078,4.4404876782
H,0,1.0514627217,1.0804995504,4.3035675812
H,0,1.7364573234,-0.5512545976,4.4613678971
H,0,4.8830729031,-0.5693135034,-1.9817029213
H,0,5.3700289206,-0.5085623486,-0.2722505156
H,0,4.3449769594,-2.8726871683,-1.5640205338
H,0,4.336080684,-2.6224059558,0.1978627019
H,0,1.778176344,4.7763357994,-1.1326408238
H,0,0.0483078989,5.0239437805,-1.4519821377
H,0,1.1953565357,4.8434737774,1.2028449636
H,0,-0.527976551,4.5993938761,0.8496708702
H,0,0.4360314533,0.1786083138,-2.163550137
H,0,1.5652019154,1.1242772506,-0.383268901

IrBpy5_B3H2
E(RB+HF-LYP) = -1363.07263387

Zero-point correction= 0.388119 (Hartree/Particle)

Thermal correction to Energy= 0.414981
Thermal correction to Enthalpy= 0.415925
Thermal correction to Gibbs Free Energy= 0.328341
Sum of electronic and zero-point Energies= -1362.684515
Sum of electronic and thermal Energies= -1362.657653
Sum of electronic and thermal Enthalpies= -1362.656709
Sum of electronic and thermal Free Energies= -1362.744293

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	260.404	99.679	184.336

N,0,-1.2404988852,-1.5061968267,-0.0341588336
C,0,-2.5551211103,-1.1579827442,-0.0138437241
C,0,-3.5337311368,-2.0863626698,0.3655877268
C,0,-3.1650102876,-3.3763476127,0.7254773249
C,0,-1.8140785225,-3.7165790506,0.7025822198
C,0,-0.8836436835,-2.7567985272,0.3208048849
C,0,-2.8831876245,0.2322880687,-0.398610716
N,0,-1.8293317319,1.0363981466,-0.6678084415
C,0,-2.0502920023,2.319374365,-0.9968124359
C,0,-3.3297564894,2.857417255,-1.0951385433
C,0,-4.4249357106,2.0335056518,-0.83987244
C,0,-4.1991099774,0.7091397941,-0.4840430322
Ir,0,0.1953869968,0.0046778997,-0.6807581721
B,0,1.8771985068,-1.1406480045,-0.9267585432
O,0,3.0414976705,-0.7408809964,-1.5774844759
C,0,3.9354646241,-1.8476545594,-1.6877163855
C,0,3.3325943945,-2.9300974854,-0.7683188819
O,0,1.996376548,-2.4806637506,-0.5244937251
B,0,1.3267766273,1.6476308183,-0.0304414258
O,0,2.6304990431,1.6711986476,0.4594147679
C,0,3.0754661156,3.029050315,0.5123580902
C,0,1.7778484718,3.853496576,0.4407630117
O,0,0.8327387136,2.9569993641,-0.1497574884
B,0,0.5044664196,0.2004136106,1.4667859023
O,0,-0.2379224064,1.0210853921,2.3148761077
C,0,-0.0189469321,0.6110594671,3.6725197572
C,0,1.1599343888,-0.381196227,3.5897983792
O,0,1.2654295423,-0.6994193514,2.1971995269
H,0,-1.1607159123,2.9161998346,-1.1589848205
H,0,-3.4564185967,3.8999634714,-1.366554758
H,0,-5.4388873127,2.4146547118,-0.9128787878
H,0,-5.0393587987,0.0565255307,-0.2813859671

H,0,-4.5775632674,-1.7997722866,0.3854445751
H,0,-3.9195039338,-4.0993729798,1.0198547574
H,0,-1.4733848684,-4.7093630418,0.9755327161
H,0,0.1792212027,-2.9656731947,0.2770225247
H,0,-0.9331705648,0.141100046,4.0573908565
H,0,0.2007517531,1.4877355384,4.2905113284
H,0,2.1031247591,0.0671673892,3.9263840312
H,0,0.9895133138,-1.296576035,4.1658807852
H,0,3.9811189435,-2.1762859553,-2.73481788
H,0,4.9422764311,-1.544926701,-1.380163999
H,0,3.3118650924,-3.9223064073,-1.2325120983
H,0,3.8676421171,-3.0056899508,0.1871419086
H,0,1.8722568829,4.7526989534,-0.1767171514
H,0,1.424055301,4.1495009106,1.4375499045
H,0,3.7353505326,3.2269365893,-0.3426906255
H,0,3.6424893139,3.1969900052,1.4335608995
H,0,-0.1601869592,-0.5653195972,-2.2020576514
H,0,1.0414123751,0.9867933889,-1.6145391529

bpyBpin3HHtsFormn2H2
E(RB+HF-LYP) = -1363.06518340

Zero-point correction= 0.385767 (Hartree/Particle)
Thermal correction to Energy= 0.412560
Thermal correction to Enthalpy= 0.413504
Thermal correction to Gibbs Free Energy= 0.325554
Sum of electronic and zero-point Energies= -1362.679416
Sum of electronic and thermal Energies= -1362.652623
Sum of electronic and thermal Enthalpies= -1362.651679
Sum of electronic and thermal Free Energies= -1362.739630

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	258.885	99.166	185.107

H,0,-1.4788404854,1.1306243453,-1.2529163214
Ir,0,-0.2662326891,0.2883936523,-0.4265561489
B,0,0.9149397576,-0.8488110285,-1.7134763459
O,0,2.0188446169,-0.4369291105,-2.4412886627
C,0,2.6399506292,-1.5801111547,-3.0288524531
C,0,1.5607627055,-2.6773416845,-2.9615954039
O,0,0.6437331657,-2.2038814701,-1.9663373188
N,0,-1.1976716665,1.0038364026,1.4504195993
C,0,-2.1985009172,0.2569718252,1.9774151167

C,0,-2.8208522099,0.6375546384,3.174306877
C,0,-2.4100351684,1.7904604206,3.8312604902
C,0,-1.3702261202,2.5399525668,3.2841672033
C,0,-0.7879773196,2.1090405651,2.0976244143
C,0,-2.5759197182,-0.9701896498,1.2386266776
N,0,-1.8245456052,-1.2721878119,0.1538331176
C,0,-2.0933608407,-2.3896891896,-0.5416264065
C,0,-3.1341054699,-3.2500477225,-0.2048695086
C,0,-3.9288340946,-2.9394444947,0.8973427379
C,0,-3.6445884138,-1.79092786,1.6269154422
B,0,0.9828210963,1.8651336946,-0.7991201956
O,0,1.7057106142,2.5531057115,0.1957892692
C,0,2.3145364206,3.7121687301,-0.3872398616
C,0,2.1772122977,3.4891950566,-1.9055564177
O,0,1.1598954779,2.4957664689,-2.0278938091
B,0,1.2420330887,-0.5448682367,0.8597019835
O,0,0.9584876253,-0.8625257416,2.1923319485
C,0,2.1092402741,-1.4693134366,2.7947399331
C,0,3.2380325944,-1.2695886289,1.7620612799
O,0,2.5687813237,-0.845449481,0.569736983
H,0,-0.6777523191,0.4538689747,-1.9797191205
H,0,-1.4266818062,-2.5848173251,-1.3744057781
H,0,-4.2536783611,-1.5359100258,2.4853112714
H,0,-3.3111831839,-4.1402832498,-0.7988547035
H,0,-4.7553138451,-3.5808088214,1.187835763
H,0,-3.6127325943,0.031872772,3.5966748916
H,0,-2.8878150226,2.0912688801,4.7586000502
H,0,-1.0048740404,3.440694355,3.7652868428
H,0,0.0452307079,2.6312647448,1.6400989013
H,0,1.9579393514,-3.6533145967,-2.664054191
H,0,1.0306711361,-2.7949393067,-3.9165017638
H,0,3.529568635,-1.8463762473,-2.4435620483
H,0,2.9516925142,-1.3489632788,-4.0526827016
H,0,2.3205571,-0.9864397908,3.7548665358
H,0,1.9000467419,-2.5302297042,2.9833211508
H,0,3.948994133,-0.4924128237,2.0693721635
H,0,3.7998813893,-2.1884751082,1.5628353777
H,0,1.7796979782,4.612142827,-0.0525426314
H,0,3.355450464,3.7886249041,-0.0564461128
H,0,1.8805060257,4.3955303992,-2.4443010608
H,0,3.108044027,3.1121340449,-2.3493270556

bpyBpin3HHconfIntTS
E(RB+HF-LYP) = -1363.06647565

Zero-point correction= 0.388449 (Hartree/Particle)
Thermal correction to Energy= 0.414342
Thermal correction to Enthalpy= 0.415286
Thermal correction to Gibbs Free Energy= 0.330561
Sum of electronic and zero-point Energies= -1362.678027
Sum of electronic and thermal Energies= -1362.652134
Sum of electronic and thermal Enthalpies= -1362.651190
Sum of electronic and thermal Free Energies= -1362.735915

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	260.003	97.381	178.319

H,0,-1.3063022338,1.5548412679,-0.9340267311
Ir,0,-0.2268437183,0.3767783355,-0.4931777673
B,0,0.8842850586,-1.3300586722,-1.1337742657
O,0,1.7942411491,-1.3729779557,-2.1844782913
C,0,2.1627121363,-2.7312151499,-2.4211337962
C,0,1.0654437142,-3.549890875,-1.7154737953
O,0,0.4882897132,-2.6275543443,-0.7832122932
N,0,-1.1218919007,0.5939380398,1.5163495424
C,0,-2.2257455489,-0.1479518724,1.7847823915
C,0,-2.8690937231,-0.0587655587,3.0277191852
C,0,-2.3825967008,0.8103306162,3.9949777973
C,0,-1.2620568484,1.5852427154,3.6965673946
C,0,-0.6619820695,1.445726329,2.451408936
C,0,-2.7179660695,-1.0082670696,0.6898992443
N,0,-2.0021957178,-0.9755648714,-0.459614219
C,0,-2.4236485429,-1.6944484026,-1.5139108123
C,0,-3.5635406471,-2.486042081,-1.4800234306
C,0,-4.3022796582,-2.5400620568,-0.2968552955
C,0,-3.8767118505,-1.7932129579,0.7932311384
B,0,0.9979048949,2.0360576856,-0.6411352466
O,0,1.2800656629,2.8822633297,0.4453127279
C,0,1.9851214118,4.033239789,-0.0366418976
C,0,2.4134271634,3.6426934174,-1.4651746085
O,0,1.5825898329,2.5289745519,-1.7968330363
B,0,1.5787880775,-0.2051829013,0.5123282051
O,0,1.5033190467,-0.6272911523,1.8432924999
C,0,2.792493079,-0.5024685305,2.4508993266
C,0,3.7557258392,-0.2625508933,1.2691082904
O,0,2.904177733,0.0548668235,0.1667490936
H,0,0.1031525727,0.4335451259,-2.0360756018

H,0,-1.8147638694,-1.6167067367,-2.4065244875
H,0,-4.4439248186,-1.816680155,1.7154045657
H,0,-3.8597893484,-3.0455975135,-2.360570175
H,0,-5.1976095828,-3.1498247662,-0.2267451769
H,0,-3.7445780663,-0.6610759879,3.2361092696
H,0,-2.8736527785,0.8860812431,4.9602141863
H,0,-0.8521779085,2.2885631622,4.413393283
H,0,0.2001719584,2.0335788183,2.1593792892
H,0,1.4514307566,-4.4227353641,-1.1794935926
H,0,0.2898754067,-3.891391496,-2.4156017247
H,0,3.1556634524,-2.9197110264,-1.9903029858
H,0,2.2148876298,-2.9189677747,-3.4983110159
H,0,2.7818979549,0.3415264365,3.1533188515
H,0,3.0226224178,-1.4135715674,3.0130341999
H,0,4.4503779013,0.5650128397,1.4470195134
H,0,4.3443343824,-1.1562976778,1.0244870735
H,0,1.3106523832,4.8997529214,-0.0288263725
H,0,2.8334910198,4.2507777871,0.6210207771
H,0,2.2602744514,4.4486733795,-2.1904005864
H,0,3.4657618017,3.333543796,-1.507905577

bpyBpin3HHconfIntTS2
E(RB+HF-LYP) = -1363.06489611

Zero-point correction= 0.385848 (Hartree/Particle)
Thermal correction to Energy= 0.412667
Thermal correction to Enthalpy= 0.413612
Thermal correction to Gibbs Free Energy= 0.325674
Sum of electronic and zero-point Energies= -1362.679048
Sum of electronic and thermal Energies= -1362.652229
Sum of electronic and thermal Enthalpies= -1362.651284
Sum of electronic and thermal Free Energies= -1362.739222

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	258.953	99.090	185.081

C,0,-4.1023100101,1.2083612297,-0.4982207969
C,0,-2.8628303232,0.5581525075,-0.4152585973
N,0,-1.705137038,1.2469690218,-0.5445806749
C,0,-1.745107219,2.5770427137,-0.7279596165
C,0,-2.941524052,3.2834593591,-0.8099815189
C,0,-4.142149382,2.5833160469,-0.7000199808
C,0,-2.7308492771,-0.8967817219,-0.168442173

N,0,-1.4730218943,-1.4068438833,-0.1943899679
C,0,-1.2828096164,-2.7124337664,0.0701777132
C,0,-2.3373415752,-3.5765001771,0.3477386342
C,0,-3.6357003872,-3.0711671251,0.3643792468
C,0,-3.8310026867,-1.7186271517,0.1104034896
Ir,0,0.1979562685,0.004577057,-0.5997488807
B,0,0.3995927131,0.0409495946,1.5398296676
O,0,0.6251241162,-1.0777095255,2.3342525044
C,0,0.5273911018,-0.7073858051,3.7152874653
C,0,0.4976424187,0.8338834712,3.7019882999
O,0,0.213998152,1.1727495567,2.338371426
B,0,1.7648631339,-1.304179785,-0.7930434283
O,0,1.7723913503,-2.615281437,-0.2920635779
C,0,3.0272605732,-3.2332673227,-0.5909554557
C,0,3.6943686421,-2.2792248734,-1.6055265492
O,0,2.9210662266,-1.0817063913,-1.5408921527
B,0,1.6104324093,1.4824892944,-0.2072029306
O,0,1.4025114167,2.8246956631,-0.5612320566
C,0,2.4427464815,3.6213031478,0.0186864466
C,0,3.5220553117,2.5965102437,0.4156675308
O,0,2.8317273694,1.344556206,0.4408035142
H,0,-0.7768650975,3.0614874672,-0.8029167889
H,0,-2.9240322838,4.3575910116,-0.9602159727
H,0,-5.0957836709,3.097803222,-0.768535665
H,0,-5.0264648609,0.6498145805,-0.4132805815
H,0,-4.8308196299,-1.3037572732,0.1410660918
H,0,-4.4830552146,-3.7146327053,0.5806343073
H,0,-2.1327247582,-4.622088287,0.5506567595
H,0,-0.2494228785,-3.0411726523,0.0592472688
H,0,-0.2734474397,1.2545599957,4.3559658052
H,0,1.465204833,1.2672589536,3.9861328792
H,0,1.3823781425,-1.1130422695,4.2657525471
H,0,-0.3895807733,-1.1361810143,4.1410193461
H,0,3.6637613604,-2.6783554643,-2.6284011761
H,0,4.7387471204,-2.0615875729,-1.3561515231
H,0,2.8599495616,-4.2374213301,-0.9966517381
H,0,3.6103518867,-3.3288037832,0.3338819
H,0,2.7955656963,4.3559731395,-0.7124461589
H,0,2.0450661492,4.1583777405,0.8896883119
H,0,4.3340531015,2.5464196864,-0.3214785245
H,0,3.9600196026,2.7979341058,1.3987372996
H,0,-0.0369704562,-0.2564449677,-2.2544308447
H,0,0.7605191314,0.6783853066,-1.9544338628

$Ir(bpy)(BPin)_3(\ ^2\text{-}H_2)$
E(RB+HF-LYP) = -1363.07458254

Zero-point correction= 0.387170 (Hartree/Particle)
Thermal correction to Energy= 0.414658
Thermal correction to Enthalpy= 0.415602
Thermal correction to Gibbs Free Energy= 0.325650
Sum of electronic and zero-point Energies= -1362.687412
Sum of electronic and thermal Energies= -1362.659925
Sum of electronic and thermal Enthalpies= -1362.658981
Sum of electronic and thermal Free Energies= -1362.748932

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	260.202	101.361	189.319

C,0,1.8316466801,-3.678366044,1.4023515373
C,0,1.4987374022,-2.4294026213,0.8609151595
N,0,0.2166535811,-2.1276280126,0.542928061
C,0,-0.7507506536,-3.0299049097,0.7797277507
C,0,-0.4873029723,-4.2831336171,1.3276055175
C,0,0.8301570717,-4.6148595232,1.6367484732
C,0,2.5075984938,-1.3683114287,0.6146504209
N,0,2.071723891,-0.2599087651,-0.0282038439
C,0,2.9215573758,0.7593359532,-0.2329198645
C,0,4.2556441456,0.7140072635,0.1592073387
C,0,4.7219483891,-0.4283362975,0.8069094257
C,0,3.8373795468,-1.4746342306,1.0437466635
Ir,0,-0.1238309159,-0.1216068331,-0.5153667771
B,0,-0.1484234961,1.6487305975,-1.5289640564
O,0,0.3529036719,2.8697147631,-1.0412248463
C,0,0.1126503541,3.8922006251,-2.0143903125
C,0,-0.2213090423,3.1208794647,-3.307721132
O,0,-0.5166420426,1.7941829842,-2.8696728345
B,0,-0.381087077,0.989487115,1.1942768057
O,0,0.6583441131,1.2096955159,2.1100457529
C,0,0.2077860625,2.1292768023,3.1095049496
C,0,-1.3247147438,2.1504170959,2.9468433113
O,0,-1.5536445114,1.5902741072,1.6524921537
B,0,-2.18541982,-0.0492290795,-0.6002190387
O,0,-2.9916598572,-1.1045511193,-0.1227444003
C,0,-4.3686529617,-0.7920189985,-0.3607424885
C,0,-4.3565716267,0.702087149,-0.7394306386
O,0,-2.9975609449,0.97380646,-1.0778188715

H,0,0.3587299365,-1.0412764009,-2.1386869765
H,0,-0.4478889908,-0.9818279491,-2.1481407466
H,0,-1.7535690334,-2.7061107802,0.5173780283
H,0,2.8615077914,-3.9231867574,1.6317421804
H,0,-1.3023515906,-4.9778535263,1.5002250621
H,0,1.0777700654,-5.585998289,2.0544994464
H,0,4.1770622375,-2.3566096189,1.5727797079
H,0,5.7541927074,-0.5006863441,1.1355158098
H,0,4.9036045526,1.5623913153,-0.0325100067
H,0,2.4922399989,1.6357458793,-0.7055141033
H,0,-4.7490417481,-1.4228160921,-1.1760558674
H,0,-4.9583772112,-1.0001780177,0.538553784
H,0,-5.0065019481,0.9307449613,-1.590994111
H,0,-4.65269858,1.3390089557,0.1044293386
H,0,0.6288871504,3.0959340247,-4.0038002903
H,0,-1.0838596501,3.5378402341,-3.8386076032
H,0,0.9981894076,4.5303642658,-2.111464041
H,0,-0.7259600876,4.5168066934,-1.6810336707
H,0,0.5291648049,1.7890222047,4.1000034037
H,0,0.6535291433,3.1149591595,2.9214896974
H,0,-1.8279104694,1.5340176592,3.7045587266
H,0,-1.7444728571,3.1608470646,2.9936836949

Bpy_lossH2TS
E(RB+HF-LYP) = -1363.06627172

Zero-point correction= 0.383505 (Hartree/Particle)
Thermal correction to Energy= 0.412344
Thermal correction to Enthalpy= 0.413288
Thermal correction to Gibbs Free Energy= 0.319255
Sum of electronic and zero-point Energies= -1362.682767
Sum of electronic and thermal Energies= -1362.653928
Sum of electronic and thermal Enthalpies= -1362.652984
Sum of electronic and thermal Free Energies= -1362.747017

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	258.750	103.364	197.909

C,0,-4.0715287284,-1.451661716,-0.288556466
C,0,-2.8874934499,-0.7041691337,-0.2664659105
N,0,-1.678272228,-1.3141465766,-0.2812810718
C,0,-1.6193486148,-2.6548105178,-0.3278431175
C,0,-2.7565730915,-3.4577660517,-0.3425469189

C,0,-4.0059014079,-2.8413490005,-0.3200782439
C,0,-2.8730083511,0.7816259308,-0.2385148472
N,0,-1.6570729105,1.372687941,-0.3412259269
C,0,-1.5727288939,2.7145758516,-0.3171096884
C,0,-2.6942204999,3.5321299432,-0.1955067435
C,0,-3.9486350755,2.9362153707,-0.0877839522
C,0,-4.0377681681,1.5473686596,-0.1061540395
Ir,0,0.1680121832,0.0085259962,-0.3295978337
B,0,0.5938215305,0.0759601998,1.6163618115
O,0,-0.1079767925,-0.7249154495,2.5296918673
C,0,0.3243328936,-0.3871226986,3.8519871229
C,0,1.6035595241,0.4476393482,3.6358881196
O,0,1.5255696161,0.8720682227,2.2734008926
B,0,1.6639440702,1.3650308597,-0.6334757204
O,0,2.8969175269,1.1278878645,-1.2492081146
C,0,3.6741666149,2.3257332321,-1.2541766541
C,0,2.6727417662,3.4414227649,-0.8891841629
O,0,1.5338054218,2.7456277124,-0.3756157974
B,0,1.623692744,-1.4064157764,-0.4093249138
O,0,1.6026486374,-2.3746106626,-1.4388339483
C,0,2.8077302654,-3.1474176122,-1.364982892
C,0,3.3457669649,-2.8717021366,0.0519231902
O,0,2.6821393512,-1.6749175018,0.4612000509
H,0,-0.6209724359,-3.0748737428,-0.3720472284
H,0,-2.6564675578,-4.5371702438,-0.3764398299
H,0,-4.9178211687,-3.4303187513,-0.3353057832
H,0,-5.0362249407,-0.9591962283,-0.2906817047
H,0,-5.004728821,1.0694033121,-0.0068406801
H,0,-4.8457259387,3.5390862398,0.0154134865
H,0,-2.575532949,4.610226301,-0.1802272682
H,0,-0.5641002481,3.1124656246,-0.3824052895
H,0,3.0992921117,-3.6841266366,0.7501114297
H,0,4.4303564449,-2.7212132322,0.0723384397
H,0,3.5047817813,-2.806907026,-2.14148438
H,0,2.5833440502,-4.2049384933,-1.5425495458
H,0,2.511592175,-0.1534845518,3.7742033259
H,0,1.6614290024,1.3207035471,4.2946037784
H,0,0.5032260948,-1.3004948297,4.4291886227
H,0,-0.4634101929,0.1897618988,4.3562088111
H,0,4.4788395527,2.2381657315,-0.5124609974
H,0,4.1306061606,2.4701403793,-2.2397208288
H,0,3.0605775382,4.1293758509,-0.1299721325
H,0,2.375473245,4.0321672866,-1.7670334656
H,0,0.0582094105,-0.8875753237,-3.9642248741

H,0,0.4590622494,-1.2237596739,-3.4323459701

Bpy_lossH2_TSgood
E(RB+HF-LYP) = -1363.06745295

Zero-point correction=	0.383540 (Hartree/Particle)
Thermal correction to Energy=	0.412242
Thermal correction to Enthalpy=	0.413186
Thermal correction to Gibbs Free Energy=	0.319235
Sum of electronic and zero-point Energies=	-1362.683913
Sum of electronic and thermal Energies=	-1362.655211
Sum of electronic and thermal Enthalpies=	-1362.654266
Sum of electronic and thermal Free Energies=	-1362.748218

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	258.686	103.160	197.737

C,0,4.0953655295,1.5009715818,-0.3133149711
C,0,2.8979654231,0.7757992852,-0.2720672814
N,0,1.7007714232,1.4094207714,-0.20491615
C,0,1.6680509234,2.7525099317,-0.1539938299
C,0,2.8239180403,3.530237975,-0.1761684877
C,0,4.0586764538,2.891366011,-0.2639718399
C,0,2.8580209849,-0.7093560097,-0.2895550426
C,0,4.0090158929,-1.5014033777,-0.1895630072
C,0,3.8892024028,-2.8875153292,-0.1830054455
C,0,2.618865924,-3.4554440396,-0.2611962712
C,0,1.5170474468,-2.6102303241,-0.3506812666
N,0,1.630378484,-1.2726519317,-0.3791197665
Ir,0,-0.1647487785,0.0939569644,-0.3626646138
B,0,-1.6395608181,-1.2297514445,-0.8183814737
O,0,-2.2715889474,-1.2460510741,-2.0690190813
C,0,-3.299857502,-2.2380460024,-2.0657531704
C,0,-3.0130599567,-3.0933730618,-0.8123268216
O,0,-2.0733013443,-2.3246611105,-0.0543675335
B,0,-1.6703416329,1.4832990106,-0.2559991677
O,0,-3.0491957623,1.2761314591,-0.2739271094
C,0,-3.7258074508,2.5002042941,0.004873925
C,0,-2.6505260599,3.5886030744,-0.1845720515
O,0,-1.4130494269,2.8698604928,-0.1508464643
B,0,-0.5671955147,-0.3203025706,1.5532524134
O,0,-1.5785338745,0.2123426316,2.3493010592
C,0,-1.5760958937,-0.4607736153,3.6096124111

C,0,-0.2160880938,-1.189357619,3.6568832851
O,0,0.236146422,-1.1944397907,2.299904638
H,0,0.3546218798,0.6202195876,-3.0632759484
H,0,-0.3111277777,0.3735049438,-2.8150172427
H,0,0.5022482134,-2.9909416522,-0.3804083109
H,0,4.9876549845,-1.0454343054,-0.1009471911
H,0,2.4758913408,-4.5304290324,-0.2442576786
H,0,4.774262957,-3.5115173206,-0.1055314201
H,0,5.0472387837,0.989952304,-0.3918006072
H,0,4.9813846269,3.4628460923,-0.2956677938
H,0,2.7468724406,4.6113226264,-0.1316350318
H,0,0.6731227462,3.1847033893,-0.0991516257
H,0,-2.5670674494,-4.0650827761,-1.06622076
H,0,-3.9100801843,-3.2786939092,-0.2117349825
H,0,-3.2615173888,-2.8186455911,-2.994321361
H,0,-4.278127253,-1.7436594634,-2.0088167116
H,0,-4.5766529104,2.6210390751,-0.6746436332
H,0,-4.1066967341,2.4772964253,1.0346551702
H,0,-2.7469735854,4.1018064837,-1.1513373123
H,0,-2.6641812338,4.344649657,0.6081297665
H,0,-0.2972300565,-2.2176418872,4.0253697278
H,0,0.5149565906,-0.6573613845,4.2811931463
H,0,-2.4188883579,-1.1632221404,3.6453450755
H,0,-1.6985960729,0.266378932,4.4195780337

Ir(bpy)(BPin)$_3$(H$_2$) TS Loss of H$_2$
E(RB+HF-LYP) = -1363.07344231

Zero-point correction= 0.386640 (Hartree/Particle)
Thermal correction to Energy= 0.414382
Thermal correction to Enthalpy= 0.415326
Thermal correction to Gibbs Free Energy= 0.324104
Sum of electronic and zero-point Energies= -1362.686802
Sum of electronic and thermal Energies= -1362.659061
Sum of electronic and thermal Enthalpies= -1362.658116
Sum of electronic and thermal Free Energies= -1362.749338

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	260.028	101.749	191.992

C,0,-4.0315064848,-1.5082024458,-0.5120889578
C,0,-2.8437606896,-0.7705165411,-0.4150428683
N,0,-1.6367042925,-1.3808734473,-0.4905710004

C,0,-1.582263526,-2.7168220179,-0.6249609821
C,0,-2.7249215354,-3.5082046809,-0.7128561722
C,0,-3.97238572,-2.8893971223,-0.6645281702
C,0,-2.8286161633,0.699437339,-0.2133262204
C,0,-3.9904858934,1.4373091351,0.050070981
C,0,-3.9022003359,2.8079783933,0.2644876259
C,0,-2.647901486,3.4144447013,0.2283101285
C,0,-1.5328049504,2.6245640664,-0.0316970458
N,0,-1.6175615263,1.3037250625,-0.2646236413
Ir,0,0.1920921172,0.0012779482,-0.5148265718
B,0,1.6263343565,1.4501210918,-0.6090978819
O,0,2.494465527,1.6447195413,-1.6867945644
C,0,3.4012857762,2.7031442756,-1.3772050399
C,0,2.755739791,3.4253820812,-0.1774061962
O,0,1.7821379685,2.4984261853,0.3172108001
B,0,1.7330859961,-1.3768116029,-0.4228955835
O,0,3.1040188673,-1.1524069956,-0.4820268661
C,0,3.7975114113,-2.3585717044,-0.1649956726
C,0,2.7345764719,-3.4639178428,-0.3138126752
O,0,1.4888433617,-2.758539717,-0.2729764876
B,0,0.4747186062,-0.0206573866,1.5186331572
O,0,1.6363158992,-0.3410604825,2.2189821393
C,0,1.4247028485,-0.117948625,3.6145742802
C,0,-0.1024907795,0.0512040163,3.7548279781
O,0,-0.563062697,0.2687660916,2.4172083888
H,0,-0.0775449098,0.0228978651,-2.4592981546
H,0,0.6481903149,-0.2875949458,-2.2961656078
H,0,-0.5278139515,3.0320042661,-0.0318312049
H,0,-4.9538164929,0.9455522096,0.1063132973
H,0,-2.5257710203,4.4772452169,0.4071101521
H,0,-4.7966353796,3.3879207136,0.4702524611
H,0,-4.9934849289,-1.0117088657,-0.4768982372
H,0,-4.8867153731,-3.4698728658,-0.7419284999
H,0,-2.629009842,-4.5834000557,-0.8201232593
H,0,-0.5805924594,-3.1349592849,-0.6483039097
H,0,2.2532452041,4.355977205,-0.4769736104
H,0,3.4740611787,3.6655451083,0.6134818117
H,0,3.5275704324,3.3544861536,-2.2490233022
H,0,4.3798917421,2.2771153702,-1.1201805587
H,0,4.6474935864,-2.489865798,-0.8432495647
H,0,4.1794177384,-2.2958959297,0.862464733
H,0,2.8212879396,-3.9947607916,-1.272066687
H,0,2.7695619361,-4.2036500631,0.4931658401
H,0,-0.3799853777,0.902123062,4.3863419838

H,0,-0.5827951408,-0.8487254144,4.1621236241
H,0,1.969019899,0.7846943217,3.9211656687
H,0,1.8138739965,-0.9652864614,4.1894998509

bpy Bpin3 Para Toluene CH Activation Transition Structure
E(RB+HF-LYP) = -1633.42680750

Zero-point correction=	0.496401 (Hartree/Particle)
Thermal correction to Energy=	0.530295
Thermal correction to Enthalpy=	0.531239
Thermal correction to Gibbs Free Energy=	0.426328
Sum of electronic and zero-point Energies=	-1632.930407
Sum of electronic and thermal Energies=	-1632.896513
Sum of electronic and thermal Enthalpies=	-1632.895569
Sum of electronic and thermal Free Energies=	-1633.000480

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	332.765	124.585	220.804

C,0,-3.0681886977,2.9015918505,-2.5380174005
C,0,-2.2553131836,3.4264743389,-1.5253813477
C,0,-1.2436612232,2.6634805539,-0.9375572242
C,0,-1.0164993117,1.3272556869,-1.3130634425
C,0,-1.8236406958,0.8156806534,-2.3439690712
C,0,-2.8306323907,1.5811850511,-2.9373533082
Ir,0,0.3389422593,0.0365045258,-0.0888122676
N,0,-1.1326091003,-1.6981863366,-0.4010226012
C,0,-2.1729096085,-1.7633224784,0.4594266748
C,0,-3.1389708147,-2.7734506726,0.3509638234
C,0,-3.0275725916,-3.7246714485,-0.6566977754
C,0,-1.9479874951,-3.6499783305,-1.5339597684
C,0,-1.0236117218,-2.6218962591,-1.3687634228
C,0,-2.2154312217,-0.7281812658,1.5200824111
N,0,-1.1912290551,0.160536017,1.5459064905
C,0,-1.1595936148,1.1022801838,2.506001345
C,0,-2.1507122243,1.2129981152,3.4767662529
C,0,-3.2156081521,0.3159062461,3.4545392215
C,0,-3.244329982,-0.6637802783,2.4688800047
B,0,1.4632127569,-1.1579213866,1.2813133421
O,0,1.4486258895,-2.5564962163,1.2748547685
C,0,2.1862389702,-3.0409753625,2.4047188057
C,0,2.8952025989,-1.7919924809,2.9668998468
O,0,2.2321619819,-0.6890122748,2.3389163932

B,0,1.9143423841,-0.7530276708,-1.186801512
O,0,3.2722215199,-0.7256892615,-0.893719781
C,0,4.0013978464,-1.3056565233,-1.978244514
C,0,2.935885799,-2.0601046793,-2.7943089982
O,0,1.6965052405,-1.4758759457,-2.3719726044
B,0,1.5515452053,1.6179902169,0.3870891741
O,0,1.4383354408,2.3733868899,1.5659415127
C,0,2.3183601406,3.5008209087,1.501661305
C,0,3.1976803054,3.2291899207,0.2630225528
O,0,2.5194091511,2.1873011713,-0.4384519795
H,0,0.5077543619,0.7030465452,-1.54461536
H,0,-0.1594724308,-2.5135223065,-2.0157425477
H,0,-3.9691558553,-2.8222761613,1.044457975
H,0,-1.8155456656,-4.3709779784,-2.3335225425
H,0,-3.7706925615,-4.510660268,-0.7507092802
H,0,-4.064434083,-1.3700128133,2.4385236822
H,0,-4.0107315149,0.3731899629,4.1916216272
H,0,-2.0790338236,1.9914114554,4.2286575469
H,0,-0.3044692081,1.7688239809,2.4752078745
H,0,2.9262973282,-3.1342929632,-2.5664483158
H,0,3.0517955255,-1.9345829694,-3.8753500286
H,0,4.7854358471,-1.9625742572,-1.5881309503
H,0,4.47635593,-0.5060630662,-2.5610578229
H,0,-0.6361823652,3.1154174979,-0.1581623657
H,0,-2.4115558738,4.4516185621,-1.1931544641
C,0,-4.1321321471,3.7431671749,-3.2038225802
H,0,-1.6655574296,-0.1997405426,-2.6977255792
H,0,-3.4373644586,1.1449673554,-3.7293438233
H,0,1.4887555009,-3.4837961192,3.1280060045
H,0,2.8851464342,-3.8203153324,2.0830911258
H,0,2.8088254287,-1.704528557,4.0550742493
H,0,3.9595800815,-1.7676662233,2.7016032256
H,0,1.7248670501,4.4189745477,1.3961430534
H,0,2.8969388401,3.5696712008,2.4287610071
H,0,3.3011649906,4.1061147213,-0.3849522686
H,0,4.2023126356,2.885081407,0.5409394953
H,0,-4.9623570602,3.128155242,-3.5660299159
H,0,-4.5409439894,4.491023139,-2.5165882178
H,0,-3.7308195418,4.2859715644,-4.0696878427

bpy Bpin3 Meta Toluene CH Activation Transition Structure
E(RB+HF-LYP) = -1633.42666181

Zero-point correction= 0.496410 (Hartree/Particle)

Thermal correction to Energy= 0.530267
Thermal correction to Enthalpy= 0.531211
Thermal correction to Gibbs Free Energy= 0.426791
Sum of electronic and zero-point Energies= -1632.930252
Sum of electronic and thermal Energies= -1632.896395
Sum of electronic and thermal Enthalpies= -1632.895451
Sum of electronic and thermal Free Energies= -1632.999871

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	332.748	124.594	219.771

C,0,-3.0773853199,2.9442794147,-2.4887063653
C,0,-2.2763056047,3.4910118131,-1.4863125318
C,0,-1.2540121803,2.7373603629,-0.9041578361
C,0,-1.0299659213,1.4035959337,-1.2905909989
C,0,-1.8352796537,0.8874288383,-2.3203462621
C,0,-2.856854629,1.6329850385,-2.9269531073
Ir,0,0.3276747939,0.1099516232,-0.0659758254
N,0,-1.1531180286,-1.6205394394,-0.3690817558
C,0,-2.1915849936,-1.6779057593,0.4942617733
C,0,-3.1666289943,-2.6796036409,0.3868743457
C,0,-3.064881236,-3.6306028536,-0.6220727851
C,0,-1.9858815291,-3.5651689911,-1.5008320329
C,0,-1.0525636229,-2.5449007937,-1.3371712944
C,0,-2.2202801928,-0.644871528,1.5575403542
N,0,-1.1906829312,0.2376762736,1.5773741582
C,0,-1.1429425195,1.1743504949,2.5413887158
C,0,-2.1236955249,1.2870167226,3.5224066941
C,0,-3.1948456786,0.3973100559,3.506045459
C,0,-3.239732072,-0.5777946955,2.5162162359
B,0,1.4507459097,-1.0891400438,1.3010359907
O,0,1.4729239646,-2.4867172121,1.2651768409
C,0,2.1996643519,-2.9784699537,2.3987292265
C,0,2.8438242565,-1.7219496278,3.0214903349
O,0,2.1781453182,-0.6232323821,2.3887958125
B,0,1.8948761839,-0.6799924901,-1.1744737131
O,0,3.2554537057,-0.6337540236,-0.8969244215
C,0,3.9789750122,-1.2209231105,-1.9812431116
C,0,2.9125080327,-1.9962398523,-2.7762909046
O,0,1.6716927323,-1.4186355355,-2.3487499973
B,0,1.5457993828,1.6910521333,0.3978064288
O,0,1.4478497384,2.4433078354,1.5803345087
C,0,2.3146721358,3.5799530095,1.4993085813

C,0,3.1836420748,3.3083938315,0.2539568179
O,0,2.4995339228,2.2655262175,-0.440522118
H,0,0.4829109802,0.7713437547,-1.5263672518
H,0,-0.1880246973,-2.443627794,-1.9851061143
H,0,-3.9964190675,-2.7219775929,1.0813555655
H,0,-1.8608420125,-4.2875801939,-2.3003390959
H,0,-3.8147347883,-4.4102707905,-0.715505451
H,0,-4.0640167109,-1.2793216429,2.4912239542
H,0,-3.9822886591,0.456251052,4.2512011333
H,0,-2.0393485804,2.0610282668,4.2775059965
H,0,-0.2829309718,1.8340963892,2.5042372797
H,0,2.9157133631,-3.0672447815,-2.5340857021
H,0,3.0159656419,-1.883775476,-3.8600445853
H,0,4.7733304114,-1.8652553047,-1.5909756606
H,0,4.4403211523,-0.42456223,-2.5793407019
H,0,-0.6420743387,3.1900094711,-0.1290305105
H,0,-2.4472120047,4.5132364094,-1.1556180563
H,0,-3.8677837042,3.5396246786,-2.9407655088
H,0,-1.6639118589,-0.1272071867,-2.6728328776
C,0,-3.6767280289,1.046194416,-4.0542392586
H,0,1.5021193262,-3.4732815025,3.0871599442
H,0,2.9380398988,-3.717983371,2.0710812996
H,0,2.7034399605,-1.6633940389,4.1060705787
H,0,3.918475955,-1.6599411769,2.8094330171
H,0,1.7099133088,4.4905570798,1.3915969896
H,0,2.9010305633,3.6628467126,2.4202974022
H,0,3.2814094592,4.1848539339,-0.3954089891
H,0,4.1906349675,2.9644289488,0.5237512042
H,0,-3.6945254225,-0.0472635034,-4.0102391781
H,0,-4.7119106235,1.4026183372,-4.02660611
H,0,-3.2658453683,1.3253067838,-5.0330976632

bpy Bpin3 Meta Toluene CH Activation Transition Structure, Isomer 2
E(RB+HF-LYP) = -1633.42667684

Zero-point correction= 0.496336 (Hartree/Particle)
Thermal correction to Energy= 0.530236
Thermal correction to Enthalpy= 0.531180
Thermal correction to Gibbs Free Energy= 0.426396
Sum of electronic and zero-point Energies= -1632.930341
Sum of electronic and thermal Energies= -1632.896441
Sum of electronic and thermal Enthalpies= -1632.895497
Sum of electronic and thermal Free Energies= -1633.000281

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	332.728	124.646	220.537

C,0,-3.9035766046,2.8568456986,-1.0381277517
C,0,-2.916390774,3.3150796461,-0.1544727119
C,0,-1.7306961405,2.5781263962,-0.0315720602
C,0,-1.5059791425,1.383389065,-0.7409115037
C,0,-2.5062224016,0.9702463452,-1.6363618885
C,0,-3.6937571008,1.6950951081,-1.7775787389
Ir,0,0.2364662357,0.0842673624,-0.2059301894
N,0,-1.0962844039,-1.7517216927,-0.5551659386
C,0,-1.8454066849,-2.1576199552,0.4940680152
C,0,-2.6918760609,-3.2705371146,0.3909829577
C,0,-2.766853171,-3.9670714243,-0.8096804747
C,0,-1.9897528277,-3.5392001325,-1.8836701678
C,0,-1.1672596857,-2.4290816034,-1.712024027
C,0,-1.705456199,-1.3740218963,1.7447025801
N,0,-0.8108180096,-0.3547462479,1.7293981603
C,0,-0.6228308311,0.3739431063,2.8445174659
C,0,-1.3231245673,0.1314971121,4.0225197907
C,0,-2.2540047291,-0.9037996079,4.0494127983
C,0,-2.4433121492,-1.6627085677,2.9003573426
B,0,1.7868047916,-1.1849620796,0.5381856793
O,0,1.8858256683,-2.5442098987,0.2259813669
C,0,2.9508247287,-3.1285571814,0.9871889244
C,0,3.6666549597,-1.9271365105,1.6404555311
O,0,2.7732360477,-0.8248862963,1.4472805164
B,0,1.5229894647,-0.2340742036,-1.8044345446
O,0,2.9050861433,-0.099180349,-1.8434139197
C,0,3.3666324074,-0.3335884579,-3.1758792984
C,0,2.1786166528,-1.0178532471,-3.8772213884
O,0,1.0548376696,-0.7055609604,-3.0430823322
B,0,1.3944511226,1.6881283489,0.3276761543
O,0,1.4906157069,2.1891243436,1.6374484386
C,0,2.2396936717,3.4093202459,1.6305175004
C,0,2.849741011,3.4728863281,0.2153640332
O,0,2.1060151751,2.5159287309,-0.5385858251
H,0,-0.0479144427,1.0468706987,-1.4645019098
H,0,-0.5342544073,-2.0519705489,-2.5085571611
H,0,-3.2858309377,-3.5946840635,1.2363646229
H,0,-2.0124110947,-4.0509871209,-2.8398455381
H,0,-3.4199782878,-4.8295793172,-0.9011645738
H,0,-3.1639491886,-2.4706724972,2.9039835922

H,0,-2.8236457764,-1.1208411784,4.9478573283
H,0,-1.1349678858,0.7492383222,4.8939592746
H,0,0.1173594355,1.1626980753,2.7652502011
H,0,2.3011338413,-2.107986888,-3.9267476004
H,0,2.0004912673,-0.6414527927,-4.8893612357
H,0,4.2655600743,-0.9579421927,-3.1517519701
H,0,3.6229429706,0.6263240033,-3.6421349505
H,0,-0.9684664926,2.9468582692,0.6505745159
C,0,-3.1273987837,4.5832990141,0.6422191329
H,0,-4.8282153971,3.4183308432,-1.1548248624
H,0,-2.3598050279,0.0793809526,-2.2406425063
H,0,-4.454457579,1.3532565851,-2.4761661575
H,0,2.5276144715,-3.8161130445,1.7311396942
H,0,3.6049491661,-3.7044499118,0.3238920423
H,0,3.8497896222,-2.0704019946,2.710734583
H,0,4.6240874335,-1.7019846869,1.154409469
H,0,1.5625353765,4.2514528525,1.8276291257
H,0,2.9961909947,3.3826296765,2.4216557978
H,0,2.7558590393,4.4625679794,-0.2440989243
H,0,3.9105582089,3.1904473088,0.2138774902
H,0,-2.2587078608,4.8100690487,1.2672923735
H,0,-3.2997898466,5.4446852703,-0.0140684233
H,0,-4.0006125804,4.5044459413,1.3012459641

bpyBpin3MetaTolHCHactTS
E(RB+HF-LYP) = -1633.42666181

Zero-point correction= 0.496410 (Hartree/Particle)
Thermal correction to Energy= 0.530267
Thermal correction to Enthalpy= 0.531211
Thermal correction to Gibbs Free Energy= 0.426791
Sum of electronic and zero-point Energies= -1632.930252
Sum of electronic and thermal Energies= -1632.896395
Sum of electronic and thermal Enthalpies= -1632.895451
Sum of electronic and thermal Free Energies= -1632.999871

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	332.748	124.594	219.771

C,0,-3.0773853199,2.9442794147,-2.4887063653
C,0,-2.2763056047,3.4910118131,-1.4863125318
C,0,-1.2540121803,2.7373603629,-0.9041578361
C,0,-1.0299659213,1.4035959337,-1.2905909989

C,0,-1.8352796537,0.8874288383,-2.3203462621
C,0,-2.856854629,1.6329850385,-2.9269531073
Ir,0,0.3276747939,0.1099516232,-0.0659758254
N,0,-1.1531180286,-1.6205394394,-0.3690817558
C,0,-2.1915849936,-1.6779057593,0.4942617733
C,0,-3.1666289943,-2.6796036409,0.3868743457
C,0,-3.064881236,-3.6306028536,-0.6220727851
C,0,-1.9858815291,-3.5651689911,-1.5008320329
C,0,-1.0525636229,-2.5449007937,-1.3371712944
C,0,-2.2202801928,-0.644871528,1.5575403542
N,0,-1.1906829312,0.2376762736,1.5773741582
C,0,-1.1429425195,1.1743504949,2.5413887158
C,0,-2.1236955249,1.2870167226,3.5224066941
C,0,-3.1948456786,0.3973100559,3.506045459
C,0,-3.239732072,-0.5777946955,2.5162162359
B,0,1.4507459097,-1.0891400438,1.3010359907
O,0,1.4729239646,-2.4867172121,1.2651768409
C,0,2.1996643519,-2.9784699537,2.3987292265
C,0,2.8438242565,-1.7219496278,3.0214903349
O,0,2.1781453182,-0.6232323821,2.3887958125
B,0,1.8948761839,-0.6799924901,-1.1744737131
O,0,3.2554537057,-0.6337540236,-0.8969244215
C,0,3.9789750122,-1.2209231105,-1.9812431116
C,0,2.9125080327,-1.9962398523,-2.7762909046
O,0,1.6716927323,-1.4186355355,-2.3487499973
B,0,1.5457993828,1.6910521333,0.3978064288
O,0,1.4478497384,2.4433078354,1.5803345087
C,0,2.3146721358,3.5799530095,1.4993085813
C,0,3.1836420748,3.3083938315,0.2539568179
O,0,2.4995339228,2.2655262175,-0.440522118
H,0,0.4829109802,0.7713437547,-1.5263672518
H,0,-0.1880246973,-2.443627794,-1.9851061143
H,0,-3.9964190675,-2.7219775929,1.0813555655
H,0,-1.8608420125,-4.2875801939,-2.3003390959
H,0,-3.8147347883,-4.4102707905,-0.715505451
H,0,-4.0640167109,-1.2793216429,2.4912239542
H,0,-3.9822886591,0.456251052,4.2512011333
H,0,-2.0393485804,2.0610282668,4.2775059965
H,0,-0.2829309718,1.8340963892,2.5042372797
H,0,2.9157133631,-3.0672447815,-2.5340857021
H,0,3.0159656419,-1.883775476,-3.8600445853
H,0,4.7733304114,-1.8652553047,-1.5909756606
H,0,4.4403211523,-0.42456223,-2.5793407019
H,0,-0.6420743387,3.1900094711,-0.1290305105

H,0,-2.4472120047,4.5132364094,-1.1556180563
H,0,-3.8677837042,3.5396246786,-2.9407655088
H,0,-1.6639118589,-0.1272071867,-2.6728328776
C,0,-3.6767280289,1.046194416,-4.0542392586
H,0,1.5021193262,-3.4732815025,3.0871599442
H,0,2.9380398988,-3.717983371,2.0710812996
H,0,2.7034399605,-1.6633940389,4.1060705787
H,0,3.918475955,-1.6599411769,2.8094330171
H,0,1.7099133088,4.4905570798,1.3915969896
H,0,2.9010305633,3.6628467126,2.4202974022
H,0,3.2814094592,4.1848539339,-0.3954089891
H,0,4.1906349675,2.9644289488,0.5237512042
H,0,-3.6945254225,-0.0472635034,-4.0102391781
H,0,-4.7119106235,1.4026183372,-4.02660611
H,0,-3.2658453683,1.3253067838,-5.0330976632

bpy Bpin3 Ortho Toluene CH Activation Transition Structure
E(RB+HF-LYP) = -1633.41948141

Zero-point correction= 0.496800 (Hartree/Particle)
Thermal correction to Energy= 0.530416
Thermal correction to Enthalpy= 0.531360
Thermal correction to Gibbs Free Energy= 0.427337
Sum of electronic and zero-point Energies= -1632.922682
Sum of electronic and thermal Energies= -1632.889065
Sum of electronic and thermal Enthalpies= -1632.888121
Sum of electronic and thermal Free Energies= -1632.992144

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	332.841	124.494	218.935

C,0,-3.422835,2.445731,-2.809270
C,0,-2.744491,3.171590,-1.831515
C,0,-1.645711,2.642578,-1.134258
C,0,-1.232558,1.311568,-1.395365
C,0,-1.904646, 0.617509,-2.418704
C,0,-2.987263,1.159492,-3.115581
Ir,0,0.244993,0.107332,-0.155795
N,0,-1.272478,-1.632863,-0.325652
C,0,-2.272498,-1.640037,0.582616
C,0,-3.286333,-2.607217,0.536883
C,0,-3.255596,-3.586093,-0.450126
C,0,-2.206506,-3.582809,-1.366192

C,0,-1.237729,-2.587269,-1.268120
C,0,-2.199612,-0.610180,1.646699
N,0,-1.125955, 0.217727,1.617517
C,0,-0.944710,1.094655,2.622246
C,0,-1.848002,1.225890,3.672375
C,0,-2.980554,0.415394,3.688979
C,0,-3.149983,-0.517075,2.672400
B,0,1.444631,-1.164083,1.079289
O,0,1.552469,-2.543259,0.874177
C,0,2.315405,-3.128545,1.936468
C,0,2.827077,-1.925400,2.760031
O,0,2.130840,-0.793410,2.226553
B,0,1.702789,-0.673925,-1.408086
O,0,3.082657,-0.568739,-1.287317
C,0,3.701480,-1.175346,-2.424974
C,0,2.580980,-2.013993,-3.067335
O,0,1.375368,-1.457977,-2.524717
B,0,1.539178,1.629108,0.287845
O,0,1.708087,2.184319,1.565811
C,0,2.562405,3.328424,1.477797
C,0,3.189627,3.224007,0.074440
O,0,2.332375,2.323990,-0.629269
H,0,0.387209,0.811314,-1.591844
H,0,-0.400922,-2.529058,-1.956065
H,0,-4.088894,-2.602791,1.263638
H,0,-2.133389,-4.331572,-2.147669
H,0,-4.035529,-4.340042,-0.496303
H,0,-4.014185,-1.169193,2.680855
H,0,-3.714551,0.495994,4.484912
H,0,-1.657777,1.952747,4.454570
H,0,-0.037591,1.686669,2.562288
H,0,2.647643,-3.073410,-2.787474
H,0,2.559733,-1.941355,-4.159115
H,0,4.556079,-1.779198,-2.103501
H,0,4.065231,-0.389124,-3.098899
C,0,-0.939007,3.548704,-0.151401
H,0,-3.064897,4.186739,-1.604955
H,0,-4.264859,2.889013,-3.334475
H,0,-1.566473,-0.376819,-2.693536
H,0,-3.475134,0.580187,-3.896018
H,0,1.667377,-3.792038,2.523185
H,0,3.128237,-3.731171,1.516771
H,0,2.609288,-2.019145,3.829520
H,0,3.906439,-1.770383,2.642622

H,0,1.961770,4.241377,1.593378
H,0,3.303346,3.298366,2.283264
H,0,3.229718,4.185591,-0.448184
H,0,4.204331,2.806314,0.109168
H,0,0.094187,3.726367,-0.465112
H,0,-1.441949,4.518905,-0.087357
H,0,-0.900856,3.122739,0.853765

bpy Bpin3 Para PhenylBPin CH Activation Transition Structure
E(RB+HF-LYP) = -1847.52939887

Zero-point correction= 0.529713 (Hartree/Particle)
Thermal correction to Energy= 0.566732
Thermal correction to Enthalpy= 0.567676
Thermal correction to Gibbs Free Energy= 0.454454
Sum of electronic and zero-point Energies= -1846.999686
Sum of electronic and thermal Energies= -1846.962667
Sum of electronic and thermal Enthalpies= -1846.961723
Sum of electronic and thermal Free Energies= -1847.074945

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	355.630	135.398	238.296

C,0,-2.8586555812,-0.9756233803,2.7353900821
C,0,-1.8136481896,-1.0672729407,1.8068405887
N,0,-0.7748621611,-0.1962494568,1.8446936812
C,0,-0.7376520637,0.746543384,2.8028743407
C,0,-1.7426351965,0.881686112,3.7561597972
C,0,-2.8270568467,0.0089996434,3.7164666727
C,0,-1.7643893405,-2.1170272436,0.7604240537
N,0,-0.7061402179,-2.0765656984,-0.0796728424
C,0,-0.5844776426,-3.0182236778,-1.0284158945
C,0,-1.5153999252,-4.0401514454,-1.1949565033
C,0,-2.6141317394,-4.0888965806,-0.3399044097
C,0,-2.7377126547,-3.1198605244,0.6492845875
Ir,0,0.771238413,-0.3471022342,0.2303679991
B,0,1.9904722928,1.2281712413,0.7085187249
O,0,2.921080121,1.8271778238,-0.1389585427
C,0,3.6154706226,2.8588951641,0.5621196585
C,0,2.7788170213,3.0925301409,1.8374146769
O,0,1.9168932703,1.9514361446,1.9096608346
C,0,-0.5611925175,0.9471693545,-1.0125198475
C,0,-0.738743618,2.3035916275,-0.6771445457

C,0,-1.7396139189,3.0737033612,-1.2689593254
C,0,-2.5960174142,2.5363405567,-2.2470500754
C,0,-2.3979160505,1.1923283301,-2.6094200353
C,0,-1.4011118184,0.4206976602,-2.0124888869
B,0,1.8625867816,-1.5581651195,1.6152182895
O,0,2.5353783008,-1.1053178368,2.7417571949
C,0,3.1820076957,-2.207466358,3.3882104956
C,0,2.6127897279,-3.4616083614,2.689245206
O,0,1.9125655008,-2.9535309223,1.5464079852
B,0,2.3601269936,-1.1442868788,-0.8442287232
O,0,2.1598645185,-1.9035354009,-2.0087188357
C,0,3.4120702835,-2.4760251037,-2.4095463166
C,0,4.4601931678,-1.6789656584,-1.6115127714
O,0,3.7158326766,-1.080291359,-0.5475508289
H,0,0.9365784902,0.2941345712,-1.2400746963
H,0,0.2939121495,-2.9284933828,-1.6589214938
H,0,-3.5818760203,-3.1495500153,1.326806026
H,0,-1.3737199823,-4.7764177541,-1.9788573101
H,0,-3.3626975917,-4.869367515,-0.4365611099
H,0,-3.692820794,-1.6645591449,2.6929455038
H,0,-3.6347147739,0.0875848926,4.4377799855
H,0,-1.6668307782,1.6601389386,4.5075514064
H,0,0.1348464216,1.3905773383,2.785786789
H,0,3.4211133894,-3.5431092078,-2.151031438
H,0,3.5300984155,-2.378858019,-3.493264352
H,0,5.2538228087,-2.3101652055,-1.1989314487
H,0,4.9239219844,-0.8885476558,-2.2155392409
H,0,-0.0963357778,2.7627958864,0.0689057929
H,0,-1.8590843346,4.1136021478,-0.9733991965
B,0,-3.6980797909,3.3926092512,-2.9117664587
H,0,-1.27151068,-0.6081798334,-2.3371357007
H,0,-3.0308462723,0.7502523901,-3.3755597069
H,0,1.9097329407,-4.0120981721,3.3276394633
H,0,3.3934160248,-4.1572861847,2.3631428562
H,0,2.9652289837,-2.1830800325,4.4616086543
H,0,4.2668655926,-2.1148880301,3.2549385952
H,0,2.1698071751,4.0042598578,1.7721307358
H,0,3.3892579095,3.1508023226,2.7445425731
H,0,3.6876894989,3.7516467302,-0.0681297667
H,0,4.6324760665,2.5178977323,0.7954661946
O,0,-4.5819025838,2.9030038842,-3.8511427077
O,0,-3.9037441955,4.7270461269,-2.6301073501
C,0,-5.4011297651,3.9859638883,-4.3046848385
C,0,-5.042682317,5.1734565963,-3.3738967403

H,0,-5.168734481,4.1962227345,-5.3556160724
H,0,-6.4559629339,3.6994095468,-4.2376923047
H,0,-4.7840997583,6.0818178637,-3.9280020365
H,0,-5.8542385891,5.4157779,-2.6770814747

bpy Bpin3 Meta PhenylBPin CH Activation Transition Structure
E(RB+HF-LYP) = -1847.52860836

Zero-point correction= 0.529596 (Hartree/Particle)
Thermal correction to Energy= 0.566664
Thermal correction to Enthalpy= 0.567608
Thermal correction to Gibbs Free Energy= 0.453681
Sum of electronic and zero-point Energies= -1846.999012
Sum of electronic and thermal Energies= -1846.961945
Sum of electronic and thermal Enthalpies= -1846.961000
Sum of electronic and thermal Free Energies= -1847.074927

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	355.587	135.472	239.780

C,0,-2.9398723002,-0.5689183751,2.8335411284
C,0,-1.8890357345,-0.6519329291,1.9105477942
N,0,-0.8508042867,0.2192338466,1.9624291807
C,0,-0.822461034,1.1562866513,2.9269450643
C,0,-1.8342789081,1.2835107186,3.8740331266
C,0,-2.9162352523,0.4082236068,3.8220076143
C,0,-1.836025345,-1.689757426,0.8526803375
N,0,-0.7727051123,-1.6427128346,0.0193595399
C,0,-0.6508746015,-2.5699933511,-0.9430837856
C,0,-1.5855854437,-3.5849366733,-1.1294929277
C,0,-2.6881794632,-3.641613936,-0.2803792205
C,0,-2.8126748526,-2.6866314217,0.7223714785
Ir,0,0.710118975,0.0732594362,0.3615893281
B,0,1.9270641094,1.6449451338,0.8571953358
O,0,2.8847645295,2.2307954517,0.0306442152
C,0,3.5681200863,3.2633466142,0.7408994851
C,0,2.7053097674,3.5086476268,1.9968961413
O,0,1.8269761486,2.379454665,2.0505250016
C,0,-0.6049427663,1.3823180587,-0.8923919203
C,0,-0.7824376332,2.735582832,-0.5474424423
C,0,-1.7754297022,3.5187456195,-1.1449469671
C,0,-2.6018865498,2.9760184401,-2.1263168628
C,0,-2.4374151235,1.6385877251,-2.5264233724

C,0,-1.4336936355,0.8703958105,-1.9039876176
B,0,1.7812266328,-1.1458361056,1.7516275831
O,0,2.451018921,-0.6983772394,2.8827887365
C,0,3.0926277415,-1.8053890558,3.5259127049
C,0,2.5045043147,-3.0542210347,2.8344083882
O,0,1.8193308359,-2.5418407356,1.6844598034
B,0,2.310529446,-0.7231406664,-0.6952978384
O,0,2.1234077008,-1.4662807315,-1.872204295
C,0,3.3746980559,-2.0512008493,-2.2560516917
C,0,4.4181811722,-1.2793439213,-1.4274633199
O,0,3.6616016879,-0.6805455875,-0.3723233753
H,0,0.8932120493,0.7115578178,-1.1069237282
H,0,0.2307833063,-2.4745674479,-1.568088843
H,0,-3.6608643156,-2.7221924191,1.3946405833
H,0,-1.4444356291,-4.3082683276,-1.9252832896
H,0,-3.440023777,-4.4168879919,-0.3924435474
H,0,-3.7724244271,-1.2591296503,2.7808961447
H,0,-3.7282683333,0.4798043172,4.5391559364
H,0,-1.7653311344,2.057438094,4.6307773494
H,0,0.0479794765,1.8033975302,2.919910472
H,0,3.3638848292,-3.1216194063,-2.0116543182
H,0,3.5152285885,-1.941917828,-3.3359693986
H,0,5.1930788027,-1.9275879456,-1.0056851675
H,0,4.9069692228,-0.4901389949,-2.0130756917
H,0,-0.1480828518,3.1868914382,0.2105762167
H,0,-1.8955340125,4.5568486638,-0.842929733
H,0,-3.3695774081,3.5857766042,-2.595059368
H,0,-1.3013568757,-0.1558937584,-2.2340882061
B,0,-3.331481675,1.0261873747,-3.6321463231
H,0,1.7881881435,-3.5863523532,3.4738994479
H,0,3.2735601932,-3.7669741888,2.5178896278
H,0,2.8865156015,-1.7768744758,4.6012445633
H,0,4.177063304,-1.7243086396,3.3812179415
H,0,2.1103894073,4.4286942876,1.9183745781
H,0,3.2963927201,3.5594464386,2.91727228
H,0,3.6583282611,4.1523290725,0.1074453036
H,0,4.5784558293,2.9196564717,0.9979864932
O,0,-3.2576335541,-0.2907275372,-4.0373589369
O,0,-4.2924601972,1.7407046698,-4.3167805473
C,0,-4.1596889391,-0.4723993657,-5.1345359198
H,0,-3.5808493203,-0.6472076091,-6.0495648117
H,0,-4.7866140065,-1.3515188601,-4.9519758727
C,0,-4.9758430616,0.8434160512,-5.1986601727
H,0,-5.0086318114,1.2732179059,-6.2050602266

H,0,-6.0066570126,0.7110667646,-4.8476849032

bpy Bpin3 2Pyrrole CH Activation Transition Structure
E(RB+HF-LYP) = -1572.03532752

Zero-point correction= 0.451410 (Hartree/Particle)
Thermal correction to Energy= 0.481894
Thermal correction to Enthalpy= 0.482838
Thermal correction to Gibbs Free Energy= 0.387151
Sum of electronic and zero-point Energies= -1571.583917
Sum of electronic and thermal Energies= -1571.553433
Sum of electronic and thermal Enthalpies= -1571.552489
Sum of electronic and thermal Free Energies= -1571.648177

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	302.393	113.804	201.391

C,0,-2.4040211185,1.50070161,-3.5863334747
C,0,-1.8596726823,2.6667746142,-3.0891314073
N,0,-0.9546810249,2.3209446222,-2.1138160341
C,0,-0.918191193,0.9510913236,-1.9366414536
C,0,-1.805193865,0.4221133499,-2.872054319
Ir,0,0.2133932144,0.0614033533,-0.2750709866
N,0,-1.4071373638,-1.5710288919,-0.2230811591
C,0,-2.5231459427,-1.2723782517,0.4808771087
C,0,-3.6267031938,-2.1365588519,0.4909990466
C,0,-3.5763728209,-3.3243662403,-0.2292051597
C,0,-2.4186860138,-3.6263396822,-0.941387582
C,0,-1.3589816782,-2.7231318715,-0.9110507294
C,0,-2.5077500252,0.0022272177,1.2371526037
N,0,-1.4111781348,0.7856355549,1.0944246405
C,0,-1.3423523838,1.9486448777,1.7646192935
C,0,-2.3551614379,2.3896089535,2.6096300432
C,0,-3.4847851881,1.5914783477,2.7722698166
C,0,-3.5587898711,0.3887419276,2.08028725
B,0,1.1259226554,-0.643778313,1.5193234963
O,0,1.3345563046,-1.9784496361,1.8650116037
C,0,1.830685395,-2.0549678996,3.2072817548
C,0,2.1103734335,-0.5896923293,3.6065070973
O,0,1.4935778871,0.1908548521,2.5743549885
B,0,1.78317918,-1.1480161213,-0.9160172821
O,0,3.1412880243,-1.035385642,-0.6709345546
C,0,3.8411626501,-2.0575097287,-1.3826314153

C,0,2.7426118558,-3.0447224606,-1.8183057318
O,0,1.5325593733,-2.2866585969,-1.7015032397
B,0,1.4795539577,1.6712983036,-0.1334179914
O,0,0.9585037063,2.9911897227,-0.0098580713
C,0,2.041368166,3.9335117257,-0.0400001157
C,0,3.2990447855,3.0628741668,0.1381511599
O,0,2.8626508897,1.7351154389,-0.1457493942
H,0,0.5371041796,0.1311234991,-1.8552630445
H,0,-0.43138134,-2.9047541878,-1.4419854392
H,0,-4.5220302619,-1.8837664037,1.0448135893
H,0,-2.3287549889,-4.5414942673,-1.5167735657
H,0,-4.4276018348,-3.9983156576,-0.2326491639
H,0,-4.427371636,-0.2459007094,2.2008934467
H,0,-4.2957901925,1.8967688836,3.4263019843
H,0,-2.2497743065,3.3383495577,3.1244521284
H,0,-0.4496994125,2.5347186193,1.5885924074
H,0,2.6873647147,-3.9183853563,-1.1559556384
H,0,2.8594913881,-3.3942066476,-2.8490647633
H,0,4.5910437528,-2.5150679267,-0.7293532301
H,0,4.3584031323,-1.6104871436,-2.2417296111
H,0,-0.4307562655,2.9487559898,-1.5174861831
H,0,-2.0451964363,3.7011522336,-3.3431612576
H,0,-3.1388376924,1.4306122686,-4.3777605807
H,0,-1.9875173757,-0.6320737429,-3.0344809219
H,0,1.0703605859,-2.5228955239,3.8457560416
H,0,2.7294911234,-2.6801135243,3.2323360229
H,0,1.678941223,-0.3235517454,4.5774932303
H,0,3.183580196,-0.3650338536,3.6327809597
H,0,2.0332660066,4.458810387,-1.003903911
H,0,1.9114217593,4.6728992476,0.7570554412
H,0,4.1085001286,3.3413468248,-0.5445770874
H,0,3.6844400299,3.1051387301,1.1652284921

bpy Bpin3 3Pyrrole CH Activation Transition Structure
E(RB+HF-LYP) = -1572.02768754

Zero-point correction= 0.450991 (Hartree/Particle)
Thermal correction to Energy= 0.482539
Thermal correction to Enthalpy= 0.483483
Thermal correction to Gibbs Free Energy= 0.384732
Sum of electronic and zero-point Energies= -1571.576696
Sum of electronic and thermal Energies= -1571.545148
Sum of electronic and thermal Enthalpies= -1571.544204
Sum of electronic and thermal Free Energies= -1571.642956

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	302.798	116.303	207.840

C,0,2.3317884728,-1.7710620075,-3.4712886288
N,0,1.2063975343,-2.5459665342,-3.6242450192
C,0,0.2325177547,-2.1180623737,-2.7491548499
C,0,0.7296274915,-1.0627990941,-1.9973255016
C,0,2.0650250023,-0.8421470895,-2.4881900031
Ir,0,-0.1889807531,-0.0562544916,-0.2579936462
N,0,1.5565827737,1.4124570288,-0.1726544688
C,0,2.6335133678,1.0229492277,0.5468983049
C,0,3.7589046294,1.8509295879,0.6661499283
C,0,3.7694024563,3.0883991721,0.0322584393
C,0,2.6520334751,3.4776241826,-0.7041277962
C,0,1.5656365422,2.6102364444,-0.7781269012
C,0,2.5412826767,-0.3059445449,1.1996241043
N,0,1.3765168844,-0.983193596,1.0435113071
C,0,1.2222114837,-2.179375101,1.6376697422
C,0,2.2252830139,-2.7669565552,2.4025244189
C,0,3.4321943199,-2.0897446034,2.5617293329
C,0,3.5880299883,-0.8475498034,1.9578057053
B,0,-0.9427209049,0.7712289624,1.5688435804
O,0,-0.7917886423,2.1133199947,1.9362960061
C,0,-1.2653915815,2.2959496989,3.2763854193
C,0,-1.9546374318,0.9608879082,3.6293049671
O,0,-1.5485880984,0.0581326484,2.5951276316
B,0,-1.705987222,1.2647740181,-0.7672652573
O,0,-3.0470599416,1.2100844558,-0.3980764671
C,0,-3.7592236933,2.2574388689,-1.0613505057
C,0,-2.6579116573,3.2131026045,-1.5549541363
O,0,-1.472857506,2.4087822531,-1.5482207313
B,0,-1.6214923365,-1.514608234,-0.2140049249
O,0,-1.7112308372,-2.5075753315,0.7733124814
C,0,-2.8652107593,-3.3166478061,0.5373876923
C,0,-3.308286271,-2.9455162618,-0.8939105587
O,0,-2.5862092202,-1.7522762266,-1.1990915305
H,0,-0.4766560069,0.0737461067,-1.8345458825
H,0,0.6605406455,2.8610293395,-1.3211008447
H,0,4.6178694828,1.5382381605,1.2469181068
H,0,2.6136667508,4.4349044737,-1.2128316631
H,0,4.6359243226,3.7373071092,0.1160407023
H,0,4.5188052045,-0.3066311147,2.0743950199

H,0,4.2396876225,-2.5171561917,3.1484156582
H,0,2.0529561603,-3.7354274917,2.8594649535
H,0,0.2558572571,-2.6489657861,1.490314719
H,0,-2.5210000312,4.0668823496,-0.8780987395
H,0,-2.8392232144,3.5943731311,-2.5650038792
H,0,-4.4563676989,2.7319728326,-0.3631288486
H,0,-4.3366758961,1.8315151932,-1.8923424241
H,0,-0.7495438541,-2.566168291,-2.743012442
H,0,1.1041114147,-3.2973363424,-4.2870374324
H,0,3.2169134407,-1.9454395763,-4.0668745508
H,0,2.7601874816,-0.0860063762,-2.1501019612
H,0,-0.4132319579,2.5116837522,3.9342521297
H,0,-1.9488042211,3.1511463898,3.3133313629
H,0,-1.6481693928,0.5674216658,4.6045181957
H,0,-3.0485678127,1.0458215068,3.6216753579
H,0,-2.6058200502,-4.3761571855,0.6423508863
H,0,-3.6328502361,-3.0745815853,1.2833904061
H,0,-3.0476520351,-3.727004547,-1.6215799884
H,0,-4.3847791352,-2.7576407718,-0.968681973

C^2-C^6 Enyne Allene Cyclization

B3LYP//6-31G unless otherwise noted**

4thmodelBirad
E(RB+HF-LYP) = -1508.41113773

Zero-point correction= .421551 (Hartree/Particle)
Thermal correction to Energy= .450543
Thermal correction to Enthalpy= .451487
Thermal correction to Gibbs Free Energy= .362131
Sum of electronic and zero-point Energies= -1507.989587
Sum of electronic and thermal Energies= -1507.960595
Sum of electronic and thermal Enthalpies= -1507.959651
Sum of electronic and thermal Free Energies= -1508.049006

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	282.720	107.748	188.065

C,0,1.6539169668,4.0971440398,-0.2658661267
C,0,0.3005816138,4.4561239005,-0.3263347307

C,0,-0.700814282,3.4874748172,-0.2984413978
C,0,-0.3276582525,2.137984796,-0.2083248019
C,0,1.0406100451,1.7781471122,-0.1548378762
C,0,2.0300858947,2.7513682577,-0.1808783841
C,0,-1.0944348903,0.9250526066,-0.1838564258
O,0,-2.4626198098,0.8782265636,-0.3587485322
C,0,1.1446268754,0.2934528202,-0.0950522578
C,0,2.2826554862,-0.3803431275,-0.0048539529
Si,0,4.0239637534,-0.9398645995,0.1332153692
C,0,-0.2754454185,-0.2379714769,-0.1379875518
C,0,-0.6461627289,-1.5834926435,-0.1400312942
C,0,0.4555990361,-2.6216209569,-0.1368893005
Si,0,-2.4327964278,-2.2512972558,-0.109670261
C,0,-3.3417078912,-1.7240299676,1.4742084938
C,0,-2.3861469507,-4.1494199587,-0.0436878843
C,0,-3.392582544,-1.8330980914,-1.6923532202
C,0,5.2236578095,0.5280322355,0.1737132174
C,0,4.4287736759,-2.0241500606,-1.3636041505
C,0,4.2096944189,-1.9338185033,1.7322443374
C,0,-3.2939403044,1.5820793165,0.4906602449
O,0,-2.9132658541,2.1263296798,1.4947642936
C,0,-4.7063752377,1.5523289963,-0.0323422951
H,0,2.4171782207,4.8691506832,-0.2873075001
H,0,0.0270897799,5.5050843529,-0.3926046416
H,0,-1.7440700362,3.779210062,-0.3324369625
H,0,3.0782770004,2.473489747,-0.1420588332
H,0,0.0743619149,-3.6399023288,-0.2192088603
H,0,1.1579610077,-2.4596156962,-0.9647861138
H,0,1.0511760775,-2.5663334921,0.7852674222
H,0,-4.418741771,-1.9105231532,1.3866451576
H,0,-2.978284056,-2.3297126865,2.3120628469
H,0,-3.1968778932,-0.678601915,1.753097609
H,0,-3.4155621051,-4.5230965229,0.0139708353
H,0,-1.9321592955,-4.5944073878,-0.9354479584
H,0,-1.8542673391,-4.5319273836,0.8337836759
H,0,-4.4155424695,-2.2239950783,-1.630519031
H,0,-3.4409811467,-0.7614772116,-1.8902358603
H,0,-2.9138824707,-2.3127088381,-2.5536040109
H,0,6.2547632784,0.1677674097,0.2708746513
H,0,5.1653894972,1.1219915529,-0.7441604976
H,0,5.0224672289,1.1910672346,1.0212911033
H,0,5.4707007907,-2.3617654923,-1.3213464175
H,0,3.7905498586,-2.9126193635,-1.4001619439
H,0,4.2934459978,-1.4755098799,-2.3012591177

H,0,5.244384507,-2.273761817,1.8558958454
H,0,3.9489026127,-1.3308674344,2.6079337021
H,0,3.5645818978,-2.8181158947,1.7304218596
H,0,-4.7524170736,2.0455001385,-1.0080099582
H,0,-5.0374265317,0.5200797958,-0.1718618633
H,0,-5.359874662,2.0639519537,0.6730993973

4thmodelBiradTS – UB3LYP//6-31G**
E(UB+HF-LYP) = -1508.44206941

Zero-point correction= 0.419118 (Hartree/Particle)
Thermal correction to Energy= 0.448695
Thermal correction to Enthalpy= 0.449640
Thermal correction to Gibbs Free Energy= 0.359101
Sum of electronic and zero-point Energies= -1508.022952
Sum of electronic and thermal Energies= -1507.993374
Sum of electronic and thermal Enthalpies= -1507.992430
Sum of electronic and thermal Free Energies= -1508.082968

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	281.561	109.541	190.554

C,0,-0.3603628844,-0.1757387289,-0.3808474133
C,0,-1.0924849276,1.0051729517,-0.3544794447
C,0,-0.258193296,2.1588671423,-0.0955360613
C,0,1.0765534863,1.6977957342,0.0380192017
C,0,1.1023403682,0.2253274449,-0.1429044376
C,0,2.1112621468,2.5936936283,0.2804608763
C,0,1.8211285416,3.9587836298,0.3694260491
C,0,0.5049313664,4.4154721985,0.232919485
C,0,-0.5445177142,3.5258046211,0.0031760183
O,0,-2.407668887,1.0623279916,-0.7917758086
C,0,-3.3541591698,1.7465212113,-0.0690768403
C,0,-4.6562565448,1.7867220017,-0.8274091608
C,0,2.1222118506,-0.6159440102,-0.0437987884
Si,0,3.905754453,-1.0751828527,0.0845564319
C,0,4.1686485624,-1.9379850067,1.7471813237
C,0,-0.7456990384,-1.5278776081,-0.4831952089
Si,0,-2.3819299574,-2.2446162639,0.159277691
C,0,-3.7091151965,-2.1345472333,-1.1921633469
C,0,5.1010821799,0.3928423766,-0.046447881
C,0,4.2787113316,-2.270614033,-1.3357622663
C,0,0.3243052018,-2.4297659491,-0.9134561725

C,0,-2.9370562707,-1.3919387362,1.7549600208
C,0,-2.1242325782,-4.0805088551,0.5604133412
O,0,-3.153317787,2.2220100946,1.0213884916
H,0,2.6243214969,4.6695661288,0.5390532308
H,0,0.2946427608,5.4780184363,0.3128804029
H,0,-1.562342767,3.8893242249,-0.0637565764
H,0,3.1311655461,2.2415677277,0.3810555282
H,0,0.1518146355,-3.4950241026,-0.7544809883
H,0,0.6893150365,-2.256141302,-1.9321839964
H,0,1.273718043,-2.0441943389,-0.3055357493
H,0,-3.9312068494,-1.747440661,2.050158514
H,0,-2.2461611725,-1.6436197446,2.5673247582
H,0,-2.9744373069,-0.3018508934,1.6921842809
H,0,-3.0459295014,-4.4930875741,0.9867533544
H,0,-1.881474273,-4.6761209059,-0.3255992173
H,0,-1.328213697,-4.2321270098,1.2972739421
H,0,-4.6825590638,-2.4691471788,-0.8147128003
H,0,-3.8143210534,-1.1143549841,-1.5695458487
H,0,-3.4453486763,-2.7738138857,-2.0416980821
H,0,6.1328054422,0.0243640478,-0.0979555882
H,0,4.9173772826,0.9895267596,-0.9455654722
H,0,5.033759884,1.0553872653,0.8224250411
H,0,5.3212105443,-2.605594621,-1.2901245537
H,0,3.6404040941,-3.1588495225,-1.2935979444
H,0,4.1255252669,-1.7932249463,-2.3092037726
H,0,5.2112084067,-2.2590564999,1.8530119115
H,0,3.9388917657,-1.2693319844,2.5830990997
H,0,3.5329710425,-2.823718636,1.8436669056
H,0,-4.4951463778,2.1419457395,-1.8483785116
H,0,-5.0775418113,0.7788694994,-0.8926036699
H,0,-5.3546827338,2.4381152274,-0.3033991467

4thmodelBiradUB
E(UB+HF-LYP) = -1508.44810618

Zero-point correction= .422109 (Hartree/Particle)
Thermal correction to Energy= .452698
Thermal correction to Enthalpy= .453643
Thermal correction to Gibbs Free Energy= .359205
Sum of electronic and zero-point Energies= -1508.025997
Sum of electronic and thermal Energies= -1507.995408
Sum of electronic and thermal Enthalpies= -1507.994464
Sum of electronic and thermal Free Energies= -1508.088901

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	284.073	111.608	198.761

C,0,1.6539169668,4.0971440398,-0.2658661267
C,0,0.3005816138,4.4561239005,-0.3263347307
C,0,-0.700814282,3.4874748172,-0.2984413978
C,0,-0.3276582525,2.137984796,-0.2083248019
C,0,1.0406100451,1.7781471122,-0.1548378762
C,0,2.0300858947,2.7513682577,-0.1808783841
C,0,-1.0944348903,0.9250526066,-0.1838564258
O,0,-2.4626198098,0.8782265636,-0.3587485322
C,0,1.1446268754,0.2934528202,-0.0950522578
C,0,2.2826554862,-0.3803431275,-0.0048539529
Si,0,4.0239637534,-0.9398645995,0.1332153692
C,0,-0.2754454185,-0.2379714769,-0.1379875518
C,0,-0.6461627289,-1.5834926435,-0.1400312942
C,0,0.4555990361,-2.6216209569,-0.1368893005
Si,0,-2.4327964278,-2.2512972558,-0.109670261
C,0,-3.3417078912,-1.7240299676,1.4742084938
C,0,-2.3861469507,-4.1494199587,-0.0436878843
C,0,-3.392582544,-1.8330980914,-1.6923532202
C,0,5.2236578095,0.5280322355,0.1737132174
C,0,4.4287736759,-2.0241500606,-1.3636041505
C,0,4.2096944189,-1.9338185033,1.7322443374
C,0,-3.2939403044,1.5820793165,0.4906602449
O,0,-2.9132658541,2.1263296798,1.4947642936
C,0,-4.7063752377,1.5523289963,-0.0323422951
H,0,2.4171782207,4.8691506832,-0.2873075001
H,0,0.0270897799,5.5050843529,-0.3926046416
H,0,-1.7440700362,3.779210062,-0.3324369625
H,0,3.0782770004,2.473489747,-0.1420588332
H,0,0.0743619149,-3.6399023288,-0.2192088603
H,0,1.1579610077,-2.4596156962,-0.9647861138
H,0,1.0511760775,-2.5663334921,0.7852674222
H,0,-4.418741771,-1.9105231532,1.3866451576
H,0,-2.978284056,-2.3297126865,2.3120628469
H,0,-3.1968778932,-0.678601915,1.753097609
H,0,-3.4155621051,-4.5230965229,0.0139708353
H,0,-1.9321592955,-4.5944073878,-0.9354479584
H,0,-1.8542673391,-4.5319273836,0.8337836759
H,0,-4.4155424695,-2.2239950783,-1.630519031
H,0,-3.4409811467,-0.7614772116,-1.8902358603
H,0,-2.9138824707,-2.3127088381,-2.5536040109

H,0,6.2547632784,0.1677674097,0.2708746513
H,0,5.1653894972,1.1219915529,-0.7441604976
H,0,5.0224672289,1.1910672346,1.0212911033
H,0,5.4707007907,-2.3617654923,-1.3213464175
H,0,3.7905498586,-2.9126193635,-1.4001619439
H,0,4.2934459978,-1.4755098799,-2.3012591177
H,0,5.244384507,-2.273761817,1.8558958454
H,0,3.9489026127,-1.3308674344,2.6079337021
H,0,3.5645818978,-2.8181158947,1.7304218596
H,0,-4.7524170736,2.0455001385,-1.0080099582
H,0,-5.0374265317,0.5200797958,-0.1718618633
H,0,-5.359874662,2.0639519537,0.6730993973

4thmodelBiradUB – B3LYP//6-31G**
E(UB+HF-LYP) = -1508.44810618

Zero-point correction= .422109 (Hartree/Particle)
Thermal correction to Energy= .452698
Thermal correction to Enthalpy= .453643
Thermal correction to Gibbs Free Energy= .359205
Sum of electronic and zero-point Energies= -1508.025997
Sum of electronic and thermal Energies= -1507.995408
Sum of electronic and thermal Enthalpies= -1507.994464
Sum of electronic and thermal Free Energies= -1508.088901

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	284.073	111.608	198.761

C,0,1.6539169668,4.0971440398,-0.2658661267
C,0,0.3005816138,4.4561239005,-0.3263347307
C,0,-0.700814282,3.4874748172,-0.2984413978
C,0,-0.3276582525,2.137984796,-0.2083248019
C,0,1.0406100451,1.7781471122,-0.1548378762
C,0,2.0300858947,2.7513682577,-0.1808783841
C,0,-1.0944348903,0.9250526066,-0.1838564258
O,0,-2.4626198098,0.8782265636,-0.3587485322
C,0,1.1446268754,0.2934528202,-0.0950522578
C,0,2.2826554862,-0.3803431275,-0.0048539529
Si,0,4.0239637534,-0.9398645995,0.1332153692
C,0,-0.2754454185,-0.2379714769,-0.1379875518
C,0,-0.6461627289,-1.5834926435,-0.1400312942
C,0,0.4555990361,-2.6216209569,-0.1368893005
Si,0,-2.4327964278,-2.2512972558,-0.109670261

C,0,-3.3417078912,-1.7240299676,1.4742084938
C,0,-2.3861469507,-4.1494199587,-0.0436878843
C,0,-3.392582544,-1.8330980914,-1.6923532202
C,0,5.2236578095,0.5280322355,0.1737132174
C,0,4.4287736759,-2.0241500606,-1.3636041505
C,0,4.2096944189,-1.9338185033,1.7322443374
C,0,-3.2939403044,1.5820793165,0.4906602449
O,0,-2.9132658541,2.1263296798,1.4947642936
C,0,-4.7063752377,1.5523289963,-0.0323422951
H,0,2.4171782207,4.8691506832,-0.2873075001
H,0,0.0270897799,5.5050843529,-0.3926046416
H,0,-1.7440700362,3.779210062,-0.3324369625
H,0,3.0782770004,2.473489747,-0.1420588332
H,0,0.0743619149,-3.6399023288,-0.2192088603
H,0,1.1579610077,-2.4596156962,-0.9647861138
H,0,1.0511760775,-2.5663334921,0.7852674222
H,0,-4.418741771,-1.9105231532,1.3866451576
H,0,-2.978284056,-2.3297126865,2.3120628469
H,0,-3.1968778932,-0.678601915,1.753097609
H,0,-3.4155621051,-4.5230965229,0.0139708353
H,0,-1.9321592955,-4.5944073878,-0.9354479584
H,0,-1.8542673391,-4.5319273836,0.8337836759
H,0,-4.4155424695,-2.2239950783,-1.630519031
H,0,-3.4409811467,-0.7614772116,-1.8902358603
H,0,-2.9138824707,-2.3127088381,-2.5536040109
H,0,6.2547632784,0.1677674097,0.2708746513
H,0,5.1653894972,1.1219915529,-0.7441604976
H,0,5.0224672289,1.1910672346,1.0212911033
H,0,5.4707007907,-2.3617654923,-1.3213464175
H,0,3.7905498586,-2.9126193635,-1.4001619439
H,0,4.2934459978,-1.4755098799,-2.3012591177
H,0,5.244384507,-2.273761817,1.8558958454
H,0,3.9489026127,-1.3308674344,2.6079337021
H,0,3.5645818978,-2.8181158947,1.7304218596
H,0,-4.7524170736,2.0455001385,-1.0080099582
H,0,-5.0374265317,0.5200797958,-0.1718618633
H,0,-5.359874662,2.0639519537,0.6730993973

4thmodelProd

E(RB+HF-LYP) = -1508.52060319

Zero-point correction=	0.424179 (Hartree/Particle)
Thermal correction to Energy=	0.454476
Thermal correction to Enthalpy=	0.455420

Thermal correction to Gibbs Free Energy= 0.361547
Sum of electronic and zero-point Energies= -1508.096424
Sum of electronic and thermal Energies= -1508.066127
Sum of electronic and thermal Enthalpies= -1508.065183
Sum of electronic and thermal Free Energies= -1508.159056

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	285.188	110.412	197.572

C,0,0.802706903,-3.8579444049,1.524104052
C,0,-0.5766901022,-4.0421499814,1.4110003259
C,0,-1.3852852048,-3.0427982366,0.85967805
C,0,-0.7833242367,-1.865257522,0.4292858414
C,0,0.6126131712,-1.6638533505,0.5438827869
C,0,1.4037877491,-2.667963252,1.0924613064
C,0,-1.3410470906,-0.6543328004,-0.1653530045
O,0,-2.6992313737,-0.4424587385,-0.3566064295
C,0,0.9268752682,-0.3090021379,0.0167157249
C,0,2.1072239861,0.350371811,-0.0540639135
Si,0,3.891286891,-0.0686400449,0.4098675664
C,0,-0.3813403607,0.2699927943,-0.424561927
C,0,-0.5679176752,1.623144751,-0.9892765831
C,0,0.0683093552,1.971054167,-2.1229545622
Si,0,-1.646778472,2.9149965902,-0.0800768442
C,0,-3.3110579804,3.1265727847,-0.9593216449
C,0,-0.7313323207,4.5742741406,-0.1013218634
C,0,-1.9277547211,2.3706021371,1.7062293459
C,0,4.5533709361,-1.5382778209,-0.5868473592
C,0,4.0828198974,-0.3533502029,2.2744197744
C,0,4.9047786469,1.4608571756,-0.0565726303
C,0,-3.3529089846,-1.206987531,-1.2989935818
O,0,-2.8038101834,-2.0292338757,-1.9855249117
C,0,-4.8154214006,-0.8433478096,-1.3368522678
H,0,1.4189916506,-4.6440052039,1.9499384217
H,0,-1.0264450054,-4.9702491387,1.7512384139
H,0,-2.4563287609,-3.1892132713,0.7670971234
H,0,2.4752699267,-2.548239529,1.1910045313
H,0,2.015483434,1.3540417141,-0.4755729192
H,0,-0.0188509172,2.9680174499,-2.548816177
H,0,0.6869381625,1.2699602618,-2.6799696581
H,0,-3.9025102353,3.9188749254,-0.4862894369
H,0,-3.1751805761,3.3948675522,-2.012286246
H,0,-3.8951167279,2.202571003,-0.9186456169

H,0,-1.3158196375,5.3421227292,0.4182993856
H,0,0.2398560759,4.4994534552,0.3987091862
H,0,-0.5533388845,4.9338680905,-1.1202429947
H,0,-2.5070042122,3.1236143408,2.2522519724
H,0,-2.478959715,1.426648554,1.7484644802
H,0,-0.9808978015,2.2292287721,2.2377974417
H,0,5.592866195,-1.7484190904,-0.3095293734
H,0,3.975874461,-2.45522017,-0.4422624962
H,0,4.5372438118,-1.3075959676,-1.6574562697
H,0,5.1274276072,-0.5773680239,2.5198263857
H,0,3.8002328919,0.5494666326,2.826533389
H,0,3.4664745116,-1.1735103108,2.6519183189
H,0,5.9640587722,1.319017405,0.1840396882
H,0,4.8356130688,1.6749986523,-1.1287721911
H,0,4.5603200901,2.3501975995,0.4826401889
H,0,-5.23099601,-0.8075661013,-0.326924031
H,0,-4.9338836181,0.151382505,-1.7781918994
H,0,-5.3505389795,-1.572023825,-1.9447662194

4thmodelSM

E(RB+HF-LYP) = -1508.47276852

Zero-point correction= 0.421576 (Hartree/Particle)
Thermal correction to Energy= 0.453560
Thermal correction to Enthalpy= 0.454504
Thermal correction to Gibbs Free Energy= 0.355897
Sum of electronic and zero-point Energies= -1508.051192
Sum of electronic and thermal Energies= -1508.019209
Sum of electronic and thermal Enthalpies= -1508.018264
Sum of electronic and thermal Free Energies= -1508.116872

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	284.613	113.716	207.536

C,0,-2.381237053,3.8838974659,0.8784074189
C,0,-1.1139896079,4.394352073,1.1646422089
C,0,0.0087178244,3.6333532255,0.8661173775
C,0,-0.0999639271,2.3524772398,0.2853216257
C,0,-1.3915867486,1.8219137792,0.0168904489
C,0,-2.5101189914,2.620689041,0.3113634075
C,0,1.126968058,1.6919640061,-0.0311280471
C,0,2.2517597976,1.2748865583,-0.2678913809
Si,0,3.9874711281,0.7597197133,-0.5919329434

C,0,-1.6117159588,0.4784812084,-0.5471703868
O,0,-2.83777568,0.3819338562,-1.2658908838
C,0,-0.8269237868,-0.5774647564,-0.4717212409
C,0,-0.1514492732,-1.6905548896,-0.3692993334
Si,0,-0.4940825427,-2.8288997709,1.1338213691
C,0,-1.590934547,-4.2593477488,0.5611642383
C,0,0.8803274976,-2.1000904202,-1.4064212001
C,0,1.1746732275,-3.4996081059,1.7339226752
C,0,-1.3314230918,-1.8483546376,2.5056910565
C,0,4.1513610487,0.1720431702,-2.3804725239
C,0,4.4654858131,-0.6250714264,0.6029427901
C,0,5.1059709855,2.2572322487,-0.3085098877
H,0,1.8677317308,-2.2096405217,-0.9449242989
H,0,0.9548645679,-1.3686028947,-2.2143595893
H,0,0.6214881608,-3.0735197041,-1.840145936
C,0,-3.750460547,-0.5811498215,-0.9523738952
H,0,-3.497370418,2.2334521166,0.0911384228
H,0,-3.2706222086,4.4668324381,1.098637561
H,0,1.002578174,4.0207653569,1.0636789282
H,0,-1.0009146497,5.3788686821,1.6078695373
H,0,-1.7564587909,-4.9715533126,1.377715673
H,0,-2.5641810772,-3.8777156518,0.2387977372
H,0,-1.1437223322,-4.8114974055,-0.2725728025
H,0,-1.5395950211,-2.4904723579,3.3689822147
H,0,-0.7016045388,-1.0202965629,2.8467978726
H,0,-2.2776505455,-1.4359771272,2.1465004011
H,0,1.0317126338,-4.1362793821,2.6145448093
H,0,1.6759792548,-4.1050301207,0.9711264264
H,0,1.8530276441,-2.6888096295,2.0205047619
H,0,6.1561504282,1.9959604944,-0.481914884
H,0,4.8482630911,3.0774992118,-0.98608054
H,0,5.0189144685,2.6305589199,0.7169093993
H,0,5.5016678338,-0.9410294031,0.4361118891
H,0,4.3806970522,-0.2922907544,1.6425049699
H,0,3.8247899935,-1.5042760609,0.4818784485
H,0,5.1864804237,-0.1146031614,-2.5987188231
H,0,3.5144993407,-0.6951169701,-2.5799157629
H,0,3.8682630796,0.9630179039,-3.0823553315
O,0,-3.640945492,-1.3763416571,-0.0489460096
C,0,-4.9145389043,-0.5074590035,-1.9119100644
H,0,-5.3187835871,0.5077527276,-1.9470135023
H,0,-4.5738557702,-0.7566825722,-2.9215252409
H,0,-5.6855506495,-1.2106662822,-1.5993068752

4thmodelTS
E(RB+HF-LYP) = -1508.43292752

Zero-point correction= 0.419670 (Hartree/Particle)
Thermal correction to Energy= 0.450177
Thermal correction to Enthalpy= 0.451121
Thermal correction to Gibbs Free Energy= 0.355928
Sum of electronic and zero-point Energies= -1508.013257
Sum of electronic and thermal Energies= -1507.982751
Sum of electronic and thermal Enthalpies= -1507.981806
Sum of electronic and thermal Free Energies= -1508.077000

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	282.490	110.692	200.351

C,0,-0.4751258211,-4.1084867277,-1.5235193383
C,0,0.9187294618,-4.1855869263,-1.4231797078
C,0,1.6551132187,-3.1158182929,-0.9124836929
C,0,0.9805251519,-1.9660585374,-0.498644357
C,0,-0.4247813102,-1.8858167413,-0.5932858489
C,0,-1.1519350879,-2.9562106857,-1.1168962606
C,0,1.527712036,-0.7368256148,0.0403223491
O,0,2.8766584599,-0.6493980482,0.3985117146
C,0,-0.9864523146,-0.6330650542,-0.0933518634
C,0,-2.0925998894,-0.0673611803,0.1636235584
Si,0,-3.8835582794,0.2026822773,0.4872777427
C,0,0.6638751773,0.2825803552,0.2015194641
C,0,0.5626384899,1.632058527,0.3545728016
C,0,-0.5263117772,2.1195014002,1.2098384812
Si,0,1.4646753171,2.8124490792,-0.8315566233
C,0,2.5345362297,3.9772891404,0.2127581174
C,0,0.179844496,3.8292590357,-1.7837444937
C,0,2.5430606502,1.8469416202,-2.0408860044
C,0,-4.8661902846,-1.3267496338,-0.0475818938
C,0,-4.4811802077,1.6998235831,-0.5007955188
C,0,-4.1245001728,0.4954157477,2.3394570554
C,0,3.2552238,-1.1722074285,1.6160725108
H,0,-2.232846325,-2.8926434938,-1.1878843913
H,0,-1.0366227965,-4.9527614339,-1.9119264516
H,0,2.7377051312,-3.1658599453,-0.8523633937
H,0,1.4329425118,-5.0853596364,-1.7481071163
H,0,-0.6694265907,3.2023967277,1.2196950481
H,0,-1.4523294508,1.5981802585,0.7580197248

H,0,-0.5111228746,1.7292576604,2.2320876321
H,0,3.0415381738,4.7139000726,-0.4210296755
H,0,1.9321162001,4.526559756,0.9440528732
H,0,3.3027820047,3.4241695805,0.762833153
H,0,3.1043438677,2.5348298729,-2.6834531146
H,0,3.2616451518,1.2099524471,-1.517178841
H,0,1.9391742433,1.2034757892,-2.6886000204
H,0,0.6724580441,4.5364484007,-2.4609628517
H,0,-0.4636014135,3.1817156248,-2.3882844147
H,0,-0.4645609855,4.4100619283,-1.1156578602
H,0,-5.9372077096,-1.1836877519,0.1387405213
H,0,-4.7400565239,-1.5279929419,-1.1166158195
H,0,-4.5465668717,-2.2168553678,0.5038025409
H,0,-5.1860352273,0.6405995155,2.5700290041
H,0,-3.7686552804,-0.3589203758,2.923949731
H,0,-3.584177733,1.3836545297,2.6818287887
H,0,-5.5526159029,1.8669894571,-0.3417218985
H,0,-3.9525657899,2.6120645844,-0.2065270089
H,0,-4.323160513,1.554412807,-1.5745155261
O,0,2.4869864586,-1.6651434902,2.4002757354
C,0,4.7445509382,-1.0160648922,1.7974503848
H,0,5.0149594323,0.043405845,1.7655920757
H,0,5.0385445855,-1.4461155368,2.7540329541
H,0,5.2781480596,-1.513091224,0.982294606

4threversedBiradUB – UB3LYP//6-31G**

E(UB+HF-LYP) = -1508.44236212

Zero-point correction= 0.421634 (Hartree/Particle)
Thermal correction to Energy= 0.452512
Thermal correction to Enthalpy= 0.453456
Thermal correction to Gibbs Free Energy= 0.358080
Sum of electronic and zero-point Energies= -1508.020728
Sum of electronic and thermal Energies= -1507.989850
Sum of electronic and thermal Enthalpies= -1507.988906
Sum of electronic and thermal Free Energies= -1508.084282

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	283.955	111.902	200.736

C,0,0.6706497456,0.5617933614,-0.0508663259
C,0,1.9803394816,0.0265118707,-0.1113639943
C,0,1.9850392522,-1.3911207182,-0.3457983778

C,0,0.6375954811,-1.8206566576,-0.402507794
C,0,-0.2440014597,-0.6423948226,-0.1527132665
C,0,0.3353221416,-3.1507743865,-0.6604026012
C,0,1.3839490877,-4.0579736271,-0.8596794949
C,0,2.7172510929,-3.6334207208,-0.800160533
C,0,3.0323885715,-2.2992351416,-0.5450273149
O,0,3.1211772299,0.8044525861,-0.1956163543
C,0,4.1177469375,0.6495545411,0.7407613312
C,0,5.2799258674,1.5467682833,0.3990673875
C,0,-1.5453879788,-0.7072107313,0.0957379306
Si,0,-3.2006760092,-1.4151101304,0.5019882209
C,0,-3.489591505,-1.1876506869,2.3577929036
C,0,0.3045953212,1.908367418,0.0796644973
Si,0,-1.347875112,2.679703107,-0.4518459864
C,0,-2.6091258022,2.6959027414,0.9655396672
C,0,-3.3002368474,-3.2658784408,0.0966756116
C,0,-4.5387334731,-0.523733898,-0.4924388157
C,0,1.3436317421,2.9057452153,0.5675490151
C,0,-2.0431046654,1.8960656344,-2.0300726846
C,0,-1.0142158735,4.4978027702,-0.8986657513
O,0,4.0373896851,-0.0905759007,1.6874928045
H,0,1.1596077103,-5.0999296867,-1.0672224704
H,0,3.5163783949,-4.3521977677,-0.9559379219
H,0,4.0667055807,-1.9774606162,-0.4937111955
H,0,-0.6945190032,-3.4829574467,-0.7231028292
H,0,0.8684420833,3.8001756595,0.9796718371
H,0,1.9739561347,2.4809794809,1.3536842587
H,0,2.008737457,3.2451651743,-0.2380463079
H,0,-2.9969177255,2.3676823587,-2.2942448412
H,0,-1.351400968,2.066311951,-2.862679449
H,0,-2.2075348853,0.8209087717,-1.9476635503
H,0,-1.9213191725,4.9309539729,-1.336244688
H,0,-0.7466572528,5.1134237061,-0.0342342966
H,0,-0.214965458,4.5979884088,-1.6408872546
H,0,-3.5436136602,3.1737588252,0.6486112791
H,0,-2.8437971133,1.6908534271,1.3227003028
H,0,-2.2191241508,3.2665553287,1.8157153801
H,0,-4.3037199126,-3.6367700794,0.3380145686
H,0,-3.1240482786,-3.4613348244,-0.9660412297
H,0,-2.5818279498,-3.8521045614,0.6776119128
H,0,-5.522636589,-0.9402171255,-0.2475884216
H,0,-4.5641984964,0.5478143777,-0.2763626886
H,0,-4.3855676423,-0.6450062619,-1.5695667252
H,0,-4.4573122824,-1.6143101303,2.6460495669

H,0,-2.7133901552,-1.6929800562,2.9412698068
H,0,-3.4906754305,-0.1326040532,2.6470999739
H,0,5.6358061295,1.3361851442,-0.6132486579
H,0,4.959459984,2.5927275158,0.420593062
H,0,6.081090325,1.3903013253,1.1202093536

4threversedTS – UB3LYP//6-31G**
E(UB+HF-LYP) = -1508.42134865

Zero-point correction= 0.419613 (Hartree/Particle)
Thermal correction to Energy= 0.450275
Thermal correction to Enthalpy= 0.451219
Thermal correction to Gibbs Free Energy= 0.356828
Sum of electronic and zero-point Energies= -1508.001736
Sum of electronic and thermal Energies= -1507.971074
Sum of electronic and thermal Enthalpies= -1507.970130
Sum of electronic and thermal Free Energies= -1508.064520

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	282.552	111.380	198.662

C,0,-0.1464490195,2.1318696514,-0.0118659322
C,0,0.4283195243,3.3803473591,0.2174726805
C,0,-0.3825956833,4.5193799793,0.2253174446
C,0,-1.7616433406,4.4143745824,-0.0014768371
C,0,-2.3499549091,3.1730301413,-0.232064143
C,0,-1.539978571,2.0290171887,-0.2365340943
C,0,-1.9298204562,0.6620043738,-0.4319781767
O,0,-3.2854181478,0.3709741095,-0.5564763964
C,0,-3.9378692186,-0.2724379748,0.4742625191
O,0,-3.4065923654,-0.6124411034,1.499001752
C,0,0.5245041679,0.8235057937,-0.0632308998
C,0,1.7791966475,0.4916085498,-0.0298100348
Si,0,3.6175235633,0.5649262887,0.0514320097
C,0,4.3116191361,0.3306601487,-1.6924052485
C,0,-0.908281518,-0.2838981558,-0.407583257
C,0,-0.8952489141,-1.641691067,-0.6397231065
C,0,-2.0280273595,-2.2573581616,-1.4477988174
Si,0,0.3737256857,-2.8653938514,0.0633133555
C,0,-0.466870026,-4.5641192575,0.1595522831
C,0,0.892238433,-2.3970963955,1.8180741212
C,0,1.8522347384,-3.0239669595,-1.114651362
C,0,4.2743862571,-0.7772431815,1.2081984559

C,0,4.1692244245,2.256033117,0.7115244003
C,0,-5.3843901768,-0.4820179896,0.1027020257
H,0,1.4941298609,3.4635701459,0.4022755187
H,0,0.0601963848,5.4925733248,0.4147755696
H,0,-3.4158157852,3.0844173733,-0.4151784295
H,0,-2.3771938631,5.3091724485,0.0042943944
H,0,-2.7315387799,-2.8030412088,-0.8035026551
H,0,-2.5927151319,-1.5128734797,-2.0124953324
H,0,-1.6373919795,-2.992937668,-2.1611513287
H,0,2.6153722983,-3.6935215449,-0.7011716091
H,0,1.5335609686,-3.4397305576,-2.0768577923
H,0,2.3165226767,-2.0542364017,-1.3099224202
H,0,1.6252813991,-3.1117904887,2.2098137459
H,0,1.3270987146,-1.3970892784,1.8706748023
H,0,0.0200233076,-2.4148115303,2.4804028376
H,0,0.2286397944,-5.2956352768,0.5870356032
H,0,-1.3518617903,-4.5398687527,0.804281209
H,0,-0.7750153472,-4.941612682,-0.8206911953
H,0,5.2610269398,2.2812503288,0.8108958823
H,0,3.8804460174,3.0677940996,0.0360929599
H,0,3.7409736771,2.4646516662,1.6971763532
H,0,5.3668940632,-0.7141596707,1.2706446103
H,0,3.8751017038,-0.6646121712,2.2209929953
H,0,4.0146254903,-1.7790697101,0.8550719344
H,0,5.4043148089,0.4167088397,-1.6801044518
H,0,4.0591938016,-0.6508350689,-2.1052360532
H,0,3.9241761665,1.0916769436,-2.3773669509
H,0,-5.4512590939,-1.1400788376,-0.7689361797
H,0,-5.9115763073,-0.9291963369,0.9444990414
H,0,-5.8481801918,0.469556871,-0.1708431444

5BBBiradTS – UB3LYP//6-311+G**
E(UB+HF-LYP) = -348.915179034

Zero-point correction= 0.151613 (Hartree/Particle)
Thermal correction to Energy= 0.160009
Thermal correction to Enthalpy= 0.160953
Thermal correction to Gibbs Free Energy= 0.118876
Sum of electronic and zero-point Energies= -348.763566
Sum of electronic and thermal Energies= -348.755170
Sum of electronic and thermal Enthalpies= -348.754226
Sum of electronic and thermal Free Energies= -348.796303

E (Thermal) CV S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	100.407	32.649	88.560

C,0,-1.1348927375,-1.7913598576,-0.1784865552
C,0,0.0636097596,-1.0452668253,-0.2031591674
C,0,-0.3188713427,0.3891250253,0.0403865999
C,0,-1.7550469327,0.3910142037,0.1803503704
C,0,-2.2131063211,-0.9182549178,0.0713738713
C,0,1.3813535114,-1.4373233191,-0.2911917644
C,0,2.4218779268,-0.4374327492,-0.4553424893
C,0,0.5606936156,1.348153433,0.3983719213
C,0,0.3712195966,2.8138586902,0.4358556783
H,0,-1.2156014893,-2.8510705337,-0.3794977116
H,0,-3.2487638937,-1.2221972197,0.1516818975
H,0,-2.3511184433,1.2548498236,0.4379336471
H,0,1.6427920638,-2.4720042277,-0.082635587
H,0,3.4263530511,-0.7593750121,-0.1790859228
H,0,1.9978119586,0.4897157776,0.2006012588
H,0,2.4364810852,0.0445421059,-1.4360923621
H,0,0.6655185094,3.2282686334,1.4055322498
H,0,1.0383360841,3.2765654677,-0.3031141552
H,0,-0.6528313811,3.135623086,0.1957258961

5BBbiradTSBrk – BD (T)//6-31+G**
E(RHF) = -346.464341085

C,0,-1.1348927375,-1.7913598576,-0.1784865552
C,0,0.0636097596,-1.0452668253,-0.2031591674
C,0,-0.3188713427,0.3891250253,0.0403865999
C,0,-1.7550469327,0.3910142037,0.1803503704
C,0,-2.2131063211,-0.9182549178,0.0713738713
C,0,1.3813535114,-1.4373233191,-0.2911917644
C,0,2.4218779268,-0.4374327492,-0.4553424893
C,0,0.5606936156,1.348153433,0.3983719213
C,0,0.3712195966,2.8138586902,0.4358556783
H,0,-1.2156014893,-2.8510705337,-0.3794977116
H,0,-3.2487638937,-1.2221972197,0.1516818975
H,0,-2.3511184433,1.2548498236,0.4379336471
H,0,1.6427920638,-2.4720042277,-0.082635587
H,0,3.4263530511,-0.7593750121,-0.1790859228
H,0,1.9978119586,0.4897157776,0.2006012588
H,0,2.4364810852,0.0445421059,-1.4360923621
H,0,0.6655185094,3.2282686334,1.4055322498
H,0,1.0383360841,3.2765654677,-0.3031141552

H,0,-0.6528313811,3.135623086,0.1957258961

5BBBiradUB – UB3LYP//6-311+G**
E(UB+HF-LYP) = -348.924583642

Zero-point correction= 0.154228 (Hartree/Particle)
Thermal correction to Energy= 0.164021
Thermal correction to Enthalpy= 0.164965
Thermal correction to Gibbs Free Energy= 0.119146
Sum of electronic and zero-point Energies= -348.770356
Sum of electronic and thermal Energies= -348.760563
Sum of electronic and thermal Enthalpies= -348.759619
Sum of electronic and thermal Free Energies= -348.805438

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.924	35.239	96.435

C,0,-0.9838679972,0.1864479313,0.0124939581
C,0,0.407279859,-0.3844918799,-0.0069972368
C,0,0.2389537152,-1.8446462135,-0.0241728365
C,0,-1.1134969256,-2.1345334527,-0.0060651637
C,0,-1.8661762607,-0.9452615285,0.0255167039
C,0,1.562332488,0.2696810493,-0.020892774
C,0,-1.3692057196,1.494634753,0.0005660547
C,0,-0.4771313606,2.6927074949,-0.0159814009
C,0,3.0028264131,0.0041995194,0.0219593358
H,0,-2.9450864244,-0.8773344481,0.0526431211
H,0,-1.5328538669,-3.1324877564,-0.0111392828
H,0,1.052222116,-2.5549755112,-0.0519946768
H,0,-2.4401484462,1.6856165357,0.0110280935
H,0,-0.9084446675,3.4946900783,-0.6231700283
H,0,0.5163312806,2.4508166334,-0.40319193
H,0,-0.3385091745,3.1007527773,0.9947061167
H,0,3.4629570605,0.473234033,0.8990262324
H,0,3.2120405561,-1.0751317183,0.0756453898
H,0,3.5124062968,0.4023933364,-0.8621128791

5BBBiradUBrk – UBD (T)//6-31+G**
E(UHF) = -346.549228226

C,0,-0.9838679972,0.1864479313,0.0124939581
C,0,0.407279859,-0.3844918799,-0.0069972368
C,0,0.2389537152,-1.8446462135,-0.0241728365

C,0,-1.1134969256,-2.1345334527,-0.0060651637
C,0,-1.8661762607,-0.9452615285,0.0255167039
C,0,1.562332488,0.2696810493,-0.020892774
C,0,-1.3692057196,1.494634753,0.0005660547
C,0,-0.4771313606,2.6927074949,-0.0159814009
C,0,3.0028264131,0.0041995194,0.0219593358
H,0,-2.9450864244,-0.8773344481,0.0526431211
H,0,-1.5328538669,-3.1324877564,-0.0111392828
H,0,1.052222116,-2.5549755112,-0.0519946768
H,0,-2.4401484462,1.6856165357,0.0110280935
H,0,-0.9084446675,3.4946900783,-0.6231700283
H,0,0.5163312806,2.4508166334,-0.40319193
H,0,-0.3385091 745,3.1007527773,0.9947061167
H,0,3.4629570605,0.473234033,0.8990262324
H,0,3.2120405561,-1.0751317183,0.0756453898
H,0,3.5124062968,0.4023933364,-0.8621128791

5BBBiradBrk- BD (T) 6-31+G**
E(RHF) = -346.469511581

C,0,-0.9838679972,0.1864479313,0.0124939581
C,0,0.407279859,-0.3844918799,-0.0069972368
C,0,0.2389537152,-1.8446462135,-0.0241728365
C,0,-1.1134969256,-2.1345334527,-0.0060651637
C,0,-1.8661762607,-0.9452615285,0.0255167039
C,0,1.562332488,0.2696810493,-0.020892774
C,0,-1.3692057196,1.494634753,0.0005660547
C,0,-0.4771313606,2.6927074949,-0.0159814009
C,0,3.0028264131,0.0041995194,0.0219593358
H,0,-2.9450864244,-0.8773344481,0.0526431211
H,0,-1.5328538669,-3.1324877564,-0.0111392828
H,0,1.052222116,-2.5549755112,-0.0519946768
H,0,-2.4401484462,1.6856165357,0.0110280935
H,0,-0.9084446675,3.4946900783,-0.6231700283
H,0,0.5163312806,2.4508166334,-0.40319193
H,0,-0.3385091745,3.1007527773,0.9947061167
H,0,3.4629570605,0.473234033,0.8990262324
H,0,3.2120405561,-1.0751317183,0.0756453898
H,0,3.5124062968,0.4023933364,-0.8621128791

5BBCarbene – B3LYP//6-311+G**
E(RB+HF-LYP) = -348.918046261

Zero-point correction= 0.155646 (Hartree/Particle)

Thermal correction to Energy= 0.164725
Thermal correction to Enthalpy= 0.165669
Thermal correction to Gibbs Free Energy= 0.122037
Sum of electronic and zero-point Energies= -348.762400
Sum of electronic and thermal Energies= -348.753322
Sum of electronic and thermal Enthalpies= -348.752377
Sum of electronic and thermal Free Energies= -348.796009

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	103.366	34.040	91.830

C,0,0.9544309432,0.2356059514,0.0593483964
C,0,-0.5367003219,0.1132960834,0.0108856165
C,0,-1.0204979315,1.436819015,0.0234421576
C,0,0.0681036866,2.3556733321,0.0723508476
C,0,1.2464378881,1.6502173622,0.1332850827
C,0,-1.2687679495,-1.0147070325,-0.3458603572
C,0,1.8894252018,-0.7441905741,-0.0099999221
C,0,1.6234369716,-2.2054298462,-0.050993459
C,0,-2.7022666526,-1.0846276221,0.0225550029
H,0,2.2385924209,2.0656583373,0.2510567941
H,0,-0.0286276639,3.4330294264,0.0868432952
H,0,-2.0593357602,1.716699715,-0.083183002
H,0,2.9291025657,-0.4244493305,-0.0661548644
H,0,2.3911303007,-2.7342721076,-0.6221864578
H,0,0.6180028274,-2.3865109306,-0.458560644
H,0,1.6296833368,-2.6243494802,0.9634617597
H,0,-2.7720120071,-1.8663105114,0.7946156041
H,0,-3.1577230435,-0.1742245154,0.4503465695
H,0,-3.3104239915,-1.4612106192,-0.806319247

5BBCarbeneBrk – BD (T)//6-31+G**
E(RHF) = -346.500221657

C,0,0.9544309432,0.2356059514,0.0593483964
C,0,-0.5367003219,0.1132960834,0.0108856165
C,0,-1.0204979315,1.436819015,0.0234421576
C,0,0.0681036866,2.3556733321,0.0723508476
C,0,1.2464378881,1.6502173622,0.1332850827
C,0,-1.2687679495,-1.0147070325,-0.3458603572
C,0,1.8894252018,-0.7441905741,-0.0099999221
C,0,1.6234369716,-2.2054298462,-0.050993459
C,0,-2.7022666526,-1.0846276221,0.0225550029

H,0,2.2385924209,2.0656583373,0.2510567941
H,0,-0.0286276639,3.4330294264,0.0868432952
H,0,-2.0593357602,1.716699715,-0.083183002
H,0,2.9291025657,-0.4244493305,-0.0661548644
H,0,2.3911303007,-2.7342721076,-0.6221864578
H,0,0.6180028274,-2.3865109306,-0.458560644
H,0,1.6296833368,-2.6243494802,0.9634617597
H,0,-2.7720120071,-1.8663105114,0.7946156041
H,0,-3.1577230435,-0.1742245154,0.4503465695
H,0,-3.3104239915,-1.4612106192,-0.806319247

5BBCarbeneTS - B3LYP//6-311+G**
E(RB+HF-LYP) = -348.914503722

Zero-point correction= 0.153204 (Hartree/Particle)
Thermal correction to Energy= 0.161316
Thermal correction to Enthalpy= 0.162260
Thermal correction to Gibbs Free Energy= 0.120767
Sum of electronic and zero-point Energies= -348.761300
Sum of electronic and thermal Energies= -348.753188
Sum of electronic and thermal Enthalpies= -348.752244
Sum of electronic and thermal Free Energies= -348.793737

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.227	31.833	87.330

C,0,-1.1380842213,-1.7784866941,-0.1905742946
C,0,0.0680961632,-1.0372684624,-0.2102275845
C,0,-0.3050418237,0.3992047482,0.0404868786
C,0,-1.7263759363,0.4071798405,0.1865881847
C,0,-2.2011967589,-0.9067265079,0.0714193864
C,0,1.3759563193,-1.4453996718,-0.3047458609
C,0,2.4384695876,-0.4660893621,-0.4648970269
C,0,0.5713614606,1.3514559213,0.4648249036
C,0,0.3106044134,2.8082866834,0.4304615209
H,0,-1.2257081945,-2.8334966282,-0.4129620748
H,0,-3.2397997686,-1.1997077416,0.1532658249
H,0,-2.3149389083,1.2681520089,0.4703800508
H,0,1.6179854489,-2.4885393444,-0.1134350915
H,0,3.4370089904,-0.825445189,-0.2148096234
H,0,2.062463577,0.4430463497,0.2080168172
H,0,2.45039544,0.0195633005,-1.443786966
H,0,0.5573117211,3.2783134604,1.387874045

H,0,1.0013611683,3.2543741028,-0.2984829863
H,0,-0.7088146983,3.09080071,0.1239233599

5BBCarbeneTSBrk – BD (T)//6-31+G**
E(RHF) = -346.471505943

C,0,-1.1380842213,-1.7784866941,-0.1905742946
C,0,0.0680961632,-1.0372684624,-0.2102275845
C,0,-0.3050418237,0.3992047482,0.0404868786
C,0,-1.7263759363,0.4071798405,0.1865881847
C,0,-2.2011967589,-0.9067265079,0.0714193864
C,0,1.3759563193,-1.4453996718,-0.3047458609
C,0,2.4384695876,-0.4660893621,-0.4648970269
C,0,0.5713614606,1.3514559213,0.4648249036
C,0,0.3106044134,2.8082866834,0.4304615209
H,0,-1.2257081945,-2.8334966282,-0.4129620748
H,0,-3.2397997686,-1.1997077416,0.1532658249
H,0,-2.3149389083,1.2681520089,0.4703800508
H,0,1.6179854489,-2.4885393444,-0.1134350915
H,0,3.4370089904,-0.825445189,-0.2148096234
H,0,2.062463577,0.4430463497,0.2080168172
H,0,2.45039544,0.0195633005,-1.443786966
H,0,0.5573117211,3.2783134604,1.387874045
H,0,1.0013611683,3.2543741028,-0.2984829863
H,0,-0.7088146983,3.09080071,0.1239233599
H,0,1.0013611683,3.2543741028,-0.2984829863
H,0,-0.7088146983,3.09080071,0.1239233599

5BBSM – B3LYP//6-311+G**
E(RB+HF-LYP) = -348.944978128

Zero-point correction= 0.155074 (Hartree/Particle)
Thermal correction to Energy= 0.166020
Thermal correction to Enthalpy= 0.166964
Thermal correction to Gibbs Free Energy= 0.116662
Sum of electronic and zero-point Energies= -348.789904
Sum of electronic and thermal Energies= -348.778958
Sum of electronic and thermal Enthalpies= -348.778014
Sum of electronic and thermal Free Energies= -348.828316

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	104.179	36.973	105.870

C,0,0.9724769804,1.8574408216,0.0663047322
C,0,1.4606692184,0.7621228502,-0.0885879885
C,0,2.1126855815,-0.4781806113,-0.280576767
C,0,1.5634721155,-1.7121920012,-0.2180233862
C,0,0.1840595985,-2.1052134827,0.0530230912
C,0,-0.8624881572,-1.3419548866,0.2941332517
C,0,-1.9429571181,-0.6551548821,0.5327783133
C,0,-2.8992987335,-0.1451831571,-0.5185665695
C,0,0.353376512,3.1585512663,0.2685836196
H,0,0.0072098918,-3.1803928289,0.0523935508
H,0,2.2367453353,-2.5455545474,-0.393487815
H,0,3.1755473921,-0.4184126759,-0.5007938623
H,0,-2.1762570835,-0.4061133255,1.5684727758
H,0,-3.9110231609,-0.5216409748,-0.335290812
H,0,-2.590462605,-0.4524985236,-1.5183364814
H,0,-2.9505157027,0.9484704127,-0.4948336243
H,0,1.003614609,3.8199232239,0.8493034772
H,0,0.1487161783,3.6514338557,-0.6872673429
H,0,-0.5955508391,3.0633698807,0.8054303528

5BBSMBrk – BD (T)//6-31+G**
E(RHF) = -346.525246849

C,0,0.9724769804,1.8574408216,0.0663047322
C,0,1.4606692184,0.7621228502,-0.0885879885
C,0,2.1126855815,-0.4781806113,-0.280576767
C,0,1.5634721155,-1.7121920012,-0.2180233862
C,0,0.1840595985,-2.1052134827,0.0530230912
C,0,-0.8624881572,-1.3419548866,0.2941332517
C,0,-1.9429571181,-0.6551548821,0.5327783133
C,0,-2.8992987335,-0.1451831571,-0.5185665695
C,0,0.353376512,3.1585512663,0.2685836196
H,0,0.0072098918,-3.1803928289,0.0523935508
H,0,2.2367453353,-2.5455545474,-0.393487815
H,0,3.1755473921,-0.4184126759,-0.5007938623
H,0,-2.1762570835,-0.4061133255,1.5684727758
H,0,-3.9110231609,-0.5216409748,-0.335290812
H,0,-2.590462605,-0.4524985236,-1.5183364814
H,0,-2.9505157027,0.9484704127,-0.4948336243
H,0,1.003614609,3.8199232239,0.8493034772
H,0,0.1487161783,3.6514338557,-0.6872673429
H,0,-0.5955508391,3.0633698807,0.8054303528

5BBTS – B3LYP//6-311+G**

E(RB+HF-LYP) = -348.891441144

Zero-point correction= 0.152374 (Hartree/Particle)
Thermal correction to Energy= 0.161449
Thermal correction to Enthalpy= 0.162393
Thermal correction to Gibbs Free Energy= 0.118572
Sum of electronic and zero-point Energies= -348.739067
Sum of electronic and thermal Energies= -348.729992
Sum of electronic and thermal Enthalpies= -348.729048
Sum of electronic and thermal Free Energies= -348.772870

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.311	33.963	92.230

C,0,0.4688658684,1.4746868646,-0.0637473392
C,0,-0.467956475,0.6315875453,-0.0707044631
C,0,-1.8913641618,0.4424797564,-0.1836971402
C,0,-2.321076316,-0.8383257827,-0.0910151472
C,0,-1.2528221603,-1.7913689582,0.1109636974
C,0,-0.0151445756,-1.2811476261,-0.0139111032
C,0,1.2974210572,-1.5031152374,-0.2610784314
C,0,2.3061524307,-0.6147618687,0.2873755993
C,0,1.0073360946,2.8230537545,0.1566638756
H,0,-1.4340744336,-2.8069119179,0.4439383532
H,0,-3.3641196875,-1.125989407,-0.1232518994
H,0,-2.537194559,1.2962030258,-0.3468443676
H,0,1.5533111138,-2.1107697129,-1.1282227243
H,0,3.3131736806,-0.7628075343,-0.1008677456
H,0,2.3140499267,-0.5363835203,1.3761034023
H,0,1.8867572824,0.4370272401,-0.028939308
H,0,1.6879977599,3.125605357,-0.6451500869
H,0,0.2102394873,3.5726521234,0.2388730498
H,0,1.581388856,2.8528436595,1.0892640385

5BBTSBrk – BD (T)//6-31+G**
E(RHF) = -346.431029216

C,0,0.4688658684,1.4746868646,-0.0637473392
C,0,-0.467956475,0.6315875453,-0.0707044631
C,0,-1.8913641618,0.4424797564,-0.1836971402
C,0,-2.321076316,-0.8383257827,-0.0910151472
C,0,-1.2528221603,-1.7913689582,0.1109636974
C,0,-0.0151445756,-1.2811476261,-0.0139111032

C,0,1.2974210572,-1.5031152374,-0.2610784314
C,0,2.3061524307,-0.6147618687,0.2873755993
C,0,1.0073360946,2.8230537545,0.1566638756
H,0,-1.4340744336,-2.8069119179,0.4439383532
H,0,-3.3641196875,-1.125989407,-0.1232518994
H,0,-2.537194559,1.2962030258,-0.3468443676
H,0,1.5533111138,-2.1107697129,-1.1282227243
H,0,3.3131736806,-0.7628075343,-0.1008677456
H,0,2.3140499267,-0.5363835203,1.3761034023
H,0,1.8867572824,0.4370272401,-0.028939308
H,0,1.6879977599,3.125605357,-0.6451500869
H,0,0.2102394873,3.5726521234,0.2388730498
H,0,1.581388856,2.8528436595,1.0892640385

5BBProd – B3LYP//6-311+G**
E(RB+HF-LYP) = -349.005755530

Zero-point correction= 0.158554 (Hartree/Particle)
Thermal correction to Energy= 0.167380
Thermal correction to Enthalpy= 0.168325
Thermal correction to Gibbs Free Energy= 0.125036
Sum of electronic and zero-point Energies= -348.847202
Sum of electronic and thermal Energies= -348.838375
Sum of electronic and thermal Enthalpies= -348.837431
Sum of electronic and thermal Free Energies= -348.880719

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	105.033	33.306	91.108

C,0,0.2713555833,-0.9489497727,-0.1109982059
C,0,-0.3503880678,0.3958836069,0.0436828193
C,0,-1.7807334168,0.159374758,0.282181425
C,0,-2.0051490812,-1.177053217,0.2172019431
C,0,-0.7441915116,-1.8605960054,-0.0356295849
C,0,0.2505303631,1.5865197035,-0.1550396142
C,0,1.6740118868,-1.2990149634,-0.2749663492
C,0,2.7581063691,-0.6052639999,0.1027670419
C,0,-0.3855123669,2.9349498494,-0.0547552162
H,0,-0.6288518549,-2.9336379147,-0.1200942938
H,0,-2.9622464453,-1.669659075,0.3252666778
H,0,-2.5243634795,0.9283808474,0.4280364547
H,0,1.8375683291,-2.2751095688,-0.7288657412
H,0,3.7521833493,-0.9999319749,-0.0709928075

H,0,2.6973199501,0.3433088583,0.6215102636
H,0,1.2986206173,1.5854844746,-0.4387660876
H,0,0.1595344217,3.5580976492,0.6635827155
H,0,-0.3276738026,3.4552571584,-1.0180047786
H,0,-1.4302696329,2.8927097895,0.2516620435

5BBProdBrk – BD (T)//6-31+G**
E(RHF) = -346.591122835

C,0,0.2701615542,-0.9534167569,-0.1078577717
C,0,-0.352342424,0.3930029269,0.0422734119
C,0,-1.7832053736,0.1590236053,0.2811809745
C,0,-2.0087408506,-1.1786099252,0.2182411
C,0,-0.747273105,-1.8645555023,-0.0306560251
C,0,0.2541507156,1.5831189333,-0.1581296703
C,0,1.6747206917,-1.2960542882,-0.2788368002
C,0,2.7552817948,-0.59608239,0.1038077444
C,0,-0.3773893074,2.9351515796,-0.05547329
H,0,-0.6326536184,-2.9398494947,-0.1104616209
H,0,-2.9672822669,-1.6723250243,0.3273966526
H,0,-2.5252898079,0.9327193281,0.4241903306
H,0,1.8435594641,-2.2684560039,-0.7426599309
H,0,3.7550705652,-0.9767946673,-0.0779816091
H,0,2.684963759,0.3464126204,0.6355608163
H,0,1.3035113893,1.5766670307,-0.4431480303
H,0,0.1669416417,3.5556625889,0.6679338178
H,0,-0.3163913809,3.461285602,-1.0168998848
H,0,-1.4246119192,2.8952089254,0.2487714181

Pd-catalyzed allylic alkylation of 1,1-dimethylallyl acetate

B3LYP//SDD on Pd 6-31G on all other atoms unless otherwise noted**

Acetate Anion
E(RB+HF-LYP) = -228.502196453

Zero-point correction= 0.048082 (Hartree/Particle)
Thermal correction to Energy= 0.052549
Thermal correction to Enthalpy= 0.053493
Thermal correction to Gibbs Free Energy= 0.020437
Sum of electronic and zero-point Energies= -228.454114
Sum of electronic and thermal Energies= -228.449648
Sum of electronic and thermal Enthalpies= -228.448703

Sum of electronic and thermal Free Energies= -228.481759

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	32.975	13.151	69.572

C,0,0.1867372076,0.,0.1162771735
O,0,0.0896113313,0.,1.3688814132
O,0,1.2119899016,0.,-0.6126821735
C,0,-1.1733959016,0.,-0.677799841
H,0,-2.0443151516,0.,-0.0114448273
H,0,-1.2242712741,0.8795345446,-1.3345065426
H,0,-1.2242712741,-0.8795345446,-1.3345065426

Acetate Anion 6-311+G**

E(RB+HF-LYP) = -228.602316623

Zero-point correction= 0.047694 (Hartree/Particle)
Thermal correction to Energy= 0.051274
Thermal correction to Enthalpy= 0.052218
Thermal correction to Gibbs Free Energy= 0.021800
Sum of electronic and zero-point Energies= -228.554623
Sum of electronic and thermal Energies= -228.551043
Sum of electronic and thermal Enthalpies= -228.550099
Sum of electronic and thermal Free Energies= -228.580516

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	32.175	11.120	64.020

C,0,0.1800956672,0.,0.1117336715
O,0,0.0913502188,0.,1.3635519743
O,0,1.2100769042,0.,-0.606807403
C,0,-1.1714754035,0.,-0.6774991346
H,0,-2.0337402538,0.,-0.0049000193
H,0,-1.2146991562,0.8814878995,-1.3272318863
H,0,-1.2146991562,-0.8814878995,-1.3272318863

Acetic Acid

E(RB+HF-LYP) = -229.086853208

Zero-point correction= 0.061943 (Hartree/Particle)
Thermal correction to Energy= 0.065696
Thermal correction to Enthalpy= 0.066640

Thermal correction to Gibbs Free Energy= 0.035912
Sum of electronic and zero-point Energies= -229.024910
Sum of electronic and thermal Energies= -229.021158
Sum of electronic and thermal Enthalpies= -229.020213
Sum of electronic and thermal Free Energies= -229.050942

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	41.225	12.198	64.673

C,0,-1.1987961232,0.,-0.7272246722
C,0,0.1442490725,0.,-0.0385028512
O,0,1.2174408306,0.,-0.5995078855
O,0,0.0259123408,0.,1.3115493205
H,0,-2.0246798446,0.,-0.0159935316
H,0,-1.26482236,0.8805169594,-1.3722848817
H,0,-1.26482236,-0.8805169594,-1.3722848817
H,0,0.9347814977,0.,1.6585969561

Acetic Acid 6-311+G**

E(RB+HF-LYP) = -229.164176416

Zero-point correction= 0.061460 (Hartree/Particle)
Thermal correction to Energy= 0.065226
Thermal correction to Enthalpy= 0.066170
Thermal correction to Gibbs Free Energy= 0.035431
Sum of electronic and zero-point Energies= -229.102716
Sum of electronic and thermal Energies= -229.098951
Sum of electronic and thermal Enthalpies= -229.098007
Sum of electronic and thermal Free Energies= -229.128745

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	40.930	12.293	64.695

C,0,-1.1978147088,0.,-0.7256357816
C,0,0.1429262586,0.,-0.0409123007
O,0,1.2103388797,0.,-0.6010068491
O,0,0.0322244969,0.,1.3109861875
H,0,-2.0208055517,0.,-0.0137825935
H,0,-1.2615547674,0.8801340185,-1.3684453682
H,0,-1.2615547674,-0.8801340185,-1.3684453682
H,0,0.9327387745,0.,1.6701271164

PH_3

E(RB+HF-LYP) = -343.142674451

Zero-point correction= 0.024065 (Hartree/Particle)
Thermal correction to Energy= 0.026970
Thermal correction to Enthalpy= 0.027914
Thermal correction to Gibbs Free Energy= 0.003021
Sum of electronic and zero-point Energies= -343.118609
Sum of electronic and thermal Energies= -343.115704
Sum of electronic and thermal Enthalpies= -343.114760
Sum of electronic and thermal Free Energies= -343.139654

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	16.924	6.779	52.393

P,0,-0.0779701498,-0.0451387326,-0.0918631569
H,0,1.3301596685,0.0772658426,-0.2658511104
H,0,0.0482385418,-0.6620439659,1.1854706972
H,0,-0.2088459637,1.2618591128,0.4583277667

Allyl Cation

E(RB+HF-LYP) = -116.976995098

Zero-point correction= 0.068464 (Hartree/Particle)
Thermal correction to Energy= 0.072295
Thermal correction to Enthalpy= 0.073239
Thermal correction to Gibbs Free Energy= 0.043883
Sum of electronic and zero-point Energies= -116.908532
Sum of electronic and thermal Energies= -116.904700
Sum of electronic and thermal Enthalpies= -116.903756
Sum of electronic and thermal Free Energies= -116.933112

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	45.366	12.021	61.785

C,0,-0.2554933368,0.,-1.1825259184
C,0,-0.4573373876,0.,0.1873511729
C,0,0.6469517639,0.,1.0222426175
H,0,0.5411323322,0.,2.1058411355
H,0,-1.4629295504,0.,0.5984235024
H,0,-1.0903555069,0.,-1.8813505097
H,0,0.7475353973,0.,-1.6072274842

H,0,1.6598910905,0.,0.621906124

1,1-Dimethylallyl acetate

E(RB+HF-LYP) = -424.421369269

Zero-point correction= 0.178973 (Hartree/Particle)
Thermal correction to Energy= 0.189772
Thermal correction to Enthalpy= 0.190716
Thermal correction to Gibbs Free Energy= 0.142775
Sum of electronic and zero-point Energies= -424.242396
Sum of electronic and thermal Energies= -424.231598
Sum of electronic and thermal Enthalpies= -424.230653
Sum of electronic and thermal Free Energies= -424.278595

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	119.084	38.929	100.901

C,0,2.4625967208,-0.7134024244,1.7779172318
C,0,1.8832462982,-0.2748905787,0.6622085257
C,0,0.4754644379,-0.5758892194,0.1874015574
O,0,-0.0185515052,0.7714991406,-0.1673713323
C,0,-1.2443743165,0.9639956277,-0.6996665054
O,0,-2.0555172632,0.0939576072,-0.9398070939
C,0,-1.4704345902,2.4390683507,-0.9556903363
H,0,2.4502113154,0.3472500427,-0.0293409479
H,0,3.494698763,-0.4642271157,2.0050654081
H,0,1.944991812,-1.3329389674,2.5035646557
C,0,-0.4163746869,-1.1934436219,1.2658174414
C,0,0.5476494466,-1.4500503284,-1.0758328094
H,0,-2.4574249168,2.5825799413,-1.3944777002
H,0,-1.3929996611,2.9980861499,-0.0184784573
H,0,-0.7007633968,2.8266122618,-1.6295245879
H,0,-1.4234808513,-1.346871436,0.8790158222
H,0,-0.0125188373,-2.1620636585,1.5744977105
H,0,-0.4634661499,-0.5429927091,2.1435364621
H,0,-0.4490010265,-1.6394775308,-1.4758141904
H,0,1.151852331,-0.9584101793,-1.8446564163
H,0,1.0238109065,-2.4035276159,-0.8288909795

1,1-Dimethylallyl acetate 6-31+G**

E(RB+HF-LYP) = -424.439842324

Zero-point correction= 0.178286 (Hartree/Particle)

Thermal correction to Energy= 0.189163
Thermal correction to Enthalpy= 0.190108
Thermal correction to Gibbs Free Energy= 0.141938
Sum of electronic and zero-point Energies= -424.261556
Sum of electronic and thermal Energies= -424.250679
Sum of electronic and thermal Enthalpies= -424.249735
Sum of electronic and thermal Free Energies= -424.297905

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	118.702	39.032	101.382

C,0,2.5466530242,0.4397729445,0.9709921022
C,0,1.9680136493,0.7124166214,-0.2001294392
C,0,0.5405489513,0.4133522418,-0.6089668823
C,0,0.5427012823,-0.5450056726,-1.812532338
O,0,-0.0676482187,-0.2384528406,0.5560194644
C,0,-1.3528934433,-0.6542372795,0.5591934918
C,0,-1.6962314613,-1.2898808185,1.8880159408
C,0,-0.1895422775,1.7311778921,-0.920996308
O,0,-2.1280929175,-0.5390422726,-0.3696730061
H,0,2.5442952133,1.2045112303,-0.9833905349
H,0,3.5847361283,0.7033079533,1.1507519956
H,0,2.0063320825,-0.0487895358,1.7745094775
H,0,-2.7412526352,-1.5996707535,1.8805861905
H,0,-1.0523371772,-2.1569520788,2.0657901889
H,0,-1.5218550452,-0.5798519581,2.7022039365
H,0,-1.2053579167,1.5426926653,-1.2721069381
H,0,-0.224284645,2.3636950577,-0.0288259251
H,0,0.356221451,2.2738786247,-1.6999898297
H,0,-0.4726915479,-0.7348282306,-2.1641371964
H,0,1.1201232307,-0.1008651001,-2.6301745628
H,0,1.0165016021,-1.492742545,-1.539447873

1,1-Dimethylallyl acetate 6-311+G**

E(RB+HF-LYP) = -424.539263621

Zero-point correction= 0.177566 (Hartree/Particle)
Thermal correction to Energy= 0.188459
Thermal correction to Enthalpy= 0.189404
Thermal correction to Gibbs Free Energy= 0.140897
Sum of electronic and zero-point Energies= -424.361697
Sum of electronic and thermal Energies= -424.350804
Sum of electronic and thermal Enthalpies= -424.349860

Sum of electronic and thermal Free Energies= -424.398367

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	118.260	39.103	102.091

C,0,2.4582541386,-0.7028395738,1.7777472525
C,0,1.879999536,-0.2793521683,0.6586055904
C,0,0.4738131593,-0.5858066837,0.1870031266
O,0,-0.0230304252,0.7665007114,-0.1678940167
C,0,-1.2457443364,0.9718004201,-0.7006113205
O,0,-2.0538155301,0.1074476689,-0.94350359
C,0,-1.4632282793,2.4460806478,-0.9492465285
H,0,2.4457613056,0.3355722013,-0.0373632743
H,0,3.4881165607,-0.4476762939,1.9997847867
H,0,1.9427517639,-1.313270984,2.5100897239
C,0,-0.4153929298,-1.2030412432,1.2651788787
C,0,0.5488372006,-1.4589640045,-1.0749952268
H,0,-2.4477647349,2.59760756,-1.3871431924
H,0,-1.3832918139,2.9978457623,-0.0098998801
H,0,-0.6919999043,2.8303122993,-1.6204856041
H,0,-1.4181510727,-1.3756374421,0.8787800709
H,0,-0.000544635,-2.162713255,1.5818144746
H,0,-0.4753454933,-0.5482871592,2.1370738139
H,0,-0.4447347241,-1.6645694343,-1.4709590582
H,0,1.1441393153,-0.9635369669,-1.8461269786
H,0,1.0366001412,-2.4044976969,-0.8264746622

1,1-Dimethylallyl acetate – Solvated with 6 HCN 6-31G*

E(RB+HF-LYP) = -984.998782786

Zero-point correction= 0.286678 (Hartree/Particle)
Thermal correction to Energy= 0.320661
Thermal correction to Enthalpy= 0.321605
Thermal correction to Gibbs Free Energy= 0.206124
Sum of electronic and zero-point Energies= -984.712104
Sum of electronic and thermal Energies= -984.678122
Sum of electronic and thermal Enthalpies= -984.677178
Sum of electronic and thermal Free Energies= -984.792658

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	201.218	103.264	243.049

C,0,2.2749712558,-3.7370737461,-1.5552519386
C,0,2.217367563,-2.4856531162,-1.0952223411
C,0,1.0282898263,-1.5489703442,-1.1892074989
C,0,1.4363592288,-0.3070062097,-1.9925485392
O,0,0.8333490833,-1.1825772304,0.2494852195
C,0,-0.0514913517,-0.2895888906,0.6756378183
C,0,-0.0092888232,-0.1510220881,2.1773195842
C,0,-0.248996887,-2.1971695624,-1.71873658
O,0,-0.8110230684,0.348777923,-0.0544558175
H,0,3.0941297875,-2.0319779134,-0.6338255508
H,0,3.1937936202,-4.3126886435,-1.4823316386
H,0,1.4359738836,-4.2300185061,-2.0386300251
H,0,-0.7175869259,0.6121410681,2.5027550393
H,0,-0.2495188223,-1.1109375125,2.6466365987
H,0,1.0030824553,0.1163264121,2.4968711247
H,0,-1.0672534268,-1.4757999611,-1.7272033004
H,0,-0.0893918721,-2.5425128977,-2.7448598314
H,0,-0.540477407,-3.0561010997,-1.1064874409
H,0,0.6146534377,0.4076331801,-2.0620498353
H,0,2.305024299,0.1750965818,-1.5345064093
H,0,1.7173294577,-0.6184082752,-3.0038951612
H,0,-0.573969711,2.3893908624,-0.141702532
C,0,-0.1156586168,3.3673687017,-0.1579855498
N,0,0.4157355822,4.394718859,-0.163660554
H,0,-2.8075732279,0.4727393892,0.0612506535
C,0,-3.8865962234,0.5331753507,0.0374686659
N,0,-5.0399495605,0.5978332405,0.0105329863
H,0,5.1266338467,2.0797884862,0.3061433563
C,0,4.9208770623,1.024063038,0.217670503
N,0,4.6540600362,-0.0972011587,0.1119425434
H,0,2.5208338612,5.0664334961,0.0423169217
C,0,3.5119456973,4.6611966704,0.163684169
N,0,4.5468972823,4.1609768288,0.291766958
H,0,1.5318859853,-3.8925297128,1.1553232644
C,0,0.9297708757,-3.8281046689,2.0424136201
N,0,0.2638560602,-3.724797067,2.9835994782
H,0,-7.1819382628,0.7095536827,-0.0882834036
C,0,-8.2573495108,0.7641996495,-0.1526218172
N,0,-9.4113764971,0.8227231714,-0.2232496431

Dimethylmalonate - 6-311+G**

E(RB+HF-LYP) = -496.411557559

Zero-point correction= 0.132643 (Hartree/Particle)

Thermal correction to Energy= 0.142947
Thermal correction to Enthalpy= 0.143891
Thermal correction to Gibbs Free Energy= 0.095074
Sum of electronic and zero-point Energies= -496.278915
Sum of electronic and thermal Energies= -496.268610
Sum of electronic and thermal Enthalpies= -496.267666
Sum of electronic and thermal Free Energies= -496.316483

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.701	33.774	102.744

C,0,-1.1190090058,0.5807960193,-3.2593792749
O,0,-1.435984706,0.0967634977,-1.9381173943
C,0,-0.4067825057,0.0298867114,-1.0718134919
O,0,0.7223677272,0.3503561665,-1.3385003323
C,0,-0.8875687492,-0.5136326512,0.263823688
C,0,0.2332487914,-0.5824804324,1.2800970318
O,0,0.8551631519,-1.578269737,1.5500254692
O,0,0.438807752,0.6173539587,1.8506047699
C,0,1.5332947173,0.692904862,2.7851092924
H,0,-1.2842568217,-1.518026942,0.1079005237
H,0,-2.0580138779,0.5581413591,-3.8073419152
H,0,-0.7275812816,1.5973099703,-3.2066609004
H,0,-0.3801474603,-0.0665495247,-3.7329318939
H,0,1.5445855095,1.7225287113,3.1348390205
H,0,1.3719257039,0.0042621984,3.615321135
H,0,2.4704775372,0.4454063924,2.2855996002
H,0,-1.6989201984,0.1224496938,0.6241508574

Acetamidine 6-31G*

E(RB+HF-LYP) = -189.316460752

Zero-point correction= 0.086727 (Hartree/Particle)
Thermal correction to Energy= 0.091689
Thermal correction to Enthalpy= 0.092634
Thermal correction to Gibbs Free Energy= 0.059507
Sum of electronic and zero-point Energies= -189.229734
Sum of electronic and thermal Energies= -189.224771
Sum of electronic and thermal Enthalpies= -189.223827
Sum of electronic and thermal Free Energies= -189.256954

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total	57.536	16.733	69.722

N,0,0.977547434,1.0392330716,0.0728627885
C,0,0.1218699693,0.0874923935,0.0116507005
C,0,-1.3705802306,0.2176144336,-0.2265763819
N,0,0.543065218,-1.215530946,0.2427798527
H,0,-1.677687409,-0.3515152855,-1.1138640341
H,0,-1.9326144619,-0.1782591835,0.6272993671
H,0,-1.6512197002,1.262550172,-0.3793209672
H,0,0.0459136313,-1.9511943673,-0.2421323062
H,0,1.5509310445,-1.3197522572,0.221421718
H,0,0.5126498991,1.9416150797,-0.0333481776

2-Methyl-2-dimethyl malonate-3-butene – more substituted product 6-311+G**

E(RB+HF-LYP) = -691.789756969

Zero-point correction= 0.249780 (Hartree/Particle)
Thermal correction to Energy= 0.266234
Thermal correction to Enthalpy= 0.267179
Thermal correction to Gibbs Free Energy= 0.205555
Sum of electronic and zero-point Energies= -691.539977
Sum of electronic and thermal Energies= -691.523523
Sum of electronic and thermal Enthalpies= -691.522578
Sum of electronic and thermal Free Energies= -691.584202

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.065	58.600	129.697

H,0,-3.2996083661,2.2389386853,-0.5257326305
C,0,-3.4708195053,1.1954614957,-0.2869474102
H,0,-4.4516958893,0.8015051433,-0.5295905803
C,0,-2.5498307595,0.4175610014,0.278771465
C,0,-1.1416110148,0.8187673394,0.6949740513
C,0,-0.1347284698,0.0586961241,-0.2507198361
C,0,-0.1895786226,-1.4709093322,-0.2002740986
O,0,-0.8913517106,-2.1550694071,0.4989259449
C,0,1.3172071965,0.4828680423,-0.0297283891
O,0,1.9871929575,0.1920673471,0.9306897702
O,0,1.7643517874,1.2435718487,-1.0472332212
C,0,3.127805419,1.6986094875,-0.9404749118
O,0,0.6743171935,-1.9780471333,-1.1040056212
C,0,0.7590613648,-3.4153536893,-1.1655143724
C,0,-0.9061030193,2.3305192745,0.5207135398

C,0,-0.9477450578,0.4522435393,2.1845388135
H,0,-2.7991838003,-0.6177411014,0.4912182312
H,0,-0.3886711661,0.3306438006,-1.2783038609
H,0,3.3108329391,2.2766543433,-1.8433196766
H,0,3.2540016291,2.3199658997,-0.052852316
H,0,3.8067176695,0.8471474291,-0.8826242698
H,0,1.4952399452,-3.6282867989,-1.9371526649
H,0,1.0821095063,-3.8160159069,-0.2040266284
H,0,-0.2093476484,-3.8423698413,-1.4287240615
H,0,0.0806029984,2.6153655178,0.8938507203
H,0,-0.9727898963,2.6425099791,-0.5246659077
H,0,-1.6460335902,2.8931284672,1.094068848
H,0,0.0704569112,0.6662887131,2.5139639279
H,0,-1.639499119,1.0440095586,2.79014049
H,0,-1.1511591323,-0.6027048281,2.3647022889

2-Methyl-5,5-methylester-2-pentene – less substituted product 6-311+G**

E(RB+HF-LYP) = -691.804162061

Zero-point correction= 0.249789 (Hartree/Particle)
Thermal correction to Energy= 0.266756
Thermal correction to Enthalpy= 0.267701
Thermal correction to Gibbs Free Energy= 0.202538
Sum of electronic and zero-point Energies= -691.554373
Sum of electronic and thermal Energies= -691.537406
Sum of electronic and thermal Enthalpies= -691.536462
Sum of electronic and thermal Free Energies= -691.601624

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.392	58.088	137.145

C,0,-1.7589565409,3.2488496319,-0.6025847962
C,0,-2.4496300996,2.0009972913,-0.1128903079
C,0,-1.8445124453,0.9745416471,0.5002525757
C,0,-0.3846792752,0.8384120788,0.8405124257
C,0,0.3512465973,-0.200822435,-0.0471147546
C,0,1.8509359678,-0.1370087618,0.2180998226
O,0,2.431794497,0.8044239527,-0.5532437408
C,0,-3.9384192946,1.9772034487,-0.3603629014
H,0,0.1361404577,1.7916312014,0.7394590218
H,0,-0.2826072148,0.5178402971,1.8815098017
H,0,-2.458446153,0.1301540631,0.8021227097
H,0,-4.396647652,1.0581400377,0.0093784457

H,0,-4.4294737385,2.8256694505,0.1308616786
H,0,-4.1596163121,2.065255328,-1.4307096351
H,0,-1.9345613487,3.3843022881,-1.6761002831
H,0,-0.6815141239,3.2429571347,-0.4404700784
H,0,-2.1714620012,4.1354252661,-0.1067671962
H,0,0.1882187819,0.0383179574,-1.1000111542
O,0,2.4463323385,-0.7966907957,1.0325561301
C,0,-0.1358733383,-1.624365885,0.2018797137
C,0,3.844137578,1.0056981525,-0.3447805523
H,0,4.1319246018,1.7842180719,-1.047589236
H,0,4.0360034391,1.3223167177,0.6812431246
H,0,4.3914192276,0.0839628695,-0.5449882673
O,0,0.2980421899,-2.4442957319,-0.7745195898
O,0,-0.8134711134,-1.9835473591,1.1301129259
C,0,-0.0350262288,-3.8382177325,-0.6246521791
H,0,0.3956594074,-4.3337064856,-1.4917400533
H,0,0.3957406323,-4.2311218038,0.2969971929
H,0,-1.1174849016,-3.9703588287,-0.6034198967

$Pd(P(CH_3)_3)_2$

E(RB+HF-LYP) = -1050.22239586

Zero-point correction= 0.229191 (Hartree/Particle)
Thermal correction to Energy= 0.245993
Thermal correction to Enthalpy= 0.246937
Thermal correction to Gibbs Free Energy= 0.182875
Sum of electronic and zero-point Energies= -1049.993205
Sum of electronic and thermal Energies= -1049.976403
Sum of electronic and thermal Enthalpies= -1049.975459
Sum of electronic and thermal Free Energies= -1050.039521

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	154.363	57.328	134.831

P,0,-1.3312038918,0.,1.8820886516
Pd,0,-0.0055242633,0.,-0.0043947649
P,0,1.3322045822,0.,-1.8827864546
C,0,0.4812565164,0.,-3.532151148
C,0,2.4965338034,1.4304246078,-2.0886904388
C,0,2.4965338034,-1.4304246078,-2.0886904388
C,0,-3.1705704826,0.,1.6330126803
C,0,-1.139333682,-1.4303784503,3.0493800238
C,0,-1.139333682,1.4303784503,3.0493800238

H,0,-1.803998059,1.339650452,3.9160233885
H,0,-0.1027909678,1.4798061342,3.3937206556
H,0,-1.3615285111,2.3612368609,2.5206445321
H,0,-1.803998059,-1.339650452,3.9160233885
H,0,-1.3615285111,-2.3612368609,2.5206445321
H,0,-0.1027909678,-1.4798061342,3.3937206556
H,0,-3.7078286675,0.,2.5884069834
H,0,-3.4590801415,0.8838200866,1.0577593291
H,0,-3.4590801415,-0.8838200866,1.0577593291
H,0,3.0908288031,1.3421672163,-3.0054844383
H,0,1.9243548799,2.3615362469,-2.1190234535
H,0,3.168774955,1.4770527776,-1.227778686
H,0,3.0908288031,-1.3421672163,-3.0054844383
H,0,3.168774955,-1.4770527776,-1.227778686
H,0,1.9243548799,-2.3615362469,-2.1190234535
H,0,1.1983362149,0.,-4.3612680301
H,0,-0.1575206837,-0.8838714297,-3.6098397949
H,0,-0.1575206837,0.8838714297,-3.6098397949

$Pd(P(CH_3)_3)_2$ – 6-311+G**

E(RB+HF-LYP) = -1050.33178490

Zero-point correction= 0.227533 (Hartree/Particle)
Thermal correction to Energy= 0.244411
Thermal correction to Enthalpy= 0.245355
Thermal correction to Gibbs Free Energy= 0.181134
Sum of electronic and zero-point Energies= -1050.104251
Sum of electronic and thermal Energies= -1050.087374
Sum of electronic and thermal Enthalpies= -1050.086430
Sum of electronic and thermal Free Energies= -1050.150651

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	153.370	57.541	135.164

P,0,-1.3326975366,0.,1.8850530414
Pd,0,-0.0059437041,0.,-0.004189558
P,0,1.3336391177,0.,-1.8845872192
C,0,0.4829019334,-0.0000000001,-3.530274325
C,0,2.4950231127,1.4286936212,-2.0895870926
C,0,2.4950231129,-1.4286936211,-2.0895870925
C,0,-3.1679812621,-0.0000000001,1.6321549782
C,0,-1.138805852,-1.4287184231,3.048489926
C,0,-1.1388058521,1.4287184232,3.0484899259

H,0,-1.8036004006,1.3393012733,3.9136034014
H,0,-0.1040358747,1.4764469366,3.392927773
H,0,-1.3591774855,2.3577742601,2.5193717196
H,0,-1.8036004004,-1.3393012732,3.9136034015
H,0,-1.3591774853,-2.3577742601,2.5193717198
H,0,-0.1040358746,-1.4764469363,3.3929277732
H,0,-3.7077792603,-0.0000000001,2.5845611142
H,0,-3.453756328,0.8824360793,1.0565972554
H,0,-3.4537563279,-0.8824360796,1.0565972554
H,0,3.088867997,1.3395105146,-3.0050129379
H,0,1.922832244,2.3577949246,-2.1206960584
H,0,3.1650672922,1.4761805515,-1.229123381
H,0,3.0888679971,-1.3395105145,-3.0050129378
H,0,3.1650672924,-1.4761805512,-1.2291233809
H,0,1.9228322442,-2.3577949246,-2.1206960582
H,0,1.2005405081,-0.0000000001,-4.3570017255
H,0,-0.1550003102,-0.8824456024,-3.6076402595
H,0,-0.1550003103,0.8824456021,-3.6076402596

$Pd(P(H)(Ph)_2)_2$ SDD on Pd, 6-31G on Ph, 6-31G* on all other atoms

E(RB+HF-LYP) = -1738.28726260

Zero-point correction= 0.390288 (Hartree/Particle)
Thermal correction to Energy= 0.415766
Thermal correction to Enthalpy= 0.416710
Thermal correction to Gibbs Free Energy= 0.325769
Sum of electronic and zero-point Energies= -1737.896974
Sum of electronic and thermal Energies= -1737.871497
Sum of electronic and thermal Enthalpies= -1737.870552
Sum of electronic and thermal Free Energies= -1737.961493

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	260.897	95.150	191.401

C,0,1.6698368642,-3.3074528839,-0.6461423669
C,0,0.3284250519,-3.2530661487,-1.0744380676
C,0,-0.065854091,-4.0462326507,-2.1684791733
C,0,0.8565988337,-4.8778623695,-2.8152990496
C,0,2.1824306922,-4.9333163972,-2.3722794153
C,0,2.5865666641,-4.1470357585,-1.2854092686
P,0,-0.8501078429,-2.1334109001,-0.2109020725
C,0,-1.4330092259,-3.1300463893,1.233746975
C,0,-1.6344862652,-2.4757308304,2.4625468888

C,0,-2.1053090513,-3.1833088169,3.57570092
C,0,-2.3732142321,-4.5522598185,3.4741131904
C,0,-2.1683596138,-5.2146490217,2.2562207119
C,0,-1.7011787864,-4.5092135115,1.1434313666
Pd,0,-0.2051292747,0.0415030416,0.1762447993
P,0,0.4492959727,2.2205985319,0.5288843813
C,0,1.810530688,2.8817418611,-0.5341891732
C,0,2.2217007877,4.2274230104,-0.4854435364
C,0,3.273314642,4.6768423646,-1.2892691149
C,0,3.9272227169,3.7886495602,-2.1539841373
C,0,3.5232517577,2.4510576284,-2.2138584374
C,0,2.4688851096,1.999588276,-1.4099157491
C,0,-0.8387081212,3.5346347081,0.4691353264
C,0,-0.9303697992,4.5330626629,1.4571889773
C,0,-1.9312969069,5.5100863227,1.3921130276
C,0,-2.8485466123,5.505576035,0.3357269786
C,0,-2.7684052527,4.5150761963,-0.6517298677
C,0,-1.7769456793,3.5322119228,-0.5819372462
H,0,-1.9513727633,-2.3278999556,-1.0846168838
H,0,0.9772602358,2.5465470157,1.8052005504
H,0,2.1455765744,0.963428117,-1.4562455286
H,0,4.0223158321,1.759851353,-2.8858593052
H,0,4.7429345897,4.1401711813,-2.7782007306
H,0,3.5813250234,5.7169480428,-1.2432221949
H,0,1.7139282269,4.9259757948,0.1723493487
H,0,-1.0930861345,-4.0114967271,-2.5194009233
H,0,0.5387915835,-5.480094798,-3.6608543388
H,0,2.8971088741,-5.5791636405,-2.8726083334
H,0,3.6160526445,-4.1806514034,-0.9427105492
H,0,1.9930909173,-2.6814889402,0.1803374121
H,0,-1.4162339618,-1.4141351196,2.5367885035
H,0,-2.2568984488,-2.6662881631,4.5181033366
H,0,-2.7353052559,-5.1021864912,4.3372771888
H,0,-2.3708765264,-6.2782009021,2.1747285849
H,0,-1.5358757638,-5.0333586084,0.2072913894
H,0,-0.2238582939,4.5447002161,2.2820306936
H,0,-1.9929517455,6.2708512939,2.1641969985
H,0,-3.6241410981,6.2632736864,0.2851307637
H,0,-3.4836764482,4.5017383103,-1.4681379876
H,0,-1.7344643947,2.7498696371,-1.33387195

$Pd(P(CH_3)_3)_2(\eta^2$-1,1-dimethylallyl acetate)

E(RB+HF-LYP) = -1474.65508028

Zero-point correction= 0.409561 (Hartree/Particle)
Thermal correction to Energy= 0.437963
Thermal correction to Enthalpy= 0.438907
Thermal correction to Gibbs Free Energy= 0.349861
Sum of electronic and zero-point Energies= -1474.245520
Sum of electronic and thermal Energies= -1474.217117
Sum of electronic and thermal Enthalpies= -1474.216173
Sum of electronic and thermal Free Energies= -1474.305219

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	274.826	101.041	187.414

C,0,0.3058560444,-1.5052301713,-0.9636161488
C,0,0.1246872148,-1.6020593027,0.4301204262
C,0,1.2628994917,-1.6821101531,1.4370623124
O,0,1.6578170798,-3.1211114193,1.583751218
C,0,2.315116289,-3.8039644917,0.6299328752
C,0,2.4488747295,-5.259153198,1.038110367
Pd,0,-0.4631860495,0.3994058945,-0.3147056406
P,0,-0.3981488456,1.5236969856,-2.3939721472
P,0,-1.5048005052,1.6886928923,1.3724679555
O,0,2.7446868028,-3.3546513448,-0.4131211344
H,0,3.1193250455,-5.7692851271,0.3464173034
H,0,1.4647918907,-5.7384718212,1.0116422233
H,0,2.8240910874,-5.3406676362,2.0616274061
C,0,2.4923097692,-0.8269825265,1.1159988802
C,0,0.7694015369,-1.3796989197,2.8554892803
H,0,-0.7762080366,-2.1007470211,0.7882124464
H,0,-0.4385686792,-1.9489618187,-1.6229529023
H,0,1.3037376544,-1.4477696036,-1.3853030821
C,0,-2.577322061,0.7639119726,2.5755387425
C,0,-0.4562720175,2.6876911146,2.5395034001
C,0,-2.7096575179,2.9968700619,0.8285368234
C,0,-1.4584938222,0.774510749,-3.7219136516
C,0,1.2653755651,1.4935011615,-3.2175647586
C,0,-0.830530125,3.3202661412,-2.6124335865
H,0,1.2392400602,1.951560291,-4.2127089491
H,0,1.9876133302,2.0314563182,-2.5966940259
H,0,1.6054092821,0.458457004,-3.3062585927
H,0,-0.7078080031,3.647129237,-3.65130396
H,0,-1.8684396151,3.4866635205,-2.3110474806
H,0,-0.1878919382,3.9323232114,-1.972703945
H,0,-1.3220124361,1.2752867459,-4.6870702423

H,0,-1.207710499,-0.2840969626,-3.8286890933
H,0,-2.5105430862,0.8431394741,-3.4305032788
H,0,-1.0659954472,3.2286070206,3.2718857795
H,0,0.2368960959,2.0309096299,3.0721059757
H,0,0.1369345692,3.4081075587,1.9690465439
H,0,-3.195214508,3.4875784875,1.6794996114
H,0,-2.1866955553,3.7515850845,0.2347983045
H,0,-3.4772347216,2.5407854599,0.1964552037
H,0,-3.0550287059,1.4323113622,3.3009433225
H,0,-3.3523094579,0.2264012208,2.0214214701
H,0,-1.9749092029,0.0247269803,3.108674188
H,0,3.2752331752,-1.0093074505,1.8598987443
H,0,2.8983540844,-1.048667567,0.1309054451
H,0,2.2092088067,0.2291138016,1.1559941423
H,0,1.5568061935,-1.5893515853,3.5855621857
H,0,0.485789585,-0.3287420482,2.9341017565
H,0,-0.0995640752,-1.9978055957,3.1014354056

Pd($P(CH_3)_3)_2$(η^2-1,1-dimethylallyl acetate) – 6-311+G**

E(RB+HF-LYP) = -1474.87855158

Zero-point correction= 0.406833 (Hartree/Particle)
Thermal correction to Energy= 0.435325
Thermal correction to Enthalpy= 0.436269
Thermal correction to Gibbs Free Energy= 0.347036
Sum of electronic and zero-point Energies= -1474.471719
Sum of electronic and thermal Energies= -1474.443227
Sum of electronic and thermal Enthalpies= -1474.442283
Sum of electronic and thermal Free Energies= -1474.531516

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	273.170	101.400	187.807

C,0,0.3279166743,-1.4927316413,-0.9663527497
C,0,0.1465001261,-1.6028230054,0.42201604
C,0,1.2809043369,-1.6828420075,1.4289241909
O,0,1.6659819392,-3.13393088,1.5839785615
C,0,2.3195680827,-3.8360161495,0.6441854577
C,0,2.4294490246,-5.2876273452,1.0616345163
Pd,0,-0.460513865,0.404610156,-0.3128891729
P,0,-0.4041983409,1.5332160426,-2.3977895578
P,0,-1.518462573,1.6947837777,1.3718726067
O,0,2.7591052249,-3.3982424887,-0.3936590185

H,0,3.1268550984,-5.8026034731,0.4032219527
H,0,1.4453770936,-5.7583326257,0.9851607174
H,0,2.753648791,-5.3693878711,2.1004019879
C,0,2.5169070454,-0.8425081497,1.1042500578
C,0,0.7920764341,-1.3735618215,2.8450078978
H,0,-0.7523872836,-2.1039395391,0.7753522681
H,0,-0.4121776961,-1.9331056945,-1.6289604124
H,0,1.3232268709,-1.4214807298,-1.3871408998
C,0,-2.5902321813,0.7691049065,2.5698529425
C,0,-0.4755220243,2.6954730101,2.5368518193
C,0,-2.7219311388,2.9977242786,0.8226185858
C,0,-1.4680146442,0.7835922867,-3.7178073039
C,0,1.2530682492,1.5089617665,-3.2268343372
C,0,-0.8420713183,3.3260572182,-2.6073764069
H,0,1.2198284014,1.9768557062,-4.2156349972
H,0,1.9779774124,2.0393265564,-2.6056548736
H,0,1.5911962889,0.4764241828,-3.328853356
H,0,-0.7188015448,3.6540864159,-3.6443185601
H,0,-1.879378781,3.4872174379,-2.3076605169
H,0,-0.2027738562,3.9368818175,-1.9661531895
H,0,-1.3425735719,1.2916663909,-4.6790901768
H,0,-1.2092882183,-0.2703472838,-3.8337172229
H,0,-2.5164213126,0.8416606252,-3.4177407848
H,0,-1.0891191888,3.2412234261,3.2602256793
H,0,0.2105973267,2.0410846689,3.0776718125
H,0,0.1221575184,3.4095955706,1.9665144622
H,0,-3.2136493483,3.4801127785,1.6729358764
H,0,-2.198064778,3.7567965454,0.2386835997
H,0,-3.4822432682,2.542876593,0.1839683429
H,0,-3.0747978225,1.4389789281,3.2871774331
H,0,-3.3576763049,0.2250964717,2.0149891221
H,0,-1.9878101865,0.0379542342,3.1105053949
H,0,3.3027811836,-1.0385237794,1.8391330848
H,0,2.9125736971,-1.0551090528,0.1146884849
H,0,2.2454199586,0.2144017172,1.1570929706
H,0,1.5785646047,-1.5854965219,3.5730623359
H,0,0.5177192488,-0.3215746117,2.9189427426
H,0,-0.0796181454,-1.9838364939,3.0924723369

Pd(P(CHCH$_2$)(Ph)$_2$)$_2$(η^2-1,1-dimethylallyl acetamidine) SDD on Pd, 6-31G on Ph, 6-31G* on all other atoms

E(RB+HF-LYP) = -2123.37379474

Zero-point correction= 0.610329 (Hartree/Particle)

Thermal correction to Energy= 0.647915
Thermal correction to Enthalpy= 0.648859
Thermal correction to Gibbs Free Energy= 0.532133
Sum of electronic and zero-point Energies= -2122.763466
Sum of electronic and thermal Energies= -2122.725880
Sum of electronic and thermal Enthalpies= -2122.724936
Sum of electronic and thermal Free Energies= -2122.841662

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	406.573	141.669	245.670

C,0,1.1338763813,-3.9966346508,-0.1071601389
C,0,1.8074379809,-2.8249324083,-0.5039941747
C,0,2.716302126,-2.8908522921,-1.576824647
C,0,2.9437957702,-4.1025517768,-2.2399318607
C,0,2.2724888717,-5.2620629431,-1.836499695
C,0,1.3696508814,-5.2067912598,-0.7667072411
P,0,1.441245192,-1.2171740278,0.3080391551
Pd,0,-0.5674306072,-0.1246731109,-0.3424517381
P,0,0.2051882659,2.0424173957,-0.9179977554
C,0,1.7794500014,2.1074453946,-1.8781624819
C,0,1.9985712348,1.1069142328,-2.8463456028
C,0,3.1587235752,1.1163569149,-3.6280511048
C,0,4.1236127129,2.1134424708,-3.4385524637
C,0,3.9207362968,3.1024095439,-2.4694498768
C,0,2.7540362183,3.1044294683,-1.6953601373
C,0,1.7254770662,-1.5249601831,2.0995632185
C,0,2.9164457133,-2.1173362414,2.5649535908
C,0,3.1144125321,-2.3262918313,3.932188336
C,0,2.1265968076,-1.9488804866,4.8526535672
C,0,0.940067228,-1.3619598583,4.4019242784
C,0,0.7402182719,-1.1509553758,3.0314336082
C,0,-2.0754364891,-1.6131340782,-0.2741225944
C,0,-2.6709205736,-0.4060134855,-0.7642668414
C,0,-3.7048705941,0.421654555,0.0004902524
C,0,-3.5575686731,1.9210929407,-0.3179467992
C,0,-3.6977398427,0.1990123658,1.5220257319
C,0,0.3885124091,3.2711323684,0.4319511018
C,0,0.8703058709,2.8591320108,1.690984334
C,0,1.0138582596,3.7812735249,2.7327784371
C,0,0.6677531688,5.123903239,2.5360564908
C,0,0.1810269975,5.5439690957,1.292528852
C,0,0.0444739569,4.6252491728,0.2456555927

N,0,-5.1185965846,0.0947557004,-0.492347417
C,0,-5.7127616768,-1.0554336493,-0.7446803909
C,0,-7.1565466302,-1.0633978886,-1.1711074425
N,0,-5.0887895276,-2.2234246462,-0.631212788
H,0,-0.6224902578,2.8170312459,-1.7714734727
H,0,2.6488989998,-0.5600434972,-0.029387568
H,0,-2.793787588,-0.3128288335,-1.8448851853
H,0,-1.7842714998,-2.3958570278,-0.9745742508
H,0,-2.2508686325,-1.9603769707,0.7435109845
H,0,-4.4236988361,0.856914331,2.0110932645
H,0,-3.94138425,-0.833515131,1.7903179359
H,0,-2.703069391,0.4281417792,1.915002499
H,0,-4.3972849164,2.4994730846,0.0910626424
H,0,-2.6436972588,2.30066364,0.140347562
H,0,-3.4965948648,2.0912133325,-1.3981517396
H,0,-7.242093332,-1.4513865133,-2.1921147974
H,0,-7.7385641684,-1.7140392207,-0.5102516861
H,0,-7.5947854133,-0.0637417349,-1.1429124296
H,0,-5.5682203368,-3.0737367814,-0.8932469154
H,0,-4.0757950907,-2.2530057617,-0.4941518403
H,0,-0.179209235,-0.6928656676,2.6780814635
H,0,0.1732882304,-1.0694712819,5.1122108836
H,0,2.2835150142,-2.1129999035,5.9136793692
H,0,4.0356131384,-2.7818657414,4.2802438255
H,0,3.683191774,-2.4205323142,1.8589145568
H,0,-0.3236263515,4.9635018383,-0.7183285945
H,0,-0.0877676905,6.5834855004,1.1357856372
H,0,0.7763338251,5.8375293765,3.346048751
H,0,1.3912194619,3.4518308334,3.695332316
H,0,1.1282822468,1.8177672662,1.8568081828
H,0,-5.7142402233,0.9079612655,-0.6010298691
H,0,1.2611339111,0.3205859266,-2.9855089923
H,0,3.3100852849,0.3471357776,-4.3786942476
H,0,5.0268739075,2.1180110912,-4.0396212868
H,0,4.6669178532,3.8753830065,-2.3169112944
H,0,2.6061760185,3.8811192015,-0.953265313
H,0,3.2506597127,-1.9990977727,-1.8915928807
H,0,3.6512655925,-4.1413331561,-3.0619255189
H,0,2.4554528373,-6.2021973614,-2.346147053
H,0,0.8554985391,-6.1061940217,-0.4430090635
H,0,0.4421367166,-3.9670379408,0.7296811256

Pd(P(CH$_3$)$_3$)$_2$(η^2-1,1-dimethylallyl acetate) – 6-31G* Solvated 6 HCN

E(RB+HF-LYP) = -2035.17916894

Zero-point correction= 0.517787 (Hartree/Particle)
Thermal correction to Energy= 0.569564
Thermal correction to Enthalpy= 0.570508
Thermal correction to Gibbs Free Energy= 0.416768
Sum of electronic and zero-point Energies= -2034.661382
Sum of electronic and thermal Energies= -2034.609605
Sum of electronic and thermal Enthalpies= -2034.608661
Sum of electronic and thermal Free Energies= -2034.762401

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	357.407	165.367	323.572

C,0,0.9731031159,-2.2452263937,2.8702163776
P,0,1.8327573187,-1.8774029908,1.2636723354
C,0,3.5704455524,-1.6682186463,1.8773548665
Pd,0,0.8896938066,-0.1286779439,-0.0587221593
P,0,2.6470983458,0.9238238872,-1.2523442617
C,0,2.3525733356,2.699947393,-1.7074429778
C,0,-0.7308921329,1.1268920889,-0.5960831507
C,0,-1.2940018194,0.0570297291,0.1478742765
C,0,-2.1502533371,-1.0308968578,-0.4478169497
C,0,-2.1258390287,-2.3121333119,0.38678853
C,0,-1.9255778312,-1.3460637236,-1.925469559
C,0,1.9466721588,-3.5761921358,0.5178114844
C,0,2.9582831004,0.1747696462,-2.9222572378
C,0,4.3816655814,1.0293878564,-0.5993181451
O,0,-3.6603521213,-0.6249351335,-0.2730560506
C,0,-4.1890174441,0.4651981351,-0.8533607156
O,0,-3.6305651694,1.156003861,-1.6878770421
C,0,-5.5816421858,0.7661998975,-0.3329875465
C,0,-2.7902478564,4.0096002511,-1.4607554252
N,0,-2.2833927969,5.0001413031,-1.1437915397
C,0,0.0969949402,5.2355434418,0.8622203063
N,0,0.9598980877,4.9403753263,1.5729465395
C,0,2.8395679732,2.7380076741,2.8916771175
N,0,3.4861424636,1.8301788685,3.2055806945
C,0,-5.734884867,-3.0451826608,-1.0602413839
N,0,-6.5078187917,-3.8460106231,-1.3781418702
C,0,-4.4533535784,-0.5290737711,2.9104051605
N,0,-4.75795506,-0.3975720082,4.0194058833
N,0,5.0661916591,-2.7914476735,-1.644791255
C,0,6.0196141656,-3.3918300817,-1.9055088355

H,0,-6.158968323,-0.1419163912,-0.1401527008
H,0,-6.1085931451,1.3934725007,-1.0540971419
H,0,-5.5026090087,1.3157191642,0.6133284717
H,0,-1.5128500628,0.2291276529,1.2025118401
H,0,-0.5798494313,2.0879221061,-0.1053979911
H,0,-0.8961545432,1.1992164852,-1.667525037
H,0,-2.6156951875,-2.1293608673,-2.2589024074
H,0,-2.0639236668,-0.4692173862,-2.5570132421
H,0,-0.901434606,-1.7111426134,-2.0513015279
H,0,-2.9041712633,-3.0146949543,0.0698582741
H,0,-1.1571583962,-2.7986764589,0.2586642651
H,0,-2.2561845984,-2.0993515032,1.4527695586
H,0,-0.7166271201,5.4636700358,0.187489197
H,0,-3.2429437324,3.0594230612,-1.7190689328
H,0,-4.1713522161,-0.6437905482,1.8785329874
H,0,-5.0179179887,-2.2988722483,-0.766862598
H,0,6.902563376,-3.9477838667,-2.1468216598
H,0,2.2349065733,3.5756543535,2.5744985616
H,0,3.7086997342,0.7427917106,-3.4859194643
H,0,3.3126262146,-0.8523482054,-2.7922834378
H,0,2.0262921584,0.1494426004,-3.4960228278
H,0,3.1649905749,3.1024185451,-2.3247412627
H,0,1.4101846688,2.7852047543,-2.2579122001
H,0,2.2656018326,3.3033376532,-0.7981962803
H,0,5.0203163514,1.6305008625,-1.2583643357
H,0,4.3775496884,1.4725263918,0.4008117527
H,0,4.8024734024,0.022349185,-0.5262336574
H,0,1.4837913345,-3.0385998829,3.4296446274
H,0,0.9544044194,-1.3379736589,3.4826243914
H,0,-0.0609251163,-2.5504439849,2.6850189857
H,0,2.3606913884,-4.3010566757,1.2294711366
H,0,0.9564123317,-3.9200911279,0.2015465641
H,0,2.5936446028,-3.5348376949,-0.3640196406
H,0,3.8530934207,-2.4866267891,2.5510647933
H,0,4.2564886264,-1.6615938985,1.0255304064
H,0,3.6654979748,-0.7162836877,2.4091371739

Pd(P(CH$_3$)$_3$)$_2$(η^2-1,1-dimethylallyl acetate) – 6-311+G Transition State for Ionization**

E(RB+HF-LYP) = -1474.84865190

Zero-point correction=	0.403940 (Hartree/Particle)
Thermal correction to Energy=	0.433038
Thermal correction to Enthalpy=	0.433982

Thermal correction to Gibbs Free Energy= 0.341379
Sum of electronic and zero-point Energies= -1474.444712
Sum of electronic and thermal Energies= -1474.415614
Sum of electronic and thermal Enthalpies= -1474.414670
Sum of electronic and thermal Free Energies= -1474.507273

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	271.735	101.009	194.900

C,0,-0.7029429502,-1.8333511865,-0.3801251307
C,0,-1.3755060466,-0.6699190346,-0.8107377596
C,0,-1.7571250563,0.3723976536,0.042571624
O,0,-4.1861186905,-1.0431588749,-0.6205404843
C,0,-5.1346422919,-0.5079343936,0.0126704464
C,0,-6.542802971,-1.0985705098,-0.1706597072
Pd,0,0.710886838,-0.2089393912,-0.1546223701
P,0,2.6045327988,-1.5846624475,0.1139529711
P,0,1.4891983683,2.0454096563,-0.0328043498
O,0,-5.0367005764,0.4920838149,0.7798751155
H,0,-7.1322737973,-0.4224025482,-0.7987669603
H,0,-7.0513481742,-1.16988212,0.7940708651
H,0,-6.5022894384,-2.0780576562,-0.6503284381
C,0,-1.9840562739,0.2075867007,1.5113791528
C,0,-2.3720295104,1.6065347153,-0.5342525525
H,0,-1.5127421354,-0.5111638011,-1.8746179246
H,0,-0.4779126861,-2.5919377068,-1.120763281
H,0,-0.8599168708,-2.214229856,0.6230068547
C,0,0.9876625759,3.1027307866,-1.4607720676
C,0,0.8942842248,3.0167158725,1.4198340734
C,0,3.3070734662,2.3899845214,0.0337958903
C,0,3.9675860163,-1.3662555548,-1.1136780521
C,0,2.3320055596,-3.4078083228,0.0309188597
C,0,3.4918796049,-1.4225124985,1.7272090398
H,0,3.2647704001,-3.9536361658,0.1980770685
H,0,1.6021267238,-3.7064099,0.7851269992
H,0,1.93355526,-3.6749769236,-0.9491481454
H,0,4.3420269684,-2.1083777144,1.7818144132
H,0,3.8513769484,-0.4004579756,1.8563125681
H,0,2.8024689799,-1.6454678125,2.5436837962
H,0,4.782822286,-2.0708449103,-0.9266653662
H,0,3.5793796596,-1.5305319148,-2.1206144603
H,0,4.3592875941,-0.3497452232,-1.0608152228
H,0,1.2579979869,4.0471447367,1.3802797234

H,0,-0.1960224851,3.0241391791,1.4383580829
H,0,1.2448397949,2.5490074814,2.3419306301
H,0,3.498644616,3.4651798963,0.0870588532
H,0,3.7490857896,1.9133995871,0.9109094653
H,0,3.7935403882,1.9935043558,-0.8593252065
H,0,1.3457501705,4.1288372801,-1.3399751049
H,0,1.3996234578,2.686507084,-2.3822372125
H,0,-0.0990223811,3.1096611435,-1.5477246649
H,0,-1.6350623262,1.0766901178,2.0761968863
H,0,-3.0855634866,0.1789780576,1.608106598
H,0,-1.5522114586,-0.696102016,1.9378774033
H,0,-3.4505341587,1.5106403929,-0.323047605
H,0,-2.0313792392,2.5146083173,-0.0272150714
H,0,-2.2135443914,1.6969384582,-1.6097657908

$Pd(P(CH_3)_3)_2(\eta^2$-1,1-dimethylallyl acetate) 6 HCN – Transition State for Ionization

E(RB+HF-LYP) = -2035.17587036

Zero-point correction= 0.516752 (Hartree/Particle)
Thermal correction to Energy= 0.568091
Thermal correction to Enthalpy= 0.569035
Thermal correction to Gibbs Free Energy= 0.417138
Sum of electronic and zero-point Energies= -2034.659119
Sum of electronic and thermal Energies= -2034.607779
Sum of electronic and thermal Enthalpies= -2034.606835
Sum of electronic and thermal Free Energies= -2034.758733

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	356.483	163.811	319.695

C,0,-0.7085612788,1.0868292162,-0.5839597223
C,0,-1.2622397029,0.0392900834,0.211241557
C,0,-1.9255956421,-1.1361873191,-0.3132067959
C,0,-1.748970384,-1.536200372,-1.7623593749
Pd,0,0.9453363662,-0.098884782,-0.0291251823
P,0,1.9875290069,-1.8250049685,1.2667195809
P,0,2.6152493877,1.0555930721,-1.2124104328
C,0,-2.0801170861,-2.3045689079,0.6384498915
O,0,-3.7898384517,-0.7142912542,-0.3104893504
C,0,-4.2466313383,0.3243738404,-0.9732484853
C,0,-5.6799588893,0.7061185529,-0.6154927465
O,0,-3.6063446739,0.9740428369,-1.8031009206
C,0,-2.9744397159,3.8049601135,-1.5376308968

N,0,-2.5236512277,4.8171370934,-1.2027734527
C,0,-0.2529869325,5.117496996,0.8908604974
N,0,0.6060919142,4.8414879811,1.6140310699
C,0,2.601788424,2.7314441807,2.8960271635
N,0,3.3055801039,1.8515242567,3.1632091079
C,0,-5.561003092,-3.20969332,-0.9215380402
N,0,-6.1786487344,-4.1559524047,-1.1741760528
C,0,-4.5224989464,-0.4387808538,2.7165045625
N,0,-4.7159449348,-0.289946986,3.8484739657
N,0,5.0613063642,-2.6170466207,-1.7521519283
C,0,5.9104033376,-3.272719387,-2.1840162374
C,0,1.1783635404,-2.1460851125,2.9061256396
C,0,2.0493414506,-3.5307673315,0.53533376
C,0,3.7481705526,-1.6127263425,1.8006504069
C,0,2.9398748797,0.3456147306,-2.8936196171
C,0,4.3383873729,1.2073396252,-0.5481559142
C,0,2.2387374116,2.8237481691,-1.6231976104
H,0,-6.3123714403,-0.1738836493,-0.4651611409
H,0,-6.1040996649,1.3327285075,-1.4028495117
H,0,-5.6821999634,1.2754640625,0.3226546218
H,0,-1.4523052898,0.235327513,1.2656556383
H,0,-0.6186676595,2.0759192502,-0.1375997571
H,0,-0.8949001142,1.1042798642,-1.654180617
H,0,-2.4471718164,-2.3355466157,-2.0270551779
H,0,-1.9103153997,-0.6928394816,-2.4330949799
H,0,-0.7281974194,-1.9119505224,-1.903314203
H,0,-2.895323571,-2.9669173585,0.3370275937
H,0,-1.1556923559,-2.891604785,0.6206593295
H,0,-2.2477475846,-1.9744055833,1.667510249
H,0,-1.0592771951,5.3236706922,0.1984693498
H,0,-3.3688560728,2.8234208748,-1.8049762703
H,0,-4.3287561616,-0.5729741193,1.6606323419
H,0,-4.9768007516,-2.3298605161,-0.688289398
H,0,6.6972859712,-3.8796835429,-2.5835767893
H,0,1.9442388233,3.5424887098,2.6152267903
H,0,3.6663210885,0.9512345538,-3.4490728299
H,0,3.3311806663,-0.6700314258,-2.7833367407
H,0,2.0057808046,0.2988985323,-3.4621321745
H,0,3.03338144,3.2734180833,-2.2305691464
H,0,1.2943022496,2.8792672883,-2.1734531745
H,0,2.1251915662,3.402523301,-0.7012141696
H,0,4.9545591749,1.844358481,-1.1943205172
H,0,4.3138742504,1.6309259952,0.4599498497
H,0,4.7953512189,0.2153623125,-0.4937323297

H,0,1.693460358,-2.9403864267,3.4596433378
H,0,1.2010396302,-1.2280503372,3.5017938351
H,0,0.1325460007,-2.4328419877,2.7626953655
H,0,2.4840911956,-4.2521533316,1.2376752768
H,0,1.0428619138,-3.8664500236,0.2643357144
H,0,2.659628504,-3.5068787871,-0.3728488646
H,0,4.0510102772,-2.4152979046,2.484154223
H,0,4.4000019445,-1.6344194556,0.9224897266
H,0,3.8633734569,-0.6485890174,2.3051506912

Pd(P(CH$_3$)$_3$)$_2$(η^2-1,1-dimethylallyl acetate) 6-31+G Onsager in Ether – Transition State for Ionization**

E(RB+HF-LYP) = -1474.66420710

Zero-point correction= 0.405639 (Hartree/Particle)
Thermal correction to Energy= 0.434748
Thermal correction to Enthalpy= 0.435692
Thermal correction to Gibbs Free Energy= 0.343527
Sum of electronic and zero-point Energies= -1474.258568
Sum of electronic and thermal Energies= -1474.229459
Sum of electronic and thermal Enthalpies= -1474.228515
Sum of electronic and thermal Free Energies= -1474.320680

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.808	101.064	193.978

C,0,-0.7289415383,-1.648884024,-0.5809330013
C,0,-1.3913391432,-0.4045033237,-0.822357497
C,0,-2.2113138183,0.2979592467,0.1035270726
O,0,-4.0427519166,-0.6723615414,-0.4244131802
C,0,-5.196829541,-0.3793165378,0.0566578967
C,0,-6.3361088271,-1.268353288,-0.4803343836
Pd,0,0.7603662531,-0.2012644436,-0.207811231
P,0,2.5864954967,-1.6368866364,0.1323540879
P,0,1.6447442971,2.0233412052,-0.0471882676
O,0,-5.4634713026,0.5114004806,0.8911533526
H,0,-6.2966203258,-1.3154177238,-1.5737691033
H,0,-7.3067060975,-0.8851224028,-0.1521406842
H,0,-6.2033457302,-2.2904322742,-0.106411751
C,0,-2.2723255135,-0.0591641556,1.5656857868
C,0,-2.6649179241,1.6931070156,-0.2416564394
H,0,-1.4604345111,-0.0602327025,-1.8521559633
H,0,-0.4909725484,-2.2683737447,-1.4433226437

H,0,-0.9617506886,-2.219824874,0.3156706901
C,0,1.004164974,3.1995339507,-1.3289487205
C,0,1.2618599898,2.9268556006,1.5253222135
C,0,3.4671620875,2.3192356248,-0.1971144002
C,0,3.9167648615,-1.557921332,-1.148979198
C,0,2.2222202388,-3.4499242965,0.17963834
C,0,3.5367407091,-1.4184436975,1.7056115044
H,0,3.137077227,-4.0319765158,0.3339192146
H,0,1.5215162527,-3.6635125183,0.9918566676
H,0,1.758654971,-3.7583002535,-0.7615065641
H,0,4.3554000857,-2.1428344865,1.773924983
H,0,3.9573045531,-0.4107594459,1.7559188491
H,0,2.8694244352,-1.5535058626,2.5616092347
H,0,4.7174648695,-2.2721999526,-0.9296572127
H,0,3.4956560498,-1.7853837414,-2.1322560195
H,0,4.3428946435,-0.5523672646,-1.1845217142
H,0,1.6372268444,3.9556342278,1.4961379016
H,0,0.1804609772,2.9444505822,1.6894460403
H,0,1.7246283794,2.4063998007,2.368877598
H,0,3.7021988011,3.3865398134,-0.1269601515
H,0,4.0062338663,1.792911686,0.595589855
H,0,3.8252835661,1.9467814065,-1.1611106092
H,0,1.4162129323,4.2053679547,-1.1909893372
H,0,1.2827529194,2.8363284424,-2.3225292661
H,0,-0.0869341901,3.2456469143,-1.2779535707
H,0,-1.4715046822,0.4666424772,2.1022646587
H,0,-3.234288713,0.2560249343,1.9754158605
H,0,-2.1452305855,-1.1300035182,1.7320402851
H,0,-3.660026518,1.8725928606,0.1708609005
H,0,-1.9736624306,2.4198197522,0.2062022905
H,0,-2.6773924813,1.8530560907,-1.3232575442

$Pd(P(CH_3)_3)_2(\eta^2$-1,1-dimethylallyl acetate) 6-31+G Onsager in THF – Transition State for Ionization**

E(RB+HF-LYP) = -1474.66750339

Zero-point correction= 0.405707 (Hartree/Particle)
Thermal correction to Energy= 0.434728
Thermal correction to Enthalpy= 0.435672
Thermal correction to Gibbs Free Energy= 0.344051
Sum of electronic and zero-point Energies= -1474.261796
Sum of electronic and thermal Energies= -1474.232775
Sum of electronic and thermal Enthalpies= -1474.231831
Sum of electronic and thermal Free Energies= -1474.323453

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.796	101.028	192.835

C,0,-0.7448612272,-1.6377724514,-0.5731506769
C,0,-1.4003922449,-0.3869913676,-0.8031766644
C,0,-2.2598490091,0.2894047152,0.1177400725
O,0,-4.0080033791,-0.6399769155,-0.413778209
C,0,-5.1772966514,-0.3749410429,0.0561528423
C,0,-6.2817118982,-1.2799479013,-0.5235621399
Pd,0,0.7536058985,-0.2015864584,-0.205479112
P,0,2.5867005743,-1.6353936002,0.1349747453
P,0,1.6500211818,2.019497349,-0.0586653691
O,0,-5.4779949219,0.4918090879,0.8999992416
H,0,-6.2237666449,-1.2948622121,-1.6169870143
H,0,-7.2671351531,-0.931642748,-0.2004737139
H,0,-6.1258744448,-2.3079511942,-0.1762515261
C,0,-2.2972666798,-0.0705306542,1.5820012602
C,0,-2.6869550948,1.6992900642,-0.2113337982
H,0,-1.471337685,-0.0377087643,-1.831413571
H,0,-0.5080750913,-2.2514093616,-1.4403220018
H,0,-0.9793168766,-2.2162470069,0.318463317
C,0,1.0097509973,3.1971837904,-1.3401467531
C,0,1.279670864,2.9314698303,1.5126165966
C,0,3.4726621608,2.3067732405,-0.218902754
C,0,3.9117543117,-1.5604737471,-1.1518751042
C,0,2.2213581392,-3.4485545094,0.1866675429
C,0,3.5442450721,-1.4161063893,1.7036968349
H,0,3.136759988,-4.0313099131,0.3347827035
H,0,1.5264301816,-3.6608546166,1.0042747041
H,0,1.7510089045,-3.7571641814,-0.7510987937
H,0,4.363378031,-2.1402084465,1.7682218588
H,0,3.9657211377,-0.4087035388,1.7515510004
H,0,2.8814880078,-1.5506848994,2.5633488503
H,0,4.7129651719,-2.2745478268,-0.934068237
H,0,3.4870664686,-1.7898186479,-2.1331831339
H,0,4.3390129142,-0.5556082198,-1.1913568856
H,0,1.6607464421,3.9579884168,1.4781421812
H,0,0.1990948669,2.9552532549,1.6822531885
H,0,1.7441809959,2.4116808917,2.3556191224
H,0,3.7134527978,3.3730027176,-0.1525187748
H,0,4.0139479373,1.7799048112,0.5718396156
H,0,3.824072835,1.9305327335,-1.1838743967

H,0,1.4293911387,4.2006024444,-1.207403796
H,0,1.2811120127,2.8296138283,-2.3341389415
H,0,-0.0808816857,3.2505554981,-1.2838734964
H,0,-1.4696452688,0.4326560184,2.0979786341
H,0,-3.240444884,0.2635282789,2.0189383313
H,0,-2.1894734918,-1.1449929177,1.7399127583
H,0,-3.6646835236,1.9087630534,0.2266815571
H,0,-1.9607003666,2.4037045358,0.2146307853
H,0,-2.7238584191,1.8598700221,-1.2924076276

$Pd(P(CH_3)_3)_2(\eta^2$-1,1-dimethylallyl acetate) 6-31+G Onsager in H_2O – Transition State for Ionization**

E(RB+HF-LYP) = -1474.67183041

Zero-point correction= 0.405718 (Hartree/Particle)
Thermal correction to Energy= 0.434674
Thermal correction to Enthalpy= 0.435619
Thermal correction to Gibbs Free Energy= 0.344252
Sum of electronic and zero-point Energies= -1474.266112
Sum of electronic and thermal Energies= -1474.237156
Sum of electronic and thermal Enthalpies= -1474.236212
Sum of electronic and thermal Free Energies= -1474.327579

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	272.762	100.997	192.298

C,0,-0.7633724412,-1.6249883689,-0.5722361262
C,0,-1.4090495213,-0.3655823756,-0.78738972
C,0,-2.3134783026,0.2802017964,0.1276178085
O,0,-3.9687071487,-0.6027837046,-0.4105712775
C,0,-5.1540543612,-0.3676689212,0.0461810484
C,0,-6.2187109674,-1.2883289397,-0.5791860234
Pd,0,0.7433997144,-0.2017371656,-0.2013335588
P,0,2.5866989649,-1.6337247089,0.1355543336
P,0,1.6561680443,2.0135722864,-0.0602751939
O,0,-5.4915070978,0.4715048004,0.8994374091
H,0,-6.1239540778,-1.2921504807,-1.6698899222
H,0,-7.220715385,-0.962038415,-0.2848730608
H,0,-6.0535055365,-2.3158809393,-0.2351411118
C,0,-2.32537673,-0.0858726469,1.5936066507
C,0,-2.7074829721,1.7081546577,-0.178405442
H,0,-1.4813403113,-0.008781715,-1.8133310228
H,0,-0.5255874678,-2.2298196015,-1.4456171616

H,0,-1.0021757557,-2.214144631,0.3115768196
C,0,1.0179499165,3.1989851131,-1.3367568757
C,0,1.3013414669,2.9292438801,1.5131701128
C,0,3.4792013261,2.2889413346,-0.2311834908
C,0,3.9050008678,-1.5591884758,-1.1579652636
C,0,2.2198768561,-3.4471401141,0.1865543734
C,0,3.552722988,-1.4184567024,1.6995380359
H,0,3.1358510511,-4.0310856068,0.3258963001
H,0,1.5315381562,-3.6605883481,1.0095611991
H,0,1.7420404464,-3.7530675485,-0.7483885248
H,0,4.3724443056,-2.1423511732,1.7570025388
H,0,3.9754116095,-0.411631518,1.747949309
H,0,2.8955024697,-1.5554848468,2.5631043437
H,0,4.7068361988,-2.2737448309,-0.944501329
H,0,3.4758666995,-1.7875430218,-2.1375796931
H,0,4.3338134452,-0.5551385311,-1.1989246455
H,0,1.6925030752,3.9519164798,1.4775620104
H,0,0.2216584371,2.9630967323,1.687952093
H,0,1.7651712818,2.40496611,2.3537451023
H,0,3.7278965544,3.3533322482,-0.1652067855
H,0,4.022388143,1.758009069,0.5553830709
H,0,3.8225486513,1.9116185601,-1.1985930106
H,0,1.4473898323,4.1984980034,-1.2057327507
H,0,1.2811276221,2.8303256092,-2.3325647071
H,0,-0.0720416515,3.2615794022,-1.2746430928
H,0,-1.4718977503,0.3931395043,2.0882354504
H,0,-3.2484719797,0.2652077557,2.0591841915
H,0,-2.2363356725,-1.1638008947,1.7411155583
H,0,-3.6667302674,1.9475711584,0.2841096259
H,0,-1.9463489399,2.3839288177,0.2300903946
H,0,-2.7659699647,1.8766884162,-1.2575241631

$Pd(P(H)(Ph)_2)_2(\eta^2$-1,1-dimethylallyl acetamidine) SDD on Pd, 6-31G on Ph, 6-31G* on all other atoms – Transition State for loss of acetamidine

E(RB+HF-LYP) = -2123.35595516

Zero-point correction= 0.606849 (Hartree/Particle)
Thermal correction to Energy= 0.645286
Thermal correction to Enthalpy= 0.646230
Thermal correction to Gibbs Free Energy= 0.526468
Sum of electronic and zero-point Energies= -2122.749106
Sum of electronic and thermal Energies= -2122.710669
Sum of electronic and thermal Enthalpies= -2122.709725
Sum of electronic and thermal Free Energies= -2122.829487

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	404.923	142.513	252.061

C,0,0.4753700224,4.104917016,-0.0172568946
C,0,-0.5582039776,3.264025016,-0.4733758946
C,0,-1.3184269776,3.655852016,-1.5917598946
C,0,-1.0469929776,4.864810016,-2.2421588946
C,0,-0.0192309776,5.695703016,-1.7817858946
C,0,0.7385040224,5.315043016,-0.6668178946
P,0,-0.8653279776,1.639875016,0.3194691054
Pd,0,0.4972670224,-0.139419984,-0.3715038946
P,0,-1.0877969776,-1.838664984,-0.8950388946
C,0,-2.5640059776,-1.304885984,-1.8570038946
C,0,-2.3834649776,-0.322440984,-2.8514088946
C,0,-3.4632599776,0.100230016,-3.6337778946
C,0,-4.7377599776,-0.439473984,-3.4195838946
C,0,-4.9273579776,-1.405788984,-2.4252248946
C,0,-3.8469229776,-1.841419984,-1.6487168946
C,0,-0.9698819776,1.979715016,2.1194681054
C,0,-1.7870409776,3.013114016,2.6206191054
C,0,-1.8679009776,3.242699016,3.9964121054
C,0,-1.1353269776,2.446548016,4.8879351054
C,0,-0.3206469776,1.419628016,4.4005741054
C,0,-0.2373269776,1.186956016,3.0218791054
C,0,2.4064430224,0.754558016,-0.2614928946
C,0,2.6176380224,-0.506041984,-0.9132388946
C,0,2.9982800224,-1.731634984,-0.2783708946
C,0,2.8239220224,-3.009594984,-1.0689388946
C,0,2.9598690224,-1.885983984,1.2255031054
C,0,-1.7075549776,-2.883781984,0.4743171054
C,0,-2.0290459776,-2.297757984,1.7152321054
C,0,-2.5014259776,-3.085625984,2.7697171054
C,0,-2.6470399776,-4.468521984,2.6036721054
C,0,-2.3233539776,-5.062615984,1.3780911054
C,0,-1.8592479776,-4.276273984,0.3178571054
N,0,5.1313600224,-1.801991984,-0.4229528946
C,0,6.0560090224,-0.900251984,-0.5426508946
C,0,7.5076540224,-1.227217984,-0.8148198946
N,0,5.7683570224,0.415622016,-0.4050558946
H,0,-0.5966559776,-2.872265984,-1.7333348946
H,0,-2.2311899776,1.500292016,-0.0202238946
H,0,2.6667740224,-0.512794984,-2.0009488946

H,0,2.4540470224,1.661040016,-0.8625398946
H,0,2.6994650224,0.893892016,0.7788611054
H,0,3.5665090224,-2.737498984,1.5420011054
H,0,3.3198070224,-0.994630984,1.7435821054
H,0,1.9254590224,-2.071317984,1.5424671054
H,0,3.4680820224,-3.808980984,-0.6930098946
H,0,1.7903390224,-3.359349984,-0.9618248946
H,0,3.0204250224,-2.857531984,-2.1336538946
H,0,7.8014340224,-0.850817984,-1.8017158946
H,0,8.1523650224,-0.752950984,-0.0670378946
H,0,7.6831720224,-2.304611984,-0.7906648946
H,0,6.4605180224,1.110528016,-0.6394138946
H,0,4.8018990224,0.711992016,-0.3627648946
H,0,0.3937690224,0.389083016,2.6415261054
H,0,0.2485020224,0.802773016,5.0883531054
H,0,-1.2003899776,2.628486016,5.9555051054
H,0,-2.5001799776,4.039709016,4.3731851054
H,0,-2.3526239776,3.639540016,1.9381321054
H,0,-1.6216409776,-4.745846984,-0.6318808946
H,0,-2.4348349776,-6.133626984,1.2455491054
H,0,-3.0094869776,-5.079034984,3.4239011054
H,0,-2.7506709776,-2.622048984,3.7184711054
H,0,-1.9066119776,-1.228810984,1.8592631054
H,0,5.4854000224,-2.748506984,-0.5314548946
H,0,-1.3985589776,0.108166016,-3.0132788946
H,0,-3.3109629776,0.847810016,-4.4056068946
H,0,-5.5766279776,-0.108200984,-4.0225128946
H,0,-5.9136069776,-1.824874984,-2.2552628946
H,0,-4.0047779776,-2.596229984,-0.8863788946
H,0,-2.1256429776,3.023664016,-1.9507508946
H,0,-1.6434639776,5.160586016,-3.0989128946
H,0,0.1853390224,6.635913016,-2.2827148946
H,0,1.5279660224,5.962687016,-0.2995738946
H,0,1.0576160224,3.826625016,0.8560931054

Pd(P(CH_3)$_3$)$_2$(η^3-1,1-dimethylallyl)

E(RB+HF-LYP) = -1245.98871731

Zero-point correction= 0.358190 (Hartree/Particle)
Thermal correction to Energy= 0.381707
Thermal correction to Enthalpy= 0.382651
Thermal correction to Gibbs Free Energy= 0.306240
Sum of electronic and zero-point Energies= -1245.630528
Sum of electronic and thermal Energies= -1245.607010

Sum of electronic and thermal Enthalpies= -1245.606066
Sum of electronic and thermal Free Energies= -1245.682477

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	239.525	83.933	160.821

C,0,0.1955591669,-1.705180093,1.9153883745
Pd,0,0.0450486177,-0.3115915499,0.256318652
P,0,0.5137157753,0.8763532056,-1.7651230218
C,0,1.0815972945,-2.1664800308,0.9052798417
C,0,2.1977855714,-1.4434836015,0.4561128203
P,0,-2.0247507761,0.4886846666,1.047343338
C,0,-2.1264673664,0.6330918189,2.883997458
C,0,-2.6445939294,2.1421836405,0.5134898013
C,0,-3.4233962774,-0.6360029732,0.625237324
C,0,2.0931024969,1.8332019287,-1.7567262708
C,0,0.6976295957,-0.2419555097,-3.2238651989
C,0,-0.6746940292,2.1307956677,-2.415240291
H,0,0.7696370651,-3.0208828764,0.3066323351
H,0,-0.6653520293,-2.3236015767,2.1514903744
H,0,0.5609761529,-1.1041802536,2.7438635227
C,0,2.9782945572,-1.9753419191,-0.7219401091
C,0,2.9527364766,-0.4611087077,1.3251295317
H,0,2.2615713137,2.3080162161,-2.7281695545
H,0,2.0534279063,2.6076215988,-0.985938312
H,0,2.9368463025,1.1748149595,-1.5381677376
H,0,-0.3070223414,2.5423056989,-3.360179744
H,0,-1.6496141557,1.6697257371,-2.593529744
H,0,-0.7956850405,2.9480727076,-1.7010401542
H,0,0.9402700722,0.333905347,-4.1223468659
H,0,1.4891896558,-0.973092876,-3.0476298287
H,0,-0.2376092822,-0.7827499539,-3.3919957009
H,0,3.384551328,-1.170208072,-1.3417424371
H,0,3.8422581619,-2.546372914,-0.3561256293
H,0,2.3811692121,-2.6398547724,-1.3510534173
H,0,3.3273378463,0.3829752891,0.7391910594
H,0,2.3683309646,-0.0669562596,2.1572368057
H,0,3.8321979164,-0.9685141192,1.7447924719
H,0,-4.3609490758,-0.2616744536,1.0478275068
H,0,-3.5269594084,-0.711944582,-0.4601933428
H,0,-3.2271732872,-1.635598139,1.0208801106
H,0,-3.117327717,0.9881933881,3.1834151596
H,0,-1.9412504142,-0.335254654,3.3531696577

H,0,-1.3745083048,1.341255886,3.2423167312
H,0,-3.583688212,2.3728415178,1.0260510177
H,0,-1.9114313304,2.915033485,0.7590857701
H,0,-2.8212260408,2.1554455611,-0.5629824813

$Pd(P(CH_3)_3)_2$(-1,1-dimethylallyl) – 6-31G Solvated with 6 HCN**

E(RB+HF-LYP) = -1806.52243762

Zero-point correction= 0.463289 (Hartree/Particle)
Thermal correction to Energy= 0.512684
Thermal correction to Enthalpy= 0.513628
Thermal correction to Gibbs Free Energy= 0.357110
Sum of electronic and zero-point Energies= -1806.059148
Sum of electronic and thermal Energies= -1806.009754
Sum of electronic and thermal Enthalpies= -1806.008810
Sum of electronic and thermal Free Energies= -1806.165328

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	321.714	150.436	329.420

C,0,2.9805090018,1.1731998249,-1.3335765686
P,0,2.126921028,0.0126027423,-0.1776572213
C,0,2.9849154099,0.3780200328,1.4125440604
Pd,0,-0.22064041,0.0672576007,-0.3715225955
P,0,-1.0512422187,0.6498395361,1.7818510072
C,0,0.1054824639,1.0630064279,3.1592133158
C,0,-0.090680569,-0.4715610148,-2.4759583059
C,0,-1.3739337818,0.0979732542,-2.2610682978
C,0,-2.3359414898,-0.46701938,-1.4060379914
C,0,-3.6104654019,0.3043751793,-1.1482331578
C,0,-2.4331113639,-1.9541086512,-1.1335138272
C,0,2.8217993951,-1.6423308625,-0.6079583735
C,0,-2.1249106763,-0.6249162224,2.57755361
C,0,-2.1147787162,2.1624958637,1.7495515221
N,0,-2.3235349974,3.512511339,-3.0436866
C,0,-2.6951176273,4.407392401,-3.674390917
N,0,1.7103166741,3.9591552738,1.3807205928
C,0,1.9913358432,5.0806371944,1.4026636541
N,0,1.2583879172,-2.5738555532,3.0898950038
C,0,1.444896335,-3.5625327951,3.6601029779
H,0,-3.4770625999,1.3799782773,-1.2940149037
H,0,-4.3853788006,-0.0354386056,-1.8517160609
H,0,-4.0069998804,0.1142053213,-0.1461846411

H,0,-3.2091748928,-2.3798126419,-1.7875031478
H,0,-2.752735694,-2.1467781273,-0.1046497256
H,0,-1.505733332,-2.4988998071,-1.3202110809
H,0,-1.5443501712,1.1227813911,-2.5881561393
H,0,0.0569010422,-1.548698385,-2.4755338287
H,0,0.6023586271,0.0815168245,-3.1041674549
H,0,0.7155030971,0.1907120341,3.4059515104
H,0,-0.4660161094,1.3587498564,4.04656564
H,0,0.756201733,1.8895439931,2.863494341
H,0,-1.5382882106,-1.5363067994,2.7292641578
H,0,-2.9907657976,-0.8618816744,1.9538957799
H,0,-2.4829677219,-0.2687835563,3.5503981128
H,0,-2.5215641621,2.3710755095,2.7456878083
H,0,-2.9413601481,2.0374971508,1.0461687404
H,0,-1.5106175178,3.0155825016,1.4255689529
H,0,1.6185645024,-4.4774172351,4.1906710475
H,0,2.6506782813,-0.3215909655,2.1825434921
H,0,2.7653595495,1.4005651049,1.7287802071
H,0,4.0651537204,0.2684216703,1.2675305234
H,0,2.4900225489,-2.3702964503,0.1389541798
H,0,2.4596695875,-1.9701414918,-1.5856571761
H,0,3.9159572875,-1.5991625236,-0.6115808034
H,0,4.0659110116,1.0666232834,-1.2372083621
H,0,2.6868361408,0.9673361919,-2.3664835818
H,0,2.6919844064,2.2000466234,-1.0887537943
H,0,2.2531448623,6.1196422365,1.4249588539
H,0,-3.0402313467,5.2361633268,-4.2592659996
N,0,-5.5097753114,-1.508076836,1.5009881591
C,0,-6.5793147895,-1.8789434636,1.7361661695
H,0,-7.5700425419,-2.2231545735,1.955018715
N,0,0.5812040816,-4.0299483507,-2.749036323
C,0,0.6478556268,-5.0154575358,-3.3498789636
H,0,0.709850059,-5.9290737968,-3.9063063386
N,0,6.3289758559,-0.2187614756,-0.3007490594
C,0,7.4795559922,-0.2743447098,-0.3999490916
H,0,8.5458757388,-0.325972512,-0.4912277253

$Pd(P(H)(Ph)_2)_2((\eta^3$-1,1-dimethylallyl) SDD on Pd, 6-31G on Ph, 6-31G* on all other atoms

E(RB+HF-LYP) = -1934.04639865

Zero-point correction=	0.519383 (Hartree/Particle)
Thermal correction to Energy=	0.551888
Thermal correction to Enthalpy=	0.552832

Thermal correction to Gibbs Free Energy= 0.448330
Sum of electronic and zero-point Energies= -1933.527015
Sum of electronic and thermal Energies= -1933.494511
Sum of electronic and thermal Enthalpies= -1933.493567
Sum of electronic and thermal Free Energies= -1933.598069

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	346.315	121.871	219.943

C,0,2.5397124579,3.7207920331,0.6958209296
C,0,1.6199140934,2.7522897747,0.2444597639
C,0,0.7627510281,3.0653603626,-0.8293380505
C,0,0.8186611813,4.3264118855,-1.432362017
C,0,1.7360153391,5.2812732054,-0.9779836627
C,0,2.5966406786,4.9769067242,0.0843098081
P,0,1.530800847,1.1115809708,1.0357346042
C,0,0.4808342112,1.2791811646,2.5319110925
C,0,0.41967265,0.1940197777,3.4304017719
C,0,-0.3729353696,0.2741556398,4.5792936354
C,0,-1.1237501576,1.4297433645,4.8355197312
C,0,-1.0748907463,2.5052262118,3.9426460441
C,0,-0.2741219667,2.4352881411,2.7951711283
Pd,0,1.0616708131,-0.7367875543,-0.3640607565
C,0,2.4772630894,-2.3006434501,-0.995401954
C,0,3.2751444566,-1.1393594964,-1.0716070638
C,0,3.3789092187,-0.287004042,-2.3207653825
P,0,-1.2850318259,-0.7774171998,-0.2163928446
C,0,-2.209268542,-0.2400152587,-1.700354033
C,0,-3.618934535,-0.25253982,-1.715195767
C,0,-4.3131675817,0.1826602252,-2.8468302677
C,0,-3.612279706,0.6337501624,-3.9738638247
C,0,-2.2137622639,0.64943446,-3.9684534292
C,0,-1.5138152123,0.2135732025,-2.8367229816
C,0,-2.0259266188,-2.3558888908,0.3338557029
C,0,-2.3035021534,-3.3844548601,-0.5873645557
C,0,-2.8153093749,-4.6071094106,-0.1416270676
C,0,-3.0483889715,-4.8174087528,1.2234431155
C,0,-2.7750977712,-3.798871461,2.143813766
C,0,-2.2671898909,-2.5715232519,1.7043525968
C,0,1.2588308919,-2.4583009699,-1.7018249529
C,0,4.4360056159,-0.9931018924,-0.1148648873
H,0,2.8177169704,1.0430481795,1.6181141458
H,0,-1.7874891336,0.0783380879,0.7884418317

H,0,2.6802448166,-2.9901067661,-0.1764912819
H,0,0.6527168269,-3.3349260656,-1.4945741221
H,0,1.1227286688,-2.0305979289,-2.6922053332
H,0,4.2909652479,-0.5718054164,-2.8652062249
H,0,2.5367117317,-0.4047651788,-3.0056989829
H,0,3.475357608,0.7750022945,-2.0722380054
H,0,5.3605824262,-1.3351386944,-0.6008898738
H,0,4.5996221816,0.0543790562,0.1616412336
H,0,4.2984282132,-1.5782585632,0.799180194
H,0,-0.4277269913,0.2249749901,-2.8353903025
H,0,-1.6693105371,0.994846093,-4.8409057517
H,0,-4.1554447518,0.9685876283,-4.8510333597
H,0,-5.397749538,0.1694691242,-2.8505610697
H,0,-4.171113133,-0.6077107559,-0.8510556808
H,0,3.2055247064,3.4982407735,1.5238749707
H,0,3.309282329,5.7149055569,0.4363150697
H,0,1.7821336603,6.2567540025,-1.4500112063
H,0,0.1524472238,4.5601686645,-2.2558935256
H,0,0.0567384458,2.3263481338,-1.1956200925
H,0,0.995560616,-0.7081334708,3.2399820456
H,0,-0.4004738809,-0.5585448148,5.274347397
H,0,-1.7387202775,1.4907294542,5.7269276556
H,0,-1.6515515165,3.4027063152,4.1395104018
H,0,-0.2318824611,3.2814193829,2.1184287748
H,0,-2.0661650406,-1.7850390873,2.4261334115
H,0,-2.9647263312,-3.9550994891,3.2004513026
H,0,-3.4462537958,-5.7664696134,1.5660562097
H,0,-3.0363637524,-5.3909468882,-0.858258707
H,0,-2.143267549,-3.2256727402,-1.6493378545

The Nature of Decarboxylation / Proton Transfer in Orotidine Decarboxylase

B3LYP//6-31+G** on all atoms unless otherwise noted

K^+
E(RB+HF-LYP) = -599.725019794

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015176

Sum of electronic and zero-point Energies= -599.725020
Sum of electronic and thermal Energies= -599.723604
Sum of electronic and thermal Enthalpies= -599.722659
Sum of electronic and thermal Free Energies= -599.740196

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
TOTAL	0.889	2.981	36.909

K,0,0.,0.,0.

Water

E(RB+HF-LYP) = -76.4340476910

Zero-point correction= 0.021287 (Hartree/Particle)
Thermal correction to Energy= 0.024123
Thermal correction to Enthalpy= 0.025067
Thermal correction to Gibbs Free Energy= 0.003638
Sum of electronic and zero-point Energies= -76.412761
Sum of electronic and thermal Energies= -76.409925
Sum of electronic and thermal Enthalpies= -76.408981
Sum of electronic and thermal Free Energies= -76.430410

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
TOTAL	15.137	6.014	45.101

H,0,-0.1065172272,0.,-0.8932457907
O,0,-0.0918033121,0.,0.0717246082
H,0,0.8409437237,0.,0.3194489253

8 Waters in a hydrogen bonded cluster – orientation A

E(RB+HF-LYP) = -611.579629323

Zero-point correction= 0.201080 (Hartree/Particle)
Thermal correction to Energy= 0.221294
Thermal correction to Enthalpy= 0.222238
Thermal correction to Gibbs Free Energy= 0.151613
Sum of electronic and zero-point Energies= -611.378549
Sum of electronic and thermal Energies= -611.358335
Sum of electronic and thermal Enthalpies= -611.357391
Sum of electronic and thermal Free Energies= -611.428016

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	138.864	66.966	148.643

O,0,1.8626151722,-0.2255565889,-0.736701768
H,0,2.297490657,-0.1665884809,-1.5957043416
H,0,1.5638211273,0.6835253424,-0.5037000941
O,0,0.7333583175,2.1653074208,0.0613790779
H,0,1.2085210941,2.8127155686,0.5967872864
H,0,0.179036219,2.6751473169,-0.5922758032
O,0,-3.0992033686,1.9604918329,-0.8204925964
H,0,-3.8925155489,2.3358114608,-0.4208761845
H,0,-2.6668983426,1.3923393321,-0.1275986296
O,0,-0.2580792297,-1.7371511215,0.4617415496
H,0,0.2397378879,-1.3234879109,-0.2688957948
H,0,0.4308285848,-1.7783614565,1.1623457025
O,0,2.2665413305,-2.0691670468,1.6010112646
H,0,2.5679901358,-1.4948806086,0.8779783774
H,0,2.2299461814,-2.9680428884,1.2269729553
O,0,-1.621696087,0.6727837569,1.0044481538
H,0,-0.7912855794,1.1771513031,0.9301580098
H,0,-1.3512137768,-0.2621228746,0.8857446627
O,0,-0.9731110207,3.4016609864,-1.5722978054
H,0,-0.8851769767,3.4113532862,-2.5324971406
H,0,-1.8369013068,2.9541575048,-1.3646047915
O,0,1.053344541,-4.2543058525,0.1556853799
H,0,0.3009468144,-3.6322216782,0.1413340294
H,0,0.6955155874,-5.1290023154,0.3466457075

8 Waters in a hydrogen bonded cluster – orientation B

E(RB+HF-LYP) = -611.586942501

Zero-point correction=	0.200146 (Hartree/Particle)
Thermal correction to Energy=	0.220477
Thermal correction to Enthalpy=	0.221422
Thermal correction to Gibbs Free Energy=	0.150369
Sum of electronic and zero-point Energies=	-611.386797
Sum of electronic and thermal Energies=	-611.366465
Sum of electronic and thermal Enthalpies=	-611.365521
Sum of electronic and thermal Free Energies=	-611.436573

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	138.352	66.657	149.542

O,0,0.572015121,2.2329982063,0.5162471169
O,0,1.0982511918,0.1942484729,2.3763766408
O,0,0.6363120817,-2.1225606499,0.8263752839
O,0,2.5432027715,-1.5915183421,-1.1330647497
O,0,2.0941222532,1.1025019933,-1.5608654362
O,0,-2.0043224124,2.2815094778,-0.0848473388
O,0,-3.0262758015,-0.032269409,-0.8791160587
O,0,-1.8224767383,-2.2648659848,-0.1144647372
H,0,-2.3737585744,1.4093951483,-0.4014166676
H,0,-2.5881092143,-0.8702150974,-0.5612011028
H,0,-2.2705391793,-2.9572373114,0.3838576147
H,0,-0.8819004024,-2.2190370932,0.2309548953
H,0,0.7809150847,-1.3641264924,1.4278269266
H,0,1.3286360156,-2.044017154,0.1341008947
H,0,0.6572713944,0.341141253,3.2209461405
H,0,0.9031220743,0.970963455,1.8118750464
H,0,0.8719231692,3.1373490321,0.6724336208
H,0,1.5414780751,1.4946335007,-0.8505372693
H,0,1.650104727,1.3034946753,-2.3934521066
H,0,2.4443256554,-0.6289480302,-1.3100192503
H,0,-0.4046553533,2.2815167342,0.3026046436
H,0,-2.658961111,2.6470438543,0.5214839308
H,0,3.4764619122,-1.7431726244,-0.9440433005
H,0,-3.2029420085,-0.1591339662,-1.8185397836

CO_2 – not perfectly linear

E(RB+HF-LYP) = -188.587511016

Zero-point correction= 0.010720 (Hartree/Particle)
Thermal correction to Energy= 0.013741
Thermal correction to Enthalpy= 0.014685
Thermal correction to Gibbs Free Energy= -0.004981
Sum of electronic and zero-point Energies= -188.576791
Sum of electronic and thermal Energies= -188.573770
Sum of electronic and thermal Enthalpies= -188.572826
Sum of electronic and thermal Free Energies= -188.592492

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	8.623	7.159	41.391

O,0,0.,0.,0.
C,0,0.,0.,1.1434

O,0,0.000287,0.,2.2868

CO_2 – linear

E(RB+HF-LYP) = -188.590392622

Zero-point correction= 0.011565 (Hartree/Particle)
Thermal correction to Energy= 0.014202
Thermal correction to Enthalpy= 0.015146
Thermal correction to Gibbs Free Energy= -0.009150
Sum of electronic and zero-point Energies= -188.578828
Sum of electronic and thermal Energies= -188.576191
Sum of electronic and thermal Enthalpies= -188.575247
Sum of electronic and thermal Free Energies= -188.599543

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	8.912	6.941	51.135

O,0,0.,0.,-1.169378144
C,0,0.,0.,0.
O,0,0.,0.,1.169378144

CO_2 – PCM acetone

E(RB+HF-LYP) = -188.594490104

Zero-point correction= 0.011482 (Hartree/Particle)
Thermal correction to Energy= 0.014118
Thermal correction to Enthalpy= 0.015062
Thermal correction to Gibbs Free Energy= -0.009232
Sum of electronic and zero-point Energies= -188.583009
Sum of electronic and thermal Energies= -188.580372
Sum of electronic and thermal Enthalpies= -188.579428
Sum of electronic and thermal Free Energies= -188.603722

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	8.859	6.938	51.131

O,0,0.,0.,-1.1691308162
C,0,0.,0.,0.
O,0,0.,0.,1.1691308162

CO_2 – PCM water

E(RB+HF-LYP) = -188.594758364

Zero-point correction= 0.011467 (Hartree/Particle)
Thermal correction to Energy= 0.014105
Thermal correction to Enthalpy= 0.015049
Thermal correction to Gibbs Free Energy= -0.009247
Sum of electronic and zero-point Energies= -188.583291
Sum of electronic and thermal Energies= -188.580653
Sum of electronic and thermal Enthalpies= -188.579709
Sum of electronic and thermal Free Energies= -188.604005

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	8.851	6.945	51.136

O,0,0.,0.,-1.1691213077
C,0,0.,0.,0.
O,0,0.,0.,1.1691213077

CO_2 – 6-311++G

E(RB+HF-LYP) = -188.562456767

Zero-point correction= 0.009210 (Hartree/Particle)
Thermal correction to Energy= 0.012251
Thermal correction to Enthalpy= 0.013196
Thermal correction to Gibbs Free Energy= -0.008292
Sum of electronic and zero-point Energies= -188.553247
Sum of electronic and thermal Energies= -188.550205
Sum of electronic and thermal Enthalpies= -188.549261
Sum of electronic and thermal Free Energies= -188.570749

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	7.688	7.290	45.225

C,0,0.0005582652,0.,0.0003357566
O,0,-0.5558600073,0.,1.0456782649
O,0,0.5554413083,0.,-1.0459300823

Acetic Acid

E(RB+HF-LYP) = -229.105826672

Zero-point correction= 0.061707 (Hartree/Particle)
Thermal correction to Energy= 0.066282

Thermal correction to Enthalpy= 0.067226
Thermal correction to Gibbs Free Energy= 0.034481
Sum of electronic and zero-point Energies= -229.044119
Sum of electronic and thermal Energies= -229.039545
Sum of electronic and thermal Enthalpies= -229.038601
Sum of electronic and thermal Free Energies= -229.071345

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	41.592	14.310	68.916

C,0,0.6529966568,-1.1310236544,0.5091210242
H,0,0.6787945194,-1.1757070023,1.5972384661
H,0,1.6716334208,-1.1323210088,0.1090891053
H,0,0.144801719,-2.0138375421,0.1090889992
C,0,-0.067215917,0.1164213958,0.0726600901
O,0,-0.1251169691,0.2167091412,-1.2814580039
O,0,-0.5510428739,0.954434332,0.8039129798
H,0,-0.6006353547,1.0403313198,-1.4857430629

Acetate Anion

E(RB+HF-LYP) = -228.543474691

Zero-point correction= 0.047933 (Hartree/Particle)
Thermal correction to Energy= 0.052411
Thermal correction to Enthalpy= 0.053355
Thermal correction to Gibbs Free Energy= 0.019821
Sum of electronic and zero-point Energies= -228.495541
Sum of electronic and thermal Energies= -228.491064
Sum of electronic and thermal Enthalpies= -228.490120
Sum of electronic and thermal Free Energies= -228.523654

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	32.888	13.092	70.578

C,0,0.6345320943,-1.0990421535,0.4739473511
H,0,0.6488281201,-1.1238037896,1.5690036498
H,0,1.6647085716,-1.1189438356,0.0944666351
H,0,0.1366790991,-2.0011518653,0.0944664842
C,0,-0.0988718101,0.1712510484,-0.0672405469
O,0,-0.1509625798,0.2614751435,-1.3252348586
O,0,-0.5570596072,0.9648556217,0.8004626593

HF

E(RB+HF-LYP) = -100.451369761

Zero-point correction= 0.009268 (Hartree/Particle)
Thermal correction to Energy= 0.011628
Thermal correction to Enthalpy= 0.012572
Thermal correction to Gibbs Free Energy= -0.007150
Sum of electronic and zero-point Energies= -100.442102
Sum of electronic and thermal Energies= -100.439742
Sum of electronic and thermal Enthalpies= -100.438797
Sum of electronic and thermal Free Energies= -100.458520

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	7.297	4.968	41.510

F,0,0.,0.,-0.0927832017
H,0,0.,0.,0.8350488154

Fluoride

E(RB+HF-LYP) = -99.8596976553

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.014159
Sum of electronic and zero-point Energies= -99.859698
Sum of electronic and thermal Energies= -99.858281
Sum of electronic and thermal Enthalpies= -99.857337
Sum of electronic and thermal Free Energies= -99.873856

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	0.889	2.981	34.768

F,0,0.,0.,0.

Formic Acid

E(RB+HF-LYP) = -189.775494786

Zero-point correction= 0.033781 (Hartree/Particle)
Thermal correction to Energy= 0.036951
Thermal correction to Enthalpy= 0.037896

Thermal correction to Gibbs Free Energy= 0.009690
Sum of electronic and zero-point Energies= -189.741714
Sum of electronic and thermal Energies= -189.738543
Sum of electronic and thermal Enthalpies= -189.737599
Sum of electronic and thermal Free Energies= -189.765805

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	23.187	8.656	59.363

C,0,-0.3057409798,0.,-0.2930667742
O,0,-0.3984902805,0.,1.0512457316
O,0,0.7283033753,0.,-0.9159516931
H,0,0.5066702281,0.,1.4123358591
H,0,-1.3107291071,0.,-0.7362875215

Formate Anion

E(RB+HF-LYP) = -189.220750692

Zero-point correction= 0.020029 (Hartree/Particle)
Thermal correction to Energy= 0.023012
Thermal correction to Enthalpy= 0.023956
Thermal correction to Gibbs Free Energy= -0.003788
Sum of electronic and zero-point Energies= -189.200722
Sum of electronic and thermal Energies= -189.197739
Sum of electronic and thermal Enthalpies= -189.196795
Sum of electronic and thermal Free Energies= -189.224539

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	14.440	7.342	58.393

C,0,-0.1388414608,-0.2865543341,0.
O,0,-0.9362599199,0.6872944502,0.
O,0,1.1196801701,-0.3086514107,0.
H,0,-0.6343132368,-1.3098183122,0.

$MeNH_2$

E(RB+HF-LYP) = -95.8718500569

Zero-point correction= 0.064052 (Hartree/Particle)
Thermal correction to Energy= 0.067478
Thermal correction to Enthalpy= 0.068422
Thermal correction to Gibbs Free Energy= 0.041130

Sum of electronic and zero-point Energies= -95.807798
Sum of electronic and thermal Energies= -95.804372
Sum of electronic and thermal Enthalpies= -95.803428
Sum of electronic and thermal Free Energies= -95.830721

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	42.343	9.575	57.442

C,0,0.0427995919,0.,-0.708237273
N,0,0.0538126889,0.,0.7577007893
H,0,-0.419908277,0.8183860668,1.128594187
H,0,-0.419908277,-0.8183860668,1.128594187
H,0,-0.9575643893,0.,-1.171363664
H,0,0.581947285,0.8811031801,-1.0701532986
H,0,0.581947285,-0.8811031801,-1.0701532986

$MeNH_3^+$ - gas phase

E(RB+HF-LYP) = -96.2282115631

Zero-point correction= 0.079429 (Hartree/Particle)
Thermal correction to Energy= 0.082887
Thermal correction to Enthalpy= 0.083831
Thermal correction to Gibbs Free Energy= 0.057274
Sum of electronic and zero-point Energies= -96.148783
Sum of electronic and thermal Energies= -96.145325
Sum of electronic and thermal Enthalpies= -96.144381
Sum of electronic and thermal Free Energies= -96.170937

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	52.012	9.775	55.893

C,0,0.,0.,-0.8037376552
N,0,0.,0.,0.7127595468
H,0,0.9548409901,0.0000962301,1.0889548205
H,0,-0.4775038328,0.826868439,1.0889548205
H,0,-0.4773371574,-0.8269646691,1.0889548205
H,0,-1.0346622469,0.0000896093,-1.1445851193
H,0,0.5174087274,0.8959989855,-1.1445851193
H,0,0.5172535196,-0.8960885948,-1.1445851193

$MeNH_3^+$ - PCM acetone

E(RB+HF-LYP) = -96.3346330432

Zero-point correction= 0.078043 (Hartree/Particle)
Thermal correction to Energy= 0.081504
Thermal correction to Enthalpy= 0.082448
Thermal correction to Gibbs Free Energy= 0.055890
Sum of electronic and zero-point Energies= -96.256590
Sum of electronic and thermal Energies= -96.253129
Sum of electronic and thermal Enthalpies= -96.252185
Sum of electronic and thermal Free Energies= -96.278743

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	51.145	9.748	55.898

C,0,0.,0.,-0.7958091567
N,0,0.,0.,0.7043475224
H,0,0.9596086136,0.0001030755,1.0880903876
H,0,-0.4798935728,0.8309938993,1.0880903876
H,0,-0.4797150408,-0.8310969748,1.0880903876
H,0,-1.034135066,0.0000965456,-1.1399496264
H,0,0.5171511439,0.8955389653,-1.1399496264
H,0,0.5169839221,-0.8956355109,-1.1399496264

$MeNH_3^+$ - PCM acetone radii=bondi

E(RB+HF-LYP) = -96.3516827379

Zero-point correction= 0.080194 (Hartree/Particle)
Thermal correction to Energy= 0.083604
Thermal correction to Enthalpy= 0.084549
Thermal correction to Gibbs Free Energy= 0.058115
Sum of electronic and zero-point Energies= -96.271489
Sum of electronic and thermal Energies= -96.268078
Sum of electronic and thermal Enthalpies= -96.267134
Sum of electronic and thermal Free Energies= -96.293568

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	52.463	9.737	55.635

C,0,0.,0.,-0.7922633723
N,0,0.,0.,0.7027966178
H,0,0.950233028,0.0001946624,1.0795309143
H,0,-0.4752850966,0.8228286106,1.0795309143
H,0,-0.4749479314,-0.823023273,1.0795309143

H,0,-1.0332628388,0.0001819718,-1.1348629447
H,0,0.5167890116,0.8947408813,-1.1348629447
H,0,0.5164738272,-0.8949228531,-1.1348629447

$MeNH_3^+$ - PCM water

E(RB+HF-LYP) = -96.3389621222

Zero-point correction= 0.077937 (Hartree/Particle)
Thermal correction to Energy= 0.081398
Thermal correction to Enthalpy= 0.082342
Thermal correction to Gibbs Free Energy= 0.055784
Sum of electronic and zero-point Energies= -96.261025
Sum of electronic and thermal Energies= -96.257564
Sum of electronic and thermal Enthalpies= -96.256620
Sum of electronic and thermal Free Energies= -96.283178

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	51.078	9.748	55.895

C,0,0.,0.,-0.7953291249
N,0,0.,0.,0.7040599059
H,0,0.9602575136,0.0001695776,1.0874586739
H,0,-0.4802756153,0.8315226122,1.0874586739
H,0,-0.4799818983,-0.8316921898,1.0874586739
H,0,-1.0341843977,0.0001584202,-1.1396068713
H,0,0.5172293948,0.8955507506,-1.1396068713
H,0,0.516955003,-0.8957091707,-1.1396068713

$MeNH_3^+$ - PCM water radii=bondi

E(RB+HF-LYP) = -96.3574775474

Zero-point correction= 0.080162 (Hartree/Particle)
Thermal correction to Energy= 0.083585
Thermal correction to Enthalpy= 0.084530
Thermal correction to Gibbs Free Energy= 0.058073
Sum of electronic and zero-point Energies= -96.277316
Sum of electronic and thermal Energies= -96.273892
Sum of electronic and thermal Enthalpies= -96.272948
Sum of electronic and thermal Free Energies= -96.299404

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	52.451	9.778	55.682

C,0,0.,0.,-0.7912948918
N,0,0.,0.,0.7028864578
H,0,0.949994944,0.0000332608,1.0790923832
H,0,-0.4750262767,0.8227031246,1.0790923832
H,0,-0.4749686673,-0.8227363854,1.0790923832
H,0,-1.0322159468,0.000032648,-1.136571001
H,0,0.5161362474,0.8939089081,-1.136571001
H,0,0.5160796994,-0.8939415561,-1.136571001

$MeNH_3^+$ - gas phase solvated with 1 water

E(RB+HF-LYP) = -172.693436369

Zero-point correction= 0.103267 (Hartree/Particle)
Thermal correction to Energy= 0.109149
Thermal correction to Enthalpy= 0.110094
Thermal correction to Gibbs Free Energy= 0.075234
Sum of electronic and zero-point Energies= -172.590169
Sum of electronic and thermal Energies= -172.584287
Sum of electronic and thermal Enthalpies= -172.583343
Sum of electronic and thermal Free Energies= -172.618202

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	68.492	18.135	73.368

C,0,0.520507236,0.6843392047,-1.4338796914
N,0,0.5062418063,0.778473698,0.0702313876
H,0,1.4566923658,0.7414247381,0.4500288218
H,0,0.0896248786,1.6598218008,0.3844837991
H,0,-0.0437287012,-0.0106480114,0.4998515246
H,0,-0.5066065492,0.7449203792,-1.7923075021
H,0,1.1104876567,1.5062832212,-1.8383984517
H,0,0.9602535445,-0.272635482,-1.7129146122
O,0,-0.9117605161,-1.3074359523,1.1629269403
H,0,-0.6897785924,-1.7912449078,1.971159185
H,0,-1.7495965345,-1.6737852338,0.8463401479

$MeNH_3^+$ - gas phase solvated with 3 waters

E(RB+HF-LYP) = -325.610614923

Zero-point correction= 0.150968 (Hartree/Particle)
Thermal correction to Energy= 0.165199

Thermal correction to Enthalpy= 0.166143
Thermal correction to Gibbs Free Energy= 0.109760
Sum of electronic and zero-point Energies= -325.459646
Sum of electronic and thermal Energies= -325.445416
Sum of electronic and thermal Enthalpies= -325.444471
Sum of electronic and thermal Free Energies= -325.500855

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	103.664	41.850	118.668

C,0,0.,0.,-1.8124990251
N,0,0.,0.,-0.3167798122
O,0,-1.5934265217,-2.1759395108,0.6107361309
H,0,0.9637311653,-0.1168811882,0.0501666676
H,0,-0.3806435045,0.8930562656,0.0501666676
H,0,-0.5830876608,-0.7761750775,0.0501666676
H,0,-1.0161700305,0.1676768404,-2.1694964135
H,0,0.6532974186,0.7961906407,-2.1694964135
H,0,0.3628726118,-0.9638674811,-2.1694964135
H,0,-1.3557775179,-2.7984603744,1.3112867094
H,0,-2.4606761785,-2.4541365549,0.2863049341
O,0,2.6811321543,-0.2919780914,0.6107361309
H,0,3.1014265347,0.2250924148,1.3112867094
H,0,3.3556826901,-0.9039398036,0.2863049341
O,0,-1.0877056326,2.4679176023,0.6107361309
H,0,-1.7456490168,2.5733679596,1.3112867094
H,0,-0.8950065116,3.3580763585,0.2863049341

$MeNH_3^+$ - PCM water solvated with 3 waters

E(RB+HF-LYP) = -325.708671090

Zero-point correction= 0.145804 (Hartree/Particle)
Thermal correction to Energy= 0.158430
Thermal correction to Enthalpy= 0.159374
Thermal correction to Gibbs Free Energy= 0.107190
Sum of electronic and zero-point Energies= -325.562867
Sum of electronic and thermal Energies= -325.550241
Sum of electronic and thermal Enthalpies= -325.549297
Sum of electronic and thermal Free Energies= -325.601481

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	99.416	37.876	109.831

C,0,0.,0.,1.7470432481
N,0,0.,0.,0.2561857599
O,0,-2.3503793665,-1.3569921599,-0.5242189005
H,0,-0.0208102427,0.9759024101,-0.10723583
H,0,0.8555614001,-0.4699290062,-0.10723583
H,0,-0.8347511574,-0.5059734039,-0.10723583
H,0,0.0272639071,-1.03025617,2.104523859
H,0,0.8785960621,0.5387393212,2.104523859
H,0,-0.9058599692,0.4915168488,2.104523859
H,0,-2.7797169691,-1.1016539793,-1.3652551648
H,0,-2.333919319,-2.3350573908,-0.5301349294
O,0,0.,2.7139843199,-0.5242189005
H,0,0.4357981524,2.9581325002,-1.3652551648
H,0,-0.8552593602,3.188762116,-0.5301349294
O,0,2.3503793665,-1.3569921599,-0.5242189005
H,0,2.3439188168,-1.856478521,-1.3652551648
H,0,3.1891786792,-0.8537047253,-0.5301349294

$EtNH_3^+$ - PCM acetone

E(RB+HF-LYP) = -135.656955699

Zero-point correction=	0.106491 (Hartree/Particle)
Thermal correction to Energy=	0.110979
Thermal correction to Enthalpy=	0.111923
Thermal correction to Gibbs Free Energy=	0.080783
Sum of electronic and zero-point Energies=	-135.550465
Sum of electronic and thermal Energies=	-135.545977
Sum of electronic and thermal Enthalpies=	-135.545033
Sum of electronic and thermal Free Energies=	-135.576172

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.640	14.564	65.540

C,0,0.460138207,0.,-0.3914198406
N,0,0.4987194945,0.,1.1186853187
H,0,1.4702872804,0.,1.4708471493
H,0,0.0326597528,0.832484012,1.5157460167
H,0,0.0326597528,-0.832484012,1.5157460167
C,0,-0.9704325647,0.,-0.9033319007
H,0,1.0107529453,0.8889270635,-0.7098190093
H,0,1.0107529453,-0.8889270635,-0.7098190093
H,0,-0.9545336892,0.,-1.996992467

H,0,-1.5159246512,-0.8908960563,-0.5739977398
H,0,-1.5159246512,0.8908960563,-0.5739977398

NMe_3 – gas phase

E(RB+HF-LYP) = -174.493080300

Zero-point correction= 0.120206 (Hartree/Particle)
Thermal correction to Energy= 0.125632
Thermal correction to Enthalpy= 0.126576
Thermal correction to Gibbs Free Energy= 0.092912
Sum of electronic and zero-point Energies= -174.372874
Sum of electronic and thermal Energies= -174.367448
Sum of electronic and thermal Enthalpies= -174.366504
Sum of electronic and thermal Free Energies= -174.400168

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.835	18.801	70.852

C,0,-0.8325584239,0.4516799578,-1.0211725843
N,0,0.2955838914,-0.0108474713,-0.2237822891
C,0,0.6057558315,0.9166701952,0.8559165014
C,0,0.0819760214,-1.3630178038,0.2749087836
H,0,-0.2218429296,1.0200195296,1.5870802029
H,0,1.4943807827,0.5736395029,1.3953710337
H,0,0.81999946,1.9076049445,0.4429588729
H,0,-0.7879599572,-1.4383520891,0.958847248
H,0,-0.0860329066,-2.0453409864,-0.5644485014
H,0,0.9702891579,-1.7029447978,0.8168945671
H,0,-1.7730078949,0.523171956,-0.4375131248
H,0,-0.6132963905,1.441443653,-1.4343164721
H,0,-1.0026571361,-0.235303509,-1.8563140066

NMe_3 – PCM acetone

E(RB+HF-LYP) = -174.495249609

Zero-point correction= 0.120052 (Hartree/Particle)
Thermal correction to Energy= 0.125458
Thermal correction to Enthalpy= 0.126403
Thermal correction to Gibbs Free Energy= 0.092787
Sum of electronic and zero-point Energies= -174.375197
Sum of electronic and thermal Energies= -174.369791
Sum of electronic and thermal Enthalpies= -174.368847
Sum of electronic and thermal Free Energies= -174.402462

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.726	18.822	70.749

C,0,-0.8336266068,0.4513112119,-1.0188324784
N,0,0,0.3082314491,-0.0115151897,-0.233486412
C,0,0.6033934763,0.9159366065,0.8563265283
C,0,0.0801740975,-1.3616579192,0.2761474565
H,0,-0.2346141756,1.0076531631,1.5755945425
H,0,1.4870590069,0.5747539039,1.4051599039
H,0,0.8139153195,1.9106824611,0.4505578299
H,0,-0.7914014849,-1.4176398706,0.9581859052
H,0,-0.0955783337,-2.0481796229,-0.5582700015
H,0,0.9634829288,-1.7056314279,0.8238057202
H,0,-1.7638363097,0.515613539,-0.4199933862
H,0,-0.623771074,1.4442875947,-1.4292918087
H,0,-1.0125218232,-0.2344728076,-1.8531928602

NMe_3 – PCM water

E(RB+HF-LYP) = -174.495532305

Zero-point correction= 0.120091 (Hartree/Particle)
Thermal correction to Energy= 0.125481
Thermal correction to Enthalpy= 0.126425
Thermal correction to Gibbs Free Energy= 0.092843
Sum of electronic and zero-point Energies= -174.375441
Sum of electronic and thermal Energies= -174.370051
Sum of electronic and thermal Enthalpies= -174.369107
Sum of electronic and thermal Free Energies= -174.402689

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.741	18.798	70.680

C,0,-0.8347686363,0.4508799308,-1.0187264695
N,0,0.3092415242,-0.0116690891,-0.2343672309
C,0,0.6046894771,0.9168825246,0.8558019061
C,0,0.0795662901,-1.3620782998,0.2769792538
H,0,-0.2347923583,1.0110436709,1.5724272589
H,0,1.4861197065,0.5735729306,1.406882341
H,0,0.8185729771,1.9105437334,0.4490733961
H,0,-0.7927039262,-1.4151524043,0.9577942475
H,0,-0.0966853581,-2.0495649488,-0.5566030208

H,0,0.9619761441,-1.7062292633,0.8259814825
H,0,-1.7651607193,0.5059382311,-0.4199624241
H,0,-0.6295614965,1.4478694978,-1.42165452
H,0,-1.0093784247,-0.2304427574,-1.857696287

Me_3NH^+ - gas phase

E(RB+HF-LYP) = -174.867401113

Zero-point correction= 0.136148 (Hartree/Particle)
Thermal correction to Energy= 0.141741
Thermal correction to Enthalpy= 0.142685
Thermal correction to Gibbs Free Energy= 0.108544
Sum of electronic and zero-point Energies= -174.731253
Sum of electronic and thermal Energies= -174.725660
Sum of electronic and thermal Enthalpies= -174.724716
Sum of electronic and thermal Free Energies= -174.758857

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.944	19.467	71.856

N,0,0.2609035532,-0.1080061803,0.1863533482
H,0,1.0511290804,-0.4352242173,0.7506075111
C,0,-0.1876909472,1.2057022425,0.7742360787
C,0,0.7634496297,0.0532233157,-1.2257047349
C,0,-0.8147867733,-1.1599701948,0.2807570508
H,0,-1.6677441912,-0.8355701777,-0.3165560004
H,0,-0.4224013921,-2.1016366942,-0.1040678812
H,0,-1.1078154795,-1.2727231774,1.3248679787
H,0,-0.0602384308,0.4071152786,-1.8469134308
H,0,1.576784146,0.7793265574,-1.2299612623
H,0,1.1185258942,-0.9125020728,-1.5862860974
H,0,-1.0345306829,1.5723328975,0.1928673507
H,0,-0.4843398208,1.0457780422,1.8111528174
H,0,0.6384745497,1.9154146449,0.7240852085

Me_3NH^+ – PCM acetone

E(RB+HF-LYP) = -174.952442584

Zero-point correction= 0.135223 (Hartree/Particle)
Thermal correction to Energy= 0.140773
Thermal correction to Enthalpy= 0.141717
Thermal correction to Gibbs Free Energy= 0.107668
Sum of electronic and zero-point Energies= -174.817220

Sum of electronic and thermal Energies= -174.811670
Sum of electronic and thermal Enthalpies= -174.810726
Sum of electronic and thermal Free Energies= -174.844774

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.336	19.351	71.661

N,0,0.2733873425,-0.113196236,0.1953837168
H,0,1.0769729033,-0.4464456885,0.7697253198
C,0,-0.1907089405,1.1988736267,0.7670473465
C,0,0.7550964112,0.0550206939,-1.2200345373
C,0,-0.8133122377,-1.1507206902,0.2749354423
H,0,-1.6542576065,-0.8139669525,-0.3338463081
H,0,-0.4237545802,-2.0963350276,-0.1048164766
H,0,-1.1182899075,-1.2601034766,1.3166777545
H,0,-0.0783163301,0.4161018551,-1.8251450038
H,0,1.5722432467,0.7777001693,-1.2280687353
H,0,1.1024291989,-0.9109999627,-1.5892093214
H,0,-1.0440492492,1.5446391113,0.1808969201
H,0,-0.4811024966,1.0453081167,1.8073707305
H,0,0.6279620255,1.9174337248,0.7070395938

Me_3NH^+ – PCM acetone radii=bondi

E(RB+HF-LYP) = -174.967805398

Zero-point correction= 0.136683 (Hartree/Particle)
Thermal correction to Energy= 0.142266
Thermal correction to Enthalpy= 0.143210
Thermal correction to Gibbs Free Energy= 0.109132
Sum of electronic and zero-point Energies= -174.831122
Sum of electronic and thermal Energies= -174.825539
Sum of electronic and thermal Enthalpies= -174.824595
Sum of electronic and thermal Free Energies= -174.858673

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	89.273	19.581	71.723

N,0,0.3060040927,-0.0573417718,0.1371172276
C,0,0.5225041014,0.7619551654,-1.100817808
C,0,-0.2985720771,-1.393167439,-0.1836427641
C,0,-0.5052446817,0.684327625,1.1584267622
H,0,-1.2832491541,-1.2277194759,-0.6225624298

H,0,-0.4482427357,0.9520258179,-1.5604824
H,0,1.1620553659,0.2014506154,-1.7814702347
H,0,0.3510784466,-1.9081769358,-0.8902389416
H,0,-0.3841395709,-1.9665910323,0.7384736491
H,0,1.0001962422,1.6993960597,-0.8190679377
H,0,-1.500724253,0.8555381302,0.7473328255
H,0,-0.564286178,0.0786422707,2.0618837261
H,0,-0.0130728721,1.6321540671,1.3725239112
H,0,1.2262320043,-0.234019222,0.5499900982

Me_3NH^+ – Onsager acetone

E(RB+HF-LYP) = -174.867582860

Zero-point correction= 0.136077 (Hartree/Particle)
Thermal correction to Energy= 0.141691
Thermal correction to Enthalpy= 0.142635
Thermal correction to Gibbs Free Energy= 0.108443
Sum of electronic and zero-point Energies= -174.731506
Sum of electronic and thermal Energies= -174.725892
Sum of electronic and thermal Enthalpies= -174.724948
Sum of electronic and thermal Free Energies= -174.759140

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	88.912	19.496	71.963

N,0,0.2611119981,-0.1081533191,0.1862953591
H,0,1.0526676403,-0.4344223521,0.7497498854
C,0,-0.1877413402,1.2053626552,0.7743089515
C,0,0.761960508,0.0540469863,-1.2264280435
C,0,-0.8132547923,-1.1604399047,0.2816906308
H,0,-1.6642775723,-0.839922961,-0.3204684608
H,0,-0.4191141425,-2.1038241803,-0.097285621
H,0,-1.110621646,-1.2687160327,1.3250837881
H,0,-0.0616656486,0.4128990561,-1.8447557504
H,0,1.5784065816,0.7767440581,-1.2313577051
H,0,1.1120481311,-0.9122084796,-1.5906617335
H,0,-1.0312966356,1.5741321375,0.1895705753
H,0,-0.4893395166,1.0444485534,1.8096880092
H,0,0.6396225692,1.9141250133,0.728940266

Me_3NH^+ – PCM water

E(RB+HF-LYP) = -174.956552090

Zero-point correction= 0.135093 (Hartree/Particle)
Thermal correction to Energy= 0.140632
Thermal correction to Enthalpy= 0.141576
Thermal correction to Gibbs Free Energy= 0.107564
Sum of electronic and zero-point Energies= -174.821459
Sum of electronic and thermal Energies= -174.815920
Sum of electronic and thermal Enthalpies= -174.814976
Sum of electronic and thermal Free Energies= -174.848988

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.248	19.348	71.586

N,0,0.2721757147,-0.1131205578,0.1945238466
H,0,1.0768777852,-0.4477461369,0.7703933513
C,0,-0.1901253191,1.1982989694,0.7672221274
C,0,0.7554321157,0.0553035272,-1.2197364535
C,0,-0.8140615102,-1.150196971,0.2746147783
H,0,-1.6549760271,-0.8146617962,-0.3350627121
H,0,-0.4230744606,-2.0959312049,-0.1033555484
H,0,-1.1185183527,-1.2576465265,1.3167311582
H,0,-0.0780952395,0.412276393,-1.8273989985
H,0,1.5699773652,0.7809634905,-1.2268735118
H,0,1.1072971718,-0.9101080504,-1.5862972569
H,0,-1.0449414416,1.5459787945,0.1842056247
H,0,-0.4770875379,1.0430889875,1.8082629551
H,0,0.6298390155,1.9151968,0.7051252988

Me_3NH^+ – Onsager water

E(RB+HF-LYP) = -174.867595594

Zero-point correction= 0.136077 (Hartree/Particle)
Thermal correction to Energy= 0.141690
Thermal correction to Enthalpy= 0.142634
Thermal correction to Gibbs Free Energy= 0.108444
Sum of electronic and zero-point Energies= -174.731518
Sum of electronic and thermal Energies= -174.725906
Sum of electronic and thermal Enthalpies= -174.724961
Sum of electronic and thermal Free Energies= -174.759152

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	88.912	19.495	71.960

N,0,0.2611098632,-0.1081528829,0.1862950343
H,0,1.0526655451,-0.4344269214,0.7497546588
C,0,-0.1877397769,1.2053630028,0.7743077917
C,0,0.7619640546,0.0540437502,-1.2264246928
C,0,-0.8132599006,-1.1604364415,0.2816871137
H,0,-1.664286342,-0.839897226,-0.3204559903
H,0,-0.4191270923,-2.1038161278,-0.0973078542
H,0,-1.1106089283,-1.2687335186,1.3250829127
H,0,-0.0616726682,0.4128702657,-1.8447540765
H,0,1.5783962841,0.776756012,-1.231357313
H,0,1.1120809976,-0.9122062019,-1.5906442291
H,0,-1.0313012794,1.5741214728,0.1895705637
H,0,-0.4893244912,1.0444543155,1.8096913417
H,0,0.6396226693,1.9141262416,0.7289334704

MeOH

E(RB+HF-LYP) = -115.734871624

Zero-point correction= 0.051239 (Hartree/Particle)
Thermal correction to Energy= 0.054573
Thermal correction to Enthalpy= 0.055517
Thermal correction to Gibbs Free Energy= 0.028477
Sum of electronic and zero-point Energies= -115.683633
Sum of electronic and thermal Energies= -115.680299
Sum of electronic and thermal Enthalpies= -115.679355
Sum of electronic and thermal Free Energies= -115.706395

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	34.245	8.810	56.911

O,0,-0.0318400433,0.0551486482,-0.7569740832
C,0,-0.0156947032,0.027184009,0.6677209482
H,0,1.0066646904,0.0455989637,1.0698390944
H,0,-0.5354122683,0.9273616421,1.002806575
H,0,-0.5428225942,-0.848997513,1.0698390496
H,0,0.4204587333,-0.7282563349,-1.0930177427

Methoxide

E(RB+HF-LYP) = -115.115520602

Zero-point correction= 0.034978 (Hartree/Particle)
Thermal correction to Energy= 0.037886
Thermal correction to Enthalpy= 0.038831

Thermal correction to Gibbs Free Energy= 0.012727
Sum of electronic and zero-point Energies= -115.080543
Sum of electronic and thermal Energies= -115.077634
Sum of electronic and thermal Enthalpies= -115.076690
Sum of electronic and thermal Free Energies= -115.102794

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	23.774	6.918	54.940

C,0,-0.5437323702,0.,0.0017192932
O,0,0.7970797927,0.,-0.0025235744
H,0,-1.0413003781,0.,-1.0251216645
H,0,-1.0364718712,0.8905876432,0.5174972503
H,0,-1.0364718712,-0.8905876432,0.5174972503

CFH_2OH

E(RB+HF-LYP) = -214.986488149

Zero-point correction= 0.044966 (Hartree/Particle)
Thermal correction to Energy= 0.048432
Thermal correction to Enthalpy= 0.049376
Thermal correction to Gibbs Free Energy= 0.020207
Sum of electronic and zero-point Energies= -214.941523
Sum of electronic and thermal Energies= -214.938056
Sum of electronic and thermal Enthalpies= -214.937112
Sum of electronic and thermal Free Energies= -214.966282

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	30.392	10.021	61.393

C,0,-0.2466151806,-0.3014102992,-0.3423280112
O,0,1.1237730045,-0.1450729915,-0.3095032595
F,0,-0.8693781434,0.5303976664,0.6042329997
H,0,-0.5878742349,0.0137599781,-1.329478683
H,0,-0.5705598811,-1.3204199449,-0.0997432029
H,0,1.4723444534,-0.4978733028,0.5211190314

CFH_2O^-

E(RB+HF-LYP) = -214.410274936

Zero-point correction= 0.029367 (Hartree/Particle)
Thermal correction to Energy= 0.032948

Thermal correction to Enthalpy= 0.033892
Thermal correction to Gibbs Free Energy= 0.004420
Sum of electronic and zero-point Energies= -214.380908
Sum of electronic and thermal Energies= -214.377327
Sum of electronic and thermal Enthalpies= -214.376382
Sum of electronic and thermal Free Energies= -214.405855

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	20.675	9.762	62.029

C,0,-0.0390092415,-0.3658189296,-0.4002750346
O,0,1.2092168247,-0.2173117252,-0.3116849216
F,0,-0.9304328682,0.579945592,0.6940883295
H,0,-0.5699558328,0.0382684177,-1.2951225764
H,0,-0.4958275018,-1.3243713665,-0.0565428089

Vinyl Alcohol

E(RB+HF-LYP) = -153.827537300

Zero-point correction= 0.056527 (Hartree/Particle)
Thermal correction to Energy= 0.060162
Thermal correction to Enthalpy= 0.061106
Thermal correction to Gibbs Free Energy= 0.032066
Sum of electronic and zero-point Energies= -153.771010
Sum of electronic and thermal Energies= -153.767375
Sum of electronic and thermal Enthalpies= -153.766431
Sum of electronic and thermal Free Energies= -153.795472

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	37.752	11.465	61.121

C,0,0.0709252143,-1.1425774144,-0.4291229521
C,0,0.1236112889,0.1918720475,-0.3803829437
H,0,0.409463618,0.801067707,-1.2321696747
H,0,-0.21627069,-1.7469058589,0.4278472133
H,0,0.32008093,-1.6596130468,-1.3476974206
O,0,-0.1585712688,0.9843907665,0.6948724721
H,0,-0.4119227271,0.4345572684,1.4500754804

Enolate of Vinyl Alcohol

E(RB+HF-LYP) = -153.251745518

Zero-point correction= 0.041822 (Hartree/Particle)
Thermal correction to Energy= 0.045300
Thermal correction to Enthalpy= 0.046244
Thermal correction to Gibbs Free Energy= 0.017597
Sum of electronic and zero-point Energies= -153.209924
Sum of electronic and thermal Energies= -153.206445
Sum of electronic and thermal Enthalpies= -153.205501
Sum of electronic and thermal Free Energies= -153.234149

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	28.426	10.453	60.294

C,0,-1.1468556693,0.3236715603,0.1265900792
C,0,0.2258383029,0.2832113034,-0.076418979
O,0,1.0310543238,-0.7034914607,-0.0525879852
H,0,-1.6789546879,1.2717176959,0.0669348511
H,0,-1.7153855644,-0.5793738647,0.3472686057
H,0,0.6720098601,1.2942906723,-0.2945261765

Ethynyl Alcohol

E(RB+HF-LYP) = -152.509709019

Zero-point correction= 0.030012 (Hartree/Particle)
Thermal correction to Energy= 0.033340
Thermal correction to Enthalpy= 0.034284
Thermal correction to Gibbs Free Energy= 0.008217
Sum of electronic and zero-point Energies= -152.479697
Sum of electronic and thermal Energies= -152.476369
Sum of electronic and thermal Enthalpies= -152.475425
Sum of electronic and thermal Free Energies= -152.501492

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	20.921	10.287	54.863

H,0,-2.4018051987,0.,0.
C,0,-1.3384810864,0.,0.
C,0,-0.1289776405,0.,0.
O,0,1.1403435063,0.,0.
H,0,2.08380951,0.,0.

Ethynyl Oxide

E(RB+HF-LYP) = -152.016569083

Zero-point correction= 0.018332 (Hartree/Particle)
Thermal correction to Energy= 0.021048
Thermal correction to Enthalpy= 0.021992
Thermal correction to Gibbs Free Energy= -0.003068
Sum of electronic and zero-point Energies= -151.998237
Sum of electronic and thermal Energies= -151.995521
Sum of electronic and thermal Enthalpies= -151.994577
Sum of electronic and thermal Free Energies= -152.019637

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	13.208	7.299	52.744

H,0,-2.3139083512,0.,0.
C,0,-1.2525780908,0.,0.
C,0,-0.0048108974,0.,0.
O,0,1.232280285,0.,0.

CH_3CNH_2 carbene

E(RB+HF-LYP) = -133.917451524

Zero-point correction= 0.067922 (Hartree/Particle)
Thermal correction to Energy= 0.071931
Thermal correction to Enthalpy= 0.072875
Thermal correction to Gibbs Free Energy= 0.042987
Sum of electronic and zero-point Energies= -133.849530
Sum of electronic and thermal Energies= -133.845521
Sum of electronic and thermal Enthalpies= -133.844577
Sum of electronic and thermal Free Energies= -133.874465

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	45.137	12.361	62.905

H,0,-1.375351751,-0.4746004192,-0.7034318302
N,0,-0.6544656119,-0.9412224718,-0.1347183321
C,0,0.4138823139,-0.3484663317,0.3488151448
C,0,0.460297255,1.1018383002,-0.0280680997
H,0,-0.8182230525,-1.9247311193,0.0400787702
H,0,1.39764762,1.2967496403,-0.563096679
H,0,-0.3862991772,1.4685839767,-0.643083409
H,0,0.5184082304,1.7023234125,0.8880792024

CH_3CNH_2 carbene – transition state for carbene rearrangement

E(RB+HF-LYP) = -133.865778415

Zero-point correction= 0.063685 (Hartree/Particle)
Thermal correction to Energy= 0.067517
Thermal correction to Enthalpy= 0.068461
Thermal correction to Gibbs Free Energy= 0.039104
Sum of electronic and zero-point Energies= -133.802094
Sum of electronic and thermal Energies= -133.798261
Sum of electronic and thermal Enthalpies= -133.797317
Sum of electronic and thermal Free Energies= -133.826674

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	42.368	12.245	61.788

H,0,-1.6344592929,-0.4189024444,-0.0882873456
N,0,-0.7459750802,-0.9014344743,0.0345336751
C,0,0.4557440493,-0.2870925212,-0.0610041449
C,0,0.4865580519,1.1098395981,-0.0796553125
H,0,-0.4055698478,1.7583978148,-0.1081056159
H,0,-0.7922289232,-1.9049180819,0.0971897314
H,0,1.440156927,1.6051978109,-0.2376624339
H,0,0.9601140913,0.3337837599,0.9390866827

$CH_3CNHC(O)H$ carbene

E(RB+HF-LYP) = -247.250275916

Zero-point correction= 0.077237 (Hartree/Particle)
Thermal correction to Energy= 0.082912
Thermal correction to Enthalpy= 0.083856
Thermal correction to Gibbs Free Energy= 0.048683
Sum of electronic and zero-point Energies= -247.173039
Sum of electronic and thermal Energies= -247.167364
Sum of electronic and thermal Enthalpies= -247.166420
Sum of electronic and thermal Free Energies= -247.201593

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	52.028	18.328	74.029

C,0,0.986669645,2.100427619,0.0130541953
C,0,0.938154066,0.6566195058,0.3863708008
N,0,-0.1382226483,0.0484831992,-0.0973809235

H,0,-0.8661958051,0.5071789226,-0.6671923093
C,0,-0.3889149211,-1.3266545703,0.1339887157
H,0,1.9324605574,2.2883604855,-0.5108879471
H,0,0.1502361428,2.4818070699,-0.600743066
H,0,1.0554858765,2.6918040257,0.9349364369
O,0,-1.3652166811,-1.8877350851,-0.3022273731
H,0,0.4018524754,-1.7890075444,0.742890064

$CH_3CNHC(O)H$ carbene – transition state for rearrangement

E(RB+HF-LYP) = -247.208218635

Zero-point correction=	0.074047 (Hartree/Particle)
Thermal correction to Energy=	0.079230
Thermal correction to Enthalpy=	0.080174
Thermal correction to Gibbs Free Energy=	0.046100
Sum of electronic and zero-point Energies=	-247.134172
Sum of electronic and thermal Energies=	-247.128989
Sum of electronic and thermal Enthalpies=	-247.128045
Sum of electronic and thermal Free Energies=	-247.162118

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	49.717	17.193	71.714

C,0,2.3004968619,0.3095181321,-0.0347225734
C,0,1.1334230547,-0.4378119843,-0.1719215872
N,0,-0.0539205,0.2329128121,-0.0117447897
H,0,-0.1170347779,1.2520348547,0.0633172729
H,0,2.3375471729,1.4004596152,0.1099766604
C,0,-1.2793346079,-0.4169010606,-0.019928406
H,0,3.2540008806,-0.1804055363,-0.2126557805
H,0,1.8832295572,-0.6112671995,0.8594480112
O,0,-2.3420452153,0.1608004339,0.0954763084
H,0,-1.1714494622,-1.5064454126,-0.1422477027

Glutarimide carbene

E(RB+HF-LYP) = -398.667350514

Zero-point correction=	0.093079 (Hartree/Particle)
Thermal correction to Energy=	0.100197
Thermal correction to Enthalpy=	0.101141
Thermal correction to Gibbs Free Energy=	0.061397
Sum of electronic and zero-point Energies=	-398.574272
Sum of electronic and thermal Energies=	-398.567154

Sum of electronic and thermal Enthalpies= -398.566209
Sum of electronic and thermal Free Energies= -398.605953

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	62.875	25.932	83.648

C,0,-0.9648104506,-0.8618103185,-0.1882551703
C,0,0.3285912759,-1.6271906586,0.0792517647
C,0,1.6539812174,-0.9751701717,0.049055147
C,0,1.5851243406,0.4989255819,-0.0221890057
C,0,0.279117339,1.2660542056,0.1678504678
N,0,-0.8804986455,0.5191179308,-0.026276737
O,0,0.2311887536,2.4532429577,0.4289264749
O,0,-2.0145285792,-1.401867545,-0.4820186543
H,0,1.8997502708,0.6542962392,-1.0762384185
H,0,2.3864672767,0.9915489398,0.5405610679
H,0,-1.7561750095,1.0353953279,-0.0523670342
H,0,0.3096140562,-2.5815408249,-0.4595872574
H,0,0.298530194,-1.949380332,1.1420270152

Glutarimide carbene – transition state for rearrangement of the carbene

E(RB+HF-LYP) = -398.655815289

Zero-point correction= 0.091424 (Hartree/Particle)
Thermal correction to Energy= 0.098094
Thermal correction to Enthalpy= 0.099038
Thermal correction to Gibbs Free Energy= 0.059968
Sum of electronic and zero-point Energies= -398.564391
Sum of electronic and thermal Energies= -398.557721
Sum of electronic and thermal Enthalpies= -398.556777
Sum of electronic and thermal Free Energies= -398.595847

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	61.555	24.310	82.230

C,0,-0.9868748859,-0.8513374778,0.0442851178
C,0,0.3212851968,-1.6371869996,0.0379279793
C,0,1.6530465748,-0.9402329917,0.0178690181
C,0,1.5723475045,0.4601179815,0.0170719127
C,0,0.2997167709,1.2800041538,-0.0940711196
N,0,-0.8718202631,0.5399162939,-0.0525822911
O,0,0.3038185479,2.4931662403,-0.196545018

O,0,-2.0840206832,-1.371710953,0.1140415037
H,0,2.4724302157,1.0683729491,-0.0886803365
H,0,1.8742642438,-0.1118316527,1.0869361523
H,0,-1.7439926666,1.0621002278,-0.0857724383
H,0,0.308868024,-2.261014933,-0.8687517755
H,0,0.2756621399,-2.3768709443,0.8458751008

N-Methyl Orotic Acid Anion

E(RB+HF-LYP) = -642.214923532

Zero-point correction= 0.115956 (Hartree/Particle)
Thermal correction to Energy= 0.126649
Thermal correction to Enthalpy= 0.127593
Thermal correction to Gibbs Free Energy= 0.077982
Sum of electronic and zero-point Energies= -642.098968
Sum of electronic and thermal Energies= -642.088275
Sum of electronic and thermal Enthalpies= -642.087331
Sum of electronic and thermal Free Energies= -642.136941

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.473	37.722	104.415

N,0,0.1462531589,0.9023129299,-0.0469415474
C,0,-1.2075582881,1.2155957541,-0.0454108931
N,0,-2.0485131902,0.1222511305,0.0075731461
C,0,-1.6967026275,-1.2443634456,0.0393373109
C,0,-0.2781472607,-1.4592611004,0.0238786751
C,0,0.5990468433,-0.4105234957,-0.006112598
C,0,1.1087323564,2.0130418727,-0.0921788851
O,0,-1.6487144465,2.3672425375,-0.0877073613
H,0,-3.0376157979,0.3362320872,0.00894283
O,0,-2.5963698464,-2.0923333396,0.0736658266
H,0,0.0922355003,-2.4753756675,0.030129508
C,0,2.1308738042,-0.6229638701,0.0368261715
O,0,2.6318537517,-1.0731523322,-1.0162651494
O,0,2.650516945,-0.3031566369,1.1327848273
H,0,1.7561108744,1.8976441311,-0.9655000326
H,0,0.5424048112,2.939231139,-0.1626220159
H,0,1.7269246347,1.9923637656,0.8067646863

N-Methyl Orotic Acid Anion – PCM acetone

E(RB+HF-LYP) = -642.309726730

Zero-point correction= 0.114954 (Hartree/Particle)
Thermal correction to Energy= 0.125580
Thermal correction to Enthalpy= 0.126524
Thermal correction to Gibbs Free Energy= 0.077114
Sum of electronic and zero-point Energies= -642.194773
Sum of electronic and thermal Energies= -642.184147
Sum of electronic and thermal Enthalpies= -642.183202
Sum of electronic and thermal Free Energies= -642.232613

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.803	37.619	103.993

N,0,0.1468818445,0.9094398644,-0.0491819794
C,0,-1.2114719741,1.213104313,-0.0370975323
N,0,-2.0548727812,0.1241222607,0.0068476143
C,0,-1.6943361056,-1.2258169262,0.0413226742
C,0,-0.2756867932,-1.4510984055,0.0311296338
C,0,0.5927653495,-0.3996879096,-0.0056873003
C,0,1.1062805818,2.026071326,-0.0948336106
O,0,-1.6452796573,2.3678849467,-0.0643791116
H,0,-3.0598732387,0.3430771417,0.0167103427
O,0,-2.5793667976,-2.0964031039,0.0795522702
H,0,0.090596597,-2.4727085444,0.0548041481
C,0,2.1119875471,-0.626794067,0.0257929623
O,0,2.6322448162,-1.0001864082,-1.0545159098
O,0,2.6594842545,-0.423568222,1.1381151033
H,0,1.8100356179,1.8683558418,-0.915032534
H,0,0.5466187164,2.9428262158,-0.2614830656
H,0,1.6546663054,2.0870267837,0.8474018861

N-Methyl Orotic Acid Anion – PCM acetone bondi=radii

E(RB+HF-LYP) = -642.320235133

Zero-point correction= 0.116099 (Hartree/Particle)
Thermal correction to Energy= 0.126568
Thermal correction to Enthalpy= 0.127513
Thermal correction to Gibbs Free Energy= 0.079246
Sum of electronic and zero-point Energies= -642.204136
Sum of electronic and thermal Energies= -642.193667
Sum of electronic and thermal Enthalpies= -642.192723
Sum of electronic and thermal Free Energies= -642.240989

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	79.423	37.619	101.586

C,0,-0.6199612143,0.7758007147,1.0889814356
C,0,-0.6494275351,-0.2380964752,0.1751514035
N,0,0.3863435222,-0.4461021433,-0.7122269902
C,0,1.5275330811,0.3417337311,-0.6777009422
N,0,1.5268162091,1.3515983285,0.2561258112
C,0,0.516020629,1.6481474534,1.1679168626
C,0,-1.8387940718,-1.2035706823,0.1295098717
O,0,-1.6674167077,-2.3031577237,0.7154356776
C,0,0.3564321275,-1.518207044,-1.7239048126
O,0,2.4856976133,0.1555836429,-1.4367453811
O,0,0.659292166,2.6017012097,1.9562995843
O,0,-2.8650392141,-0.7918286793,-0.4702952631
H,0,0.7368867904,-1.125212218,-2.6654914291
H,0,-0.6698817653,-1.848344256,-1.8642177615
H,0,0.9744674851,-2.3605605235,-1.4049281198
H,0,2.3613165575,1.9298395262,0.2795011443
H,0,-1.445996145,0.9325703908,1.7705645659

N-Methyl Orotic Acid Anion – PCM water

E(RB+HF-LYP) = -642.314719085

Zero-point correction= 0.114895 (Hartree/Particle)
Thermal correction to Energy= 0.125467
Thermal correction to Enthalpy= 0.126411
Thermal correction to Gibbs Free Energy= 0.077518
Sum of electronic and zero-point Energies= -642.199824
Sum of electronic and thermal Energies= -642.189252
Sum of electronic and thermal Enthalpies= -642.188308
Sum of electronic and thermal Free Energies= -642.237201

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	78.732	37.605	102.904

N,0,0.1488974339,0.9088926314,-0.050424087
C,0,-1.208840916,1.2127382582,-0.0158003082
N,0,-2.0535784213,0.1264585041,0.023762409
C,0,-1.6948837479,-1.2230144221,0.0445797095
C,0,-0.2763983776,-1.4510879792,0.0228602177
C,0,0.5925007686,-0.3996690638,-0.0148220803
C,0,1.1009607443,2.0310429336,-0.0970550436

O,0,-1.6372753913,2.3700491706,-0.0216071678
H,0,-3.0592194009,0.3489817825,0.0466935279
O,0,-2.5807656119,-2.0934617536,0.0804334034
H,0,0.0891069065,-2.4733220843,0.0407758976
C,0,2.1093758607,-0.6310299395,0.0058403192
O,0,2.6344124737,-0.9399143287,-1.0931311504
O,0,2.6554817719,-0.4968088698,1.1299617098
H,0,1.9011663813,1.7955680727,-0.799861373
H,0,0.5662256823,2.9160955841,-0.4338903884
H,0,1.5243754114,2.2124262259,0.8940428353

N-Methyl Orotic Acid Anion Hydrogen Bonded to 1 Water

E(RB+HF-LYP) = -718.673058473

Zero-point correction= 0.141100 (Hartree/Particle)
Thermal correction to Energy= 0.154720
Thermal correction to Enthalpy= 0.155664
Thermal correction to Gibbs Free Energy= 0.098761
Sum of electronic and zero-point Energies= -718.531958
Sum of electronic and thermal Energies= -718.518339
Sum of electronic and thermal Enthalpies= -718.517395
Sum of electronic and thermal Free Energies= -718.574297

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	97.088	47.201	119.762

C,0,0.0730181463,-0.2975572777,-0.0175456901
N,0,-0.4028722824,1.0022109781,-0.1267438661
C,0,-1.7618163028,1.2764593498,-0.2437382451
N,0,-2.576227754,0.1609134884,-0.2361058995
C,0,-2.1945034983,-1.1933655285,-0.1477675272
C,0,-0.7714223951,-1.3695821393,-0.0413824815
C,0,0.5265045485,2.1429297318,-0.1290694366
O,0,-2.2266698712,2.4129087728,-0.3487765832
O,0,-3.0663184322,-2.0672929868,-0.1694148025
C,0,1.5899328868,-0.485562548,0.178186509
O,0,2.0364949171,-0.0042234065,1.2510715244
O,0,2.1822299556,-1.0973255203,-0.7409517177
H,0,-3.5672146382,0.3490581097,-0.3201933849
H,0,-0.3742172948,-2.3736301357,0.0153596722
H,0,1.2900597967,1.9882997181,-0.8952423281
H,0,-0.0524007414,3.0371336031,-0.3496023878
H,0,1.0173790045,2.2191470502,0.8419786519

H,0,4.0778000431,-0.3908950101,1.1591651199
O,0,4.7626469088,-0.7837399751,0.5869541185
H,0,4.1849459478,-1.0935292029,-0.1346760716

N-Methyl Orotic Acid Anion in a Cluster of 8 Waters – Orientation A

E(RB+HF-LYP) = -1253.83450792

Zero-point correction= 0.317692 (Hartree/Particle)
Thermal correction to Energy= 0.349973
Thermal correction to Enthalpy= 0.350917
Thermal correction to Gibbs Free Energy= 0.249072
Sum of electronic and zero-point Energies= -1253.516816
Sum of electronic and thermal Energies= -1253.484535
Sum of electronic and thermal Enthalpies= -1253.483591
Sum of electronic and thermal Free Energies= -1253.585436

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	219.611	108.959	214.351

C,0,4.4360829354,-0.9820040711,0.8503278513
C,0,3.0110241143,-0.9894182669,1.0913371593
C,0,2.1574262011,-0.3229740362,0.2665411773
N,0,2.6074044626,0.4256868427,-0.8111135802
C,0,3.9668673539,0.492972201,-1.1222280428
N,0,4.7940582603,-0.2281312727,-0.2787914341
C,0,0.651454953,-0.4757159191,0.4882886453
O,0,-0.0424061935,-0.7517297624,-0.5294395269
C,0,1.6936822487,1.2276813478,-1.6459633573
O,0,4.417223933,1.1393142209,-2.0635088281
O,0,5.3031846496,-1.5501606643,1.5127041216
O,0,0.2561879434,-0.3603833123,1.6781726675
O,0,-2.2869291884,-0.7665193595,2.0639678193
O,0,-2.5736414442,1.9134172163,3.1392210753
O,0,-2.5718031171,0.4550982278,-0.6529515965
O,0,-3.867433581,4.122188373,1.6399320596
O,0,-4.4284937721,-0.7368915365,-2.659087564
O,0,-1.8921391293,-2.8927455921,0.0016567265
O,0,-3.6812039031,-3.4940060302,-2.0249881399
O,0,-3.0190481583,3.1825783358,-1.0068728213
H,0,5.7805668054,-0.1818299543,-0.5036242183
H,0,2.6275267747,-1.5412941288,1.9374488151
H,0,1.0017745702,1.7794759216,-1.0081876949
H,0,2.3053359248,1.9213951487,-2.2183391539

H,0,1.1227650077,0.582422374,-2.3137378345
H,0,-1.6700832306,0.0643807981,-0.7060297154
H,0,-2.8975065036,0.1718403151,0.2159962402
H,0,-1.2850676722,-0.6507586281,1.9478429268
H,0,-2.4235338509,-1.2424899507,2.8929813627
H,0,-2.8070904261,2.2290338682,-0.9007449415
H,0,-3.7307903578,3.2091000125,-1.6577984432
H,0,-2.264415734,-2.32326753,0.697749042
H,0,-1.1610090516,-2.3450016457,-0.3461724334
H,0,-3.8092466788,-0.3053141286,-2.0462050168
H,0,-4.2328333452,-1.6874369975,-2.5678661349
H,0,-2.5733702628,1.0320462729,2.7177853018
H,0,-1.6496888198,2.193959495,3.1232380837
H,0,-3.5554784532,3.3883912752,2.1966568838
H,0,-3.582881278,3.8844444465,0.7381894727
H,0,-3.032841443,-3.3201244066,-1.3026642016
H,0,-4.3795821862,-4.0263900133,-1.6274517854

N-Methyl Orotic Acid Anion in a Cluster of 8 Waters – Orientation B

E(RB+HF-LYP) = -1253.84141206

Zero-point correction=	0.320354 (Hartree/Particle)
Thermal correction to Energy=	0.352221
Thermal correction to Enthalpy=	0.353165
Thermal correction to Gibbs Free Energy=	0.251427
Sum of electronic and zero-point Energies=	-1253.521058
Sum of electronic and thermal Energies=	-1253.489191
Sum of electronic and thermal Enthalpies=	-1253.488247
Sum of electronic and thermal Free Energies=	-1253.589985

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	221.022	107.622	214.126

C,0,-2.6508161328,0.3831335991,-1.2750059219
C,0,-2.198896876,-0.3059565877,-0.1912508002
N,0,-3.0641875815,-0.9288204706,0.6967519304
C,0,-4.4445642748,-0.9053234096,0.498369784
N,0,-4.8558516336,-0.222693738,-0.631371846
C,0,-4.0621253206,0.4575788757,-1.5721401061
C,0,-0.6915246758,-0.4794123712,0.0242235877
O,0,-0.0126516143,0.5907575928,0.0378614674
C,0,-2.5705842862,-1.6112964376,1.9048501562
O,0,-5.2503763814,-1.4396048837,1.2569729256

O,0,-4.5948532058,1.0292609454,-2.5226259112
O,0,-0.2858070503,-1.6553550549,0.1269484406
O,0,2.4312590027,-2.1517309621,0.6143970721
H,0,-5.8571207723,-0.2041860596,-0.7819034292
H,0,-1.953930483,0.8777111186,-1.9369353272
H,0,-1.855215496,-0.968366754,2.4212882027
H,0,-3.4306840993,-1.8016953625,2.542988059
H,0,-2.0746091055,-2.5443280537,1.6356830591
H,0,1.4692542149,-2.0880654442,0.4155922869
H,0,2.6778481606,-1.2313014465,0.8083568414
H,0,1.6520282692,0.6540424615,0.3240790198
O,0,2.6076761831,0.8371867355,0.5504403517
H,0,2.5677942449,1.3393578625,1.3939099271
H,0,-0.1450412178,2.4293825749,0.4215732545
O,0,0.19167037,3.3202730712,0.6523597006
H,0,0.8392771262,3.5157617047,-0.0521210464
H,0,4.064368173,0.3942999397,-0.616879848
O,0,4.7470672377,0.100962083,-1.248889432
H,0,4.4225889353,-0.7653702586,-1.5808801733
H,0,3.5246930136,-2.6324833354,-0.7669311057
O,0,4.2109034668,-2.6499577708,-1.473591595
H,0,5.0571560881,-2.7484128906,-1.0071103793
H,0,2.7276953447,2.395415883,-0.5103720898
O,0,2.5760711372,3.2712233885,-0.9276062824
H,0,2.8027180722,3.1566435358,-1.8581705842
H,0,2.5811627217,3.3997101413,2.7416627845
O,0,1.9900159702,2.649165139,2.6100067315
H,0,1.2705563481,2.9762088953,2.0096696102
H,0,6.1123462324,-0.7985827724,-0.4061039716
O,0,6.6585263536,-1.5324108206,-0.0395304367
H,0,6.5424463755,-1.4856399992,0.9167198631

N-Methyl Orotic Acid Anion – 6-311++G

E(RB+HF-LYP) = -642.159803399

Zero-point correction= 0.115213 (Hartree/Particle)
Thermal correction to Energy= 0.124903
Thermal correction to Enthalpy= 0.125847
Thermal correction to Gibbs Free Energy= 0.079224
Sum of electronic and zero-point Energies= -642.044590
Sum of electronic and thermal Energies= -642.034900
Sum of electronic and thermal Enthalpies= -642.033956
Sum of electronic and thermal Free Energies= -642.080580

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	78.378	35.663	98.128

N,0,-2.0571495862,0.076670931,0.0319379425
C,0,-1.6540565862,-1.275044069,0.0728749425
C,0,-0.2346505862,-1.450732069,0.0377539425
C,0,0.6159844138,-0.382150069,-0.0117380575
N,0,0.1223064138,0.924697931,-0.0612620575
C,0,-1.2439205862,1.192780931,-0.0501630575
H,0,-3.0501695862,0.256207931,0.0455069425
O,0,-2.5370805862,-2.172466069,0.1308549425
H,0,0.1640054138,-2.450743069,0.0355589425
O,0,-1.7294275862,2.350974931,-0.1105870575
C,0,2.1370234138,-0.589789069,0.0315179425
O,0,2.7260954138,-0.014549069,1.0106899425
O,0,2.6147014138,-1.324612069,-0.8901110575
C,0,1.0537994138,2.076804931,-0.1554720575
H,0,1.7693074138,2.010579931,0.6500069425
H,0,1.5726204138,2.047878931,-1.1093960575
H,0,0.4487524138,2.980488931,-0.0918240575

N-Methyl Orotic Acid Anion – 6-311++G**

E(RB+HF-LYP) = -642.365595338

Zero-point correction= 0.114882 (Hartree/Particle)
Thermal correction to Energy= 0.124206
Thermal correction to Enthalpy= 0.125150
Thermal correction to Gibbs Free Energy= 0.080131
Sum of electronic and zero-point Energies= -642.250713
Sum of electronic and thermal Energies= -642.241390
Sum of electronic and thermal Enthalpies= -642.240446
Sum of electronic and thermal Free Energies= -642.285465

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.940	35.580	94.751

N,0,-2.0571495862,0.076670931,0.0319379425
C,0,-1.6540565862,-1.275044069,0.0728749425
C,0,-0.2346505862,-1.450732069,0.0377539425
C,0,0.6159844138,-0.382150069,-0.0117380575
N,0,0.1223064138,0.924697931,-0.0612620575
C,0,-1.2439205862,1.192780931,-0.0501630575

H,0,-3.0501695862,0.256207931,0.0455069425
O,0,-2.5370805862,-2.172466069,0.1308549425
H,0,0.1640054138,-2.450743069,0.0355589425
O,0,-1.7294275862,2.350974931,-0.1105870575
C,0,2.1370234138,-0.589789069,0.0315179425
O,0,2.7260954138,-0.014549069,1.0106899425
O,0,2.6147014138,-1.324612069,-0.8901110575
C,0,1.0537994138,2.076804931,-0.1554720575
H,0,1.7693074138,2.010579931,0.6500069425
H,0,1.5726204138,2.047878931,-1.1093960575
H,0,0.4487524138,2.980488931,-0.0918240575

Potassium salt of N-Methyl Orotic Acid

E(RB+HF-LYP) = -1242.10943368

Zero-point correction= 0.117889 (Hartree/Particle)
Thermal correction to Energy= 0.130270
Thermal correction to Enthalpy= 0.131214
Thermal correction to Gibbs Free Energy= 0.077113
Sum of electronic and zero-point Energies= -1241.991545
Sum of electronic and thermal Energies= -1241.979164
Sum of electronic and thermal Enthalpies= -1241.978220
Sum of electronic and thermal Free Energies= -1242.032321

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	81.746	42.897	113.866

C,0,-2.6417990178,-0.6729264405,0.2914688932
C,0,-1.2435681642,-1.038046058,0.2000457837
C,0,-0.2911726868,-0.1100687791,-0.0859607234
N,0,-0.6131703046,1.2153720746,-0.3478008833
C,0,-1.9378139335,1.6616425464,-0.2825961308
N,0,-2.8662674187,0.6911157976,0.0480426327
C,0,1.1762886941,-0.5367533354,-0.0195337862
O,0,1.9965652357,0.272137173,0.5059900651
C,0,0.3884834206,2.2064666958,-0.7756916166
O,0,-2.2688530288,2.821358257,-0.5032838736
O,0,-3.5802098121,-1.4194476241,0.5553772934
O,0,1.4496570507,-1.695188813,-0.4404708949
K,0,3.8831658995,-1.501536803,0.3884452095
H,0,-3.8257850802,1.0135728313,0.0961622607
H,0,-0.9616044491,-2.0668147983,0.3707776814
H,0,1.0495777666,1.7607683902,-1.5199445975

H,0,-0.1536428028,3.0445672144,-1.2087212491
H,0,0.9875810993,2.5389307932,0.0722794391

Tetramethylammonium salt of N-Methyl Orotic Acid

E(RB+HF-LYP) = -856.526880770

Zero-point correction= .281498 (Hartree/Particle)
Thermal correction to Energy= .300216
Thermal correction to Enthalpy= .301160
Thermal correction to Gibbs Free Energy= .231820
Sum of electronic and zero-point Energies= -856.245383
Sum of electronic and thermal Energies= -856.226665
Sum of electronic and thermal Enthalpies= -856.225721
Sum of electronic and thermal Free Energies= -856.295061

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	188.388	67.476	145.940

C,0,-2.2595642796,-0.7975996545,-0.0987949092
C,0,-1.337068746,0.1555002797,-0.4032439998
N,0,-1.7060231718,1.4565253628,-0.7151387132
C,0,-3.0455685023,1.8557138657,-0.6942659257
N,0,-3.9416330289,0.8633345646,-0.3431686866
C,0,-3.6690918507,-0.482230808,-0.0406895672
C,0,0.1526918742,-0.200000336,-0.3116280994
O,0,0.5079778304,-1.2665070787,-0.8670947415
C,0,-0.7207096676,2.4631216604,-1.1389569709
O,0,-3.4154744251,2.9940078078,-0.9656962465
O,0,-4.5878299337,-1.249194095,0.2393524495
O,0,0.8708738086,0.5887246374,0.3702875099
C,0,3.9483864067,0.1383308227,0.1197309378
H,0,-4.9136608782,1.1484416838,-0.3236551057
H,0,-1.9453087474,-1.8109650712,0.1062790937
H,0,-0.0639293925,2.0342213489,-1.8986780759
H,0,-1.2738592581,3.3022643628,-1.5555907362
H,0,-0.116729966,2.7841428397,-0.2898712149
H,0,2.9224237331,0.4453349134,-0.1111132132
H,0,4.5437204012,-0.0153906275,-0.7815703804
H,0,4.4275442602,0.8758845267,0.7663751567
N,0,3.8718154688,-1.1714931898,0.8692260492
C,0,5.2386419431,-1.586147405,1.3209849525
C,0,2.9657986859,-0.9909289874,2.065157362
C,0,3.2897465346,-2.2288136259,-0.0421722205

H,0,2.848433288,-1.9567780867,2.5587327915
H,0,3.4329237625,-0.2752825228,2.7442395052
H,0,2.0116130282,-0.5967687178,1.7022212768
H,0,3.2305507087,-3.1641695164,0.5174233266
H,0,2.2899114948,-1.9032549949,-0.3720785639
H,0,3.961577668,-2.3474921407,-0.8944052552
H,0,5.1634764731,-2.5315458684,1.8605102281
H,0,5.8797289052,-1.7089290107,0.4467160048
H,0,5.6485170099,-0.8162053248,1.9765134865

N-Methyl Orotic Acid Anion protonated at C5

E(RB+HF-LYP) = -642.688478889

Zero-point correction= 0.127408 (Hartree/Particle)
Thermal correction to Energy= 0.138626
Thermal correction to Enthalpy= 0.139570
Thermal correction to Gibbs Free Energy= 0.088810
Sum of electronic and zero-point Energies= -642.561070
Sum of electronic and thermal Energies= -642.549853
Sum of electronic and thermal Enthalpies= -642.548909
Sum of electronic and thermal Free Energies= -642.599669

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	86.989	39.213	106.833

C,0,-0.7449614359,0.1422664638,-1.3317145474
C,0,-2.0390351587,-0.0013142887,-0.5646343593
N,0,-1.8934678914,0.0014096399,0.822505088
C,0,-0.7264346055,0.0822508982,1.5563973376
N,0,0.4885442282,0.1612202676,0.7896028737
C,0,0.5147791094,0.0981728273,-0.5340043915
O,0,-3.129705816,-0.0953341856,-1.0832022413
H,0,-2.7429463138,-0.0793150071,1.3735558619
O,0,-0.7048258379,0.0876284812,2.7653465448
C,0,1.7433650029,0.1946383963,1.5809702013
C,0,1.8248465965,-0.1197873884,-1.2774457604
O,0,2.5701091396,0.8101939642,-1.5745766135
O,0,1.8273791198,-1.3674367836,-1.427643813
H,0,-0.7683192465,1.103733737,-1.866638505
H,0,2.5195101025,0.6398689872,0.9616018802
H,0,1.5693984018,0.7890256689,2.4751165825
H,0,2.016912218,-0.8236711212,1.8646121265
H,0,-0.6990994159,-0.6258248787,-2.1098055765

N-Methyl Orotic Acid Anion – protonated at O4

E(RB+HF-LYP) = -642.687552572

Zero-point correction= 0.128122 (Hartree/Particle)
Thermal correction to Energy= 0.139302
Thermal correction to Enthalpy= 0.140247
Thermal correction to Gibbs Free Energy= 0.089381
Sum of electronic and zero-point Energies= -642.559431
Sum of electronic and thermal Energies= -642.548250
Sum of electronic and thermal Enthalpies= -642.547306
Sum of electronic and thermal Free Energies= -642.598172

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	87.414	39.705	107.056

N,0,0.2344343596,0.9201618399,-0.0150308131
C,0,-1.1134526398,1.3104139551,0.0277679724
N,0,-2.0128922473,0.2403146837,0.021208572
C,0,-1.6537695545,-1.0701478133,0.0045504159
C,0,-0.3248067698,-1.4114129555,-0.0144071782
C,0,0.6273067498,-0.3799146504,-0.0227252011
C,0,1.2478778777,2.0006795326,-0.0213184344
O,0,-1.499300311,2.4615440293,0.0627165637
H,-2.9944609448,0.4938147486,0.0459325292
O,0,-2.702782129,-1.8985979822,0.0123015073
H,0,0.0044392547,-2.4425730472,-0.0126752206
C,0,2.1290374065,-0.7092690937,-0.0249799823
O,0,2.6395242191,-0.6841972892,-1.1582667752
O,0,2.5529382376,-0.9469081119,1.1197875595
H,0,2.0150895931,1.7399981792,-0.7499042086
H,0,0.7495335966,2.9293242117,-0.2877119216
H,0,1.691781357,2.0824240322,0.9731925589
H,0,-2.4133761959,-2.8231428062,0.0022855541

5H N-Methyl Orotic Acid Zwitterion

E(RB+HF-LYP) = -642.688479055

Zero-point correction= 0.127402 (Hartree/Particle)
Thermal correction to Energy= 0.138622
Thermal correction to Enthalpy= 0.139566
Thermal correction to Gibbs Free Energy= 0.088785
Sum of electronic and zero-point Energies= -642.561078
Sum of electronic and thermal Energies= -642.549857

Sum of electronic and thermal Enthalpies= -642.548913
Sum of electronic and thermal Free Energies= -642.599694

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	86.987	39.215	106.879

C,0,0.7587094686,1.3288746327,0.0786585453
C,0,0.7266821613,-0.1624086888,0.0674016191
C,0,-0.572907561,2.0371520178,-0.0144815009
O,0,-0.6983688974,3.2371204307,-0.1224254082
N,0,-1.6828865401,1.1952401465,0.0527949649
C,0,-1.7027121652,-0.1814168117,0.1597515206
O,0,-2.724442671,-0.8249522037,0.2224386854
N,0,-0.4151636837,-0.8231308228,0.193531145
C,0,2.0308406716,-0.9035925022,-0.1908537849
O,0,2.1096880797,-0.8563032404,-1.4439451827
C,0,-0.4403990851,-2.3054911071,0.2569846864
O,0,2.7087310878,-1.3666622549,0.7229456539
H,0,1.4091672471,1.6750494909,-0.7305272984
H,0,1.2519329175,1.6459737148,1.0098610141
H,0,-2.5969245238,1.6358694865,0.0061744311
H,0,0.5087092626,-2.640275459,0.6709726702
H,0,-0.5819625598,-2.7060487983,-0.748876047
H,0,-1.2707125107,-2.6076607992,0.8912359597

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 1.8A

E(RB+HF-LYP) = -642.204523100

Zero-point correction= 0.114943 (Hartree/Particle)
Thermal correction to Energy= 0.125764
Thermal correction to Enthalpy= 0.126708
Thermal correction to Gibbs Free Energy= 0.076480
Sum of electronic and zero-point Energies= -642.089581
Sum of electronic and thermal Energies= -642.078759
Sum of electronic and thermal Enthalpies= -642.077815
Sum of electronic and thermal Free Energies= -642.128043

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	78.918	38.431	105.713

N,0,-0.1008801434,-0.9693185353,0.0123290073
C,0,-1.4918704898,-0.976884183,0.0337412541

N,0,-2.082923026,0.2708577863,0.0106450745
C,0,-1.4425008467,1.5265086116,0.0213074165
C,0,-0.0075629505,1.4205172686,0.0273112364
C,0,0.6266544332,0.2131337266,0.0165862137
C,0,0.5333046318,-2.2958588276,0.0823361555
O,0,-2.1618463055,-2.0126745868,0.0709969615
H,0,-3.0949561195,0.2736079845,0.0242762049
O,0,-2.1340022671,2.5517911435,0.0223388832
H,0,0.5907399584,2.3215558039,0.0491470378
C,0,2.4231329442,0.2708894873,-0.0800005837
O,0,2.9463316758,-0.74953782,-0.5501038296
O,0,2.8383645458,1.3596367536,0.3149081878
H,0,1.5965843204,-2.1623287076,-0.1055235239
H,0,0.0824951351,-2.9474822478,-0.6691298632
H,0,0.3540313653,-2.7396880132,1.0675997929

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.0A

E(RB+HF-LYP) = -642.193320776

Zero-point correction= 0.114208 (Hartree/Particle)
Thermal correction to Energy= 0.124499
Thermal correction to Enthalpy= 0.125443
Thermal correction to Gibbs Free Energy= 0.077050
Sum of electronic and zero-point Energies= -642.079112
Sum of electronic and thermal Energies= -642.068822
Sum of electronic and thermal Enthalpies= -642.067878
Sum of electronic and thermal Free Energies= -642.116271

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	78.124	36.971	101.852

N,0,-0.1559667,-0.9771845955,0.
C,0,-1.5463316847,-0.9771691258,0.
N,0,-2.1233642561,0.2768971804,0.
C,0,-1.4682277452,1.5274626276,0.
C,0,-0.0341227146,1.4055456798,0.
C,0,0.5893174799,0.1918743608,0.
C,0,0.4760413961,-2.3038875654,0.
O,0,-2.2243957632,-2.009694014,0.
H,0,-3.1353323663,0.2922761078,0.
O,0,-2.1536906296,2.5581231584,0.
H,0,0.5696487079,2.304495108,0.
C,0,2.5873828412,0.2798246224,0.

O,0,2.8911427339,1.4576765445,0.
O,0,3.1151260729,-0.8250271047,0.
H,0,0.1586894208,-2.8647370772,0.8843758036
H,0,0.1586894208,-2.8647370772,-0.8843758036
H,0,1.5538047613,-2.1558174255,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.1A

E(RB+HF-LYP) = -642.188137471

Zero-point correction= 0.113995 (Hartree/Particle)
Thermal correction to Energy= 0.124378
Thermal correction to Enthalpy= 0.125322
Thermal correction to Gibbs Free Energy= 0.076790
Sum of electronic and zero-point Energies= -642.074143
Sum of electronic and thermal Energies= -642.063759
Sum of electronic and thermal Enthalpies= -642.062815
Sum of electronic and thermal Free Energies= -642.111348

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	78.048	37.186	102.145

N,0,-0.985199309,-0.1352012261,0.
C,0,-1.4218890414,1.1834133218,0.
N,0,-0.4101609667,2.1227901678,0.
C,0,0.9828477913,1.8895062086,0.
C,0,1.3144417005,0.4886207589,0.
C,0,0.356767441,-0.4851099688,0.
C,0,-2.0411270319,-1.1554840653,0.
O,0,-2.6153536979,1.5051232991,0.
H,0,-0.7104620354,3.0892346788,0.
O,0,1.7475923072,2.8637197499,0.
H,0,2.3601906609,0.2046618875,0.
C,0,1.1069247625,-2.4465555539,0.
O,0,2.3109541214,-2.3290541802,0.
O,0,0.2113607708,-3.2710442287,0.
H,0,-2.6748201738,-1.0369872106,0.8844753061
H,0,-2.6748201738,-1.0369872106,-0.8844753061
H,0,-1.5567880916,-2.1293460664,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.2A

E(RB+HF-LYP) = -642.183533562

Zero-point correction= 0.113768 (Hartree/Particle)

Thermal correction to Energy= 0.124250
Thermal correction to Enthalpy= 0.125194
Thermal correction to Gibbs Free Energy= 0.076439
Sum of electronic and zero-point Energies= -642.069766
Sum of electronic and thermal Energies= -642.059284
Sum of electronic and thermal Enthalpies= -642.058339
Sum of electronic and thermal Free Energies= -642.107095

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.968	37.394	102.615

N,0,-0.9925774057,-0.1137460648,0.
C,0,-1.4312782986,1.203596562,0.
N,0,-0.4195778335,2.1424950937,0.
C,0,0.9741483207,1.9080187245,0.
C,0,1.3043835841,0.5073544627,0.
C,0,0.3486382991,-0.4708528455,0.
C,0,-2.0438655954,-1.1373192288,0.
O,0,-2.6256289504,1.5248874643,0.
H,0,-0.7184852907,3.1093233388,0.
O,0,1.7382719695,2.8836586854,0.
H,0,2.3515952838,0.2276343744,0.
C,0,1.1397530476,-2.523689246,0.
O,0,2.3344446566,-2.3742966149,0.
O,0,0.2297610359,-3.3220451928,0.
H,0,-2.679224246,-1.0247480394,0.8844060018
H,0,-2.679224246,-1.0247480394,-0.8844060018
H,0,-1.555040663,-2.1089901451,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.3A

E(RB+HF-LYP) = -642.179574272

Zero-point correction= 0.113526 (Hartree/Particle)
Thermal correction to Energy= 0.124126
Thermal correction to Enthalpy= 0.125070
Thermal correction to Gibbs Free Energy= 0.075948
Sum of electronic and zero-point Energies= -642.066048
Sum of electronic and thermal Energies= -642.055448
Sum of electronic and thermal Enthalpies= -642.054504
Sum of electronic and thermal Free Energies= -642.103626

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

TOTAL	77.890	37.599	103.386

N,0,-0.1541049428,0.9938868287,0.
C,0,-1.5382890606,1.097968062,0.
N,0,-2.2004637428,-0.1126817869,0.
C,0,-1.6304744529,-1.4064717243,0.
C,0,-0.1920553969,-1.381894522,0.
C,0,0.5279544455,-0.2165552834,0.
C,0,0.5792599201,2.2636001346,0.
O,0,-2.1430700431,2.1777175128,0.
H,0,-3.2110540995,-0.0603228059,0.
O,0,-2.3903934974,-2.3863865571,0.
H,0,0.331730623,-2.3314307068,0.
C,0,2.8098359544,-0.5046826681,0.
O,0,2.9168922412,-1.6981800733,0.
O,0,3.3353675532,0.5785608438,0.
H,0,0.315858297,2.8534351692,-0.8841783593
H,0,0.315858297,2.8534351692,0.8841783593
H,0,1.6418291938,2.0309700784,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.4A

E(RB+HF-LYP) = -642.176274741

Zero-point correction= 0.113321 (Hartree/Particle)
Thermal correction to Energy= 0.124026
Thermal correction to Enthalpy= 0.124970
Thermal correction to Gibbs Free Energy= 0.075496
Sum of electronic and zero-point Energies= -642.062954
Sum of electronic and thermal Energies= -642.052249
Sum of electronic and thermal Enthalpies= -642.051304
Sum of electronic and thermal Free Energies= -642.100778

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.828	37.778	104.127

N,0,-0.1754506831,0.9945275279,0.
C,0,-1.5588053058,1.1015538503,0.
N,0,-2.2221975603,-0.1081126923,0.
C,0,-1.652091313,-1.4021153142,0.
C,0,-0.2139437066,-1.3779295209,0.
C,0,0.5135002668,-0.2144144147,0.
C,0,0.5598461394,2.2622709551,0.
O,0,-2.1629556495,2.1824701507,0.

H,0,-3.2327422365,-0.0555725959,0.
O,0,-2.4138011937,-2.3816383256,0.
H,0,0.3022610009,-2.3320207153,0.
C,0,2.8943028777,-0.5173648113,0.
O,0,2.9686789932,-1.7080566876,0.
O,0,3.387511091,0.574594367,0.
H,0,0.3003974165,2.8541960153,-0.8842436861
H,0,0.3003974165,2.8541960153,0.8842436861
H,0,1.6209044279,2.023336929,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.5A

E(RB+HF-LYP) = -642.173593550

Zero-point correction= 0.113142 (Hartree/Particle)
Thermal correction to Energy= 0.123945
Thermal correction to Enthalpy= 0.124889
Thermal correction to Gibbs Free Energy= 0.075079
Sum of electronic and zero-point Energies= -642.060452
Sum of electronic and thermal Energies= -642.049649
Sum of electronic and thermal Enthalpies= -642.048704
Sum of electronic and thermal Free Energies= -642.098514

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.777	37.931	104.833

N,0,-0.2720074749,-0.9790680716,0.
C,0,-1.6584571865,-0.9825359298,0.
N,0,-2.2292927219,0.2733976043,0.
C,0,-1.562060472,1.5198865119,0.
C,0,-0.1302312731,1.3862449514,0.
C,0,0.5144039177,0.1723121976,0.
C,0,0.3647215811,-2.2984553619,0.
O,0,-2.3433988941,-2.0151183037,0.
H,0,-3.2408654735,0.2974583515,0.
O,0,-2.247915628,2.5548815313,0.
H,0,0.4514317173,2.3023345187,0.
C,0,3.0108621464,0.3053397184,0.
O,0,3.1397430594,1.48660433,0.
O,0,3.3886008548,-0.8261880071,0.
H,0,0.0632814888,-2.8704750764,0.8842824679
H,0,0.0632814888,-2.8704750764,-0.8842824679
H,0,1.4403047374,-2.1373383761,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.5A

E(RB+HF-LYP) = -642.173593550

Zero-point correction= 0.113142 (Hartree/Particle)
Thermal correction to Energy= 0.123945
Thermal correction to Enthalpy= 0.124889
Thermal correction to Gibbs Free Energy= 0.075079
Sum of electronic and zero-point Energies= -642.060452
Sum of electronic and thermal Energies= -642.049649
Sum of electronic and thermal Enthalpies= -642.048704
Sum of electronic and thermal Free Energies= -642.098514

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.777	37.931	104.833

N,0,-0.2720074749,-0.9790680716,0.
C,0,-1.6584571865,-0.9825359298,0.
N,0,-2.2292927219,0.2733976043,0.
C,0,-1.562060472,1.5198865119,0.
C,0,-0.1302312731,1.3862449514,0.
C,0,0.5144039177,0.1723121976,0.
C,0,0.3647215811,-2.2984553619,0.
O,0,-2.3433988941,-2.0151183037,0.
H,0,-3.2408654735,0.2974583515,0.
O,0,-2.247915628,2.5548815313,0.
H,0,0.4514317173,2.3023345187,0.
C,0,3.0108621464,0.3053397184,0.
O,0,3.1397430594,1.48660433,0.
O,0,3.3886008548,-0.8261880071,0.
H,0,0.0632814888,-2.8704750764,0.8842824679
H,0,0.0632814888,-2.8704750764,-0.8842824679
H,0,1.4403047374,-2.1373383761,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.6A

E(RB+HF-LYP) = -642.171447125

Zero-point correction= 0.112947 (Hartree/Particle)
Thermal correction to Energy= 0.123881
Thermal correction to Enthalpy= 0.124825
Thermal correction to Gibbs Free Energy= 0.074433
Sum of electronic and zero-point Energies= -642.058500
Sum of electronic and thermal Energies= -642.047566
Sum of electronic and thermal Enthalpies= -642.046622

Sum of electronic and thermal Free Energies= -642.097014

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.737	38.070	106.059

N,0,-0.2885664598,-0.9780086557,0.0000017859
C,0,-1.6749180268,-0.9893705647,0.0000116834
N,0,-2.2518024778,0.2633350081,-0.0000015479
C,0,-1.5895230795,1.5127986915,-0.0000169978
C,0,-0.1577010336,1.3850766635,-0.000000848
C,0,0.4990235241,0.1747644464,-0.000000128
C,0,0.3522095029,-2.2948235038,-0.0000004915
O,0,-2.3552811326,-2.0256482051,-0.0000007822
H,0,-3.2634547776,0.2831297943,-0.0000016506
O,0,-2.281427966,2.544639377,0.0000062669
H,0,0.4153835069,2.306981546,0.0000057331
C,0,3.0949578816,0.3201074353,-0.0000003225
O,0,3.1875247806,1.500272614,0.0000010506
O,0,3.4429592177,-0.815720148,-0.000001669
H,0,0.0545300919,-2.8693401244,0.8842484865
H,0,0.0545287993,-2.8693389666,-0.8842497955
H,0,1.4271031339,-2.1283848292,-0.000000743

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 2.8A

E(RB+HF-LYP) = -642.168426056

Zero-point correction= 0.112779 (Hartree/Particle)
Thermal correction to Energy= 0.123834
Thermal correction to Enthalpy= 0.124778
Thermal correction to Gibbs Free Energy= 0.073734
Sum of electronic and zero-point Energies= -642.055648
Sum of electronic and thermal Energies= -642.044592
Sum of electronic and thermal Enthalpies= -642.043648
Sum of electronic and thermal Free Energies= -642.094693

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.707	38.202	107.433

N,0,-0.3364386282,-0.9685812784,0.
C,0,-1.72178917,-0.9755420911,0.
N,0,-2.2948441495,0.2786262956,0.
C,0,-1.6259237494,1.5241351911,0.

C,0,-0.1955411134,1.3891405763,0.
C,0,0.4678098861,0.1784754514,0.
C,0,0.2958990864,-2.2888284482,0.
O,0,-2.4076593481,-2.0095732485,0.
H,0,-3.3063077125,0.3025638737,0.
O,0,-2.3138253882,2.5601261739,0.
H,0,0.3736994623,2.3138699507,0.
C,0,3.2653748028,0.2952621989,0.
O,0,3.325517613,1.4710449336,0.
O,0,3.5298737358,-0.8554487907,0.
H,0,-0.0032437346,-2.8632269647,0.8842267638
H,0,-0.0032437346,-2.8632269647,-0.8842267638
H,0,1.3718438079,-2.1253448325,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 3.0A

E(RB+HF-LYP) = -642.166420137

Zero-point correction= 0.112682 (Hartree/Particle)
Thermal correction to Energy= 0.123856
Thermal correction to Enthalpy= 0.124800
Thermal correction to Gibbs Free Energy= 0.072926
Sum of electronic and zero-point Energies= -642.053738
Sum of electronic and thermal Energies= -642.042564
Sum of electronic and thermal Enthalpies= -642.041620
Sum of electronic and thermal Free Energies= -642.093495

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.721	38.233	109.179

N,0,-0.3879745615,-0.9686336925,0.
C,0,-1.7725471482,-0.9650218265,0.
N,0,-2.3361028141,0.2934552973,0.
C,0,-1.6564333683,1.5328234884,0.
C,0,-0.2275572806,1.3852913154,0.
C,0,0.4327426441,0.1703134775,0.
C,0,0.2299870941,-2.2950478388,0.
O,0,-2.4681182379,-1.993471071,0.
H,0,-3.3473197406,0.3252514617,0.
O,0,-2.3363393952,2.5749739241,0.
H,0,0.3457166747,2.3079987092,0.
C,0,3.4306495867,0.2824920912,0.
O,0,3.4477404701,1.4556063748,0.
O,0,3.6428247011,-0.874232508,0.

H,0,-0.0735768902,-2.8674114867,0.8843035582
H,0,-0.0735768902,-2.8674114867,-0.8843035582
H,0,1.3073890044,-2.1402964345,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 3.4A

E(RB+HF-LYP) = -642.163503430

Zero-point correction= 0.112626 (Hartree/Particle)
Thermal correction to Energy= 0.123909
Thermal correction to Enthalpy= 0.124853
Thermal correction to Gibbs Free Energy= 0.071992
Sum of electronic and zero-point Energies= -642.050877
Sum of electronic and thermal Energies= -642.039595
Sum of electronic and thermal Enthalpies= -642.038651
Sum of electronic and thermal Free Energies= -642.091511

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.754	38.189	111.254

N,0,-0.4677258773,-0.9539067347,0.
C,0,-1.8521657438,-0.9706409738,0.
N,0,-2.4338448831,0.2791138545,0.
C,0,-1.7714542403,1.5280659293,0.
C,0,-0.3415561713,1.4002016956,0.
C,0,0.3421037157,0.1952240934,0.
C,0,0.1658220802,-2.2723342369,0.
O,0,-2.5339063345,-2.0090811144,0.
H,0,-3.4453971803,0.2968783922,0.
O,0,-2.4676720106,2.5603719023,0.
H,0,0.2167326252,2.3321185901,0.
C,0,3.7410300288,0.280803214,0.
O,0,3.7592578997,1.4510477186,0.
O,0,3.8492569218,-0.8863273092,0.
H,0,-0.1298593619,-2.8492615598,0.8843109293
H,0,-0.1298593619,-2.8492615598,-0.8843109293
H,0,1.2412087749,-2.1029316076,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 3.55A

E(RB+HF-LYP) = -642.162609586

Zero-point correction= 0.112613 (Hartree/Particle)
Thermal correction to Energy= 0.123934
Thermal correction to Enthalpy= 0.124878

Thermal correction to Gibbs Free Energy= 0.071570
Sum of electronic and zero-point Energies= -642.049997
Sum of electronic and thermal Energies= -642.038676
Sum of electronic and thermal Enthalpies= -642.037732
Sum of electronic and thermal Free Energies= -642.091040

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.770	38.168	112.197

N,0,-0.5031038282,-0.9552962107,0.
C,0,-1.8872233845,-0.973991622,0.
N,0,-2.4706241069,0.2752222219,0.
C,0,-1.809540973,1.5247500999,0.
C,0,-0.3794278546,1.3983499001,0.
C,0,0.3066350804,0.1948104978,0.
C,0,0.1323705373,-2.2725798231,0.
O,0,-2.5679254623,-2.0132116184,0.
H,0,-3.4821629631,0.2917476314,0.
O,0,-2.5067781126,2.5564460588,0.
H,0,0.1767544926,2.3317061756,0.
C,0,3.8554153772,0.2878901926,0.
O,0,3.8473686324,1.4576311406,0.
O,0,3.9682944272,-0.8781326863,0.
H,0,-0.1615276458,-2.8501844675,0.8844807776
H,0,-0.1615276458,-2.8501844675,-0.8844807776
H,0,1.2075107338,-2.0998055798,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 3.7A

E(RB+HF-LYP) = -642.161783274

Zero-point correction= 0.112566 (Hartree/Particle)
Thermal correction to Energy= 0.123940
Thermal correction to Enthalpy= 0.124884
Thermal correction to Gibbs Free Energy= 0.071050
Sum of electronic and zero-point Energies= -642.049217
Sum of electronic and thermal Energies= -642.037843
Sum of electronic and thermal Enthalpies= -642.036899
Sum of electronic and thermal Free Energies= -642.090734

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.773	38.161	113.304

N,0,-0.5385508864,-0.9567696722,0.
C,0,-1.9225318186,-0.9776800003,0.
N,0,-2.5077539784,0.2704949572,0.
C,0,-1.8482538117,1.5209639259,0.
C,0,-0.4180985143,1.3967243464,0.
C,0,0.2704163942,0.1940803001,0.
C,0,0.0988051564,-2.2732054192,0.
O,0,-2.6016338974,-2.018143663,0.
H,0,-3.5193348351,0.2855717107,0.
O,0,-2.5470909503,2.5518125187,0.
H,0,0.1362374557,2.3311592099,0.
C,0,3.9689866677,0.2968289881,0.
O,0,3.957559285,1.4663179748,0.
O,0,4.0693744482,-0.8698630358,0.
H,0,-0.1938890211,-2.8514541105,0.8845200765
H,0,-0.1938890211,-2.8514541105,-0.8845200765
H,0,1.1733939475,-2.097162898,0.

Decarboxylation of N-Methyl Orotic Acid – distance of CO_2 loss fixed 4.2A

E(RB+HF-LYP) = -642.159649383

Zero-point correction= 0.112522 (Hartree/Particle)
Thermal correction to Energy= 0.123963
Thermal correction to Enthalpy= 0.124907
Thermal correction to Gibbs Free Energy= 0.070013
Sum of electronic and zero-point Energies= -642.047127
Sum of electronic and thermal Energies= -642.035687
Sum of electronic and thermal Enthalpies= -642.034743
Sum of electronic and thermal Free Energies= -642.089636

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	77.788	38.123	115.533

N,0,-0.6627903838,-0.9550083664,0.
C,0,-2.0467985297,-0.9761207483,0.
N,0,-2.632000435,0.2720026643,0.
C,0,-1.9721513641,1.5224415574,0.
C,0,-0.5423593748,1.3976415123,0.
C,0,0.1477445005,0.1951486347,0.
C,0,-0.0255332395,-2.2714134609,0.
O,0,-2.7262131234,-2.0166362209,0.
H,0,-3.6435688451,0.2871477663,0.
O,0,-2.6713280614,2.5534167043,0.

H,0,0.0117521783,2.3322979957,0.
C,0,4.3465937739,0.2934423863,0.
O,0,4.3672832905,1.4627008311,0.
O,0,4.3848477635,-0.8759571808,0.
H,0,-0.3176892013,-2.8499495163,0.8845966086
H,0,-0.3176892013,-2.8499495163,-0.8845966086
H,0,1.0490372493,-2.0935391745,0.

Transition State for decarboxylation of 5H N-Methyl Orotic Acid Anion – protonated at C5

E(RB+HF-LYP) = -642.672227051

Zero-point correction= 0.125331 (Hartree/Particle)
Thermal correction to Energy= 0.136443
Thermal correction to Enthalpy= 0.137387
Thermal correction to Gibbs Free Energy= 0.085977
Sum of electronic and zero-point Energies= -642.546897
Sum of electronic and thermal Energies= -642.535784
Sum of electronic and thermal Enthalpies= -642.534840
Sum of electronic and thermal Free Energies= -642.586250

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	85.619	38.870	108.203

C,0,0.1354282101,-1.4160011019,-0.0010175043
C,0,-0.6124855632,-0.1315273079,0.003133133
C,0,1.6452307363,-1.3945030879,-0.0088387741
O,0,2.3581751611,-2.3756616925,-0.0128708314
N,0,2.1964065409,-0.1094163615,-0.0112267543
C,0,1.522779334,1.0917678821,-0.0073956069
O,0,2.0732728199,2.1681444174,-0.0098632841
N,0,0.0689342215,0.991348168,-0.0000177579
C,0,-2.7106049461,-0.4577568337,0.0136470587
O,0,-2.750201317,-1.6533219279,0.0128037787
C,0,-0.6164356268,2.3099503688,0.003831522
O,0,-3.2433017959,0.6134311346,0.0173551379
H,0,-0.22422493,-2.0093482131,-0.8532219953
H,0,-0.215319042,-2.0096625068,0.8546741636
H,0,3.2100085018,-0.0413771189,-0.0164228689
H,0,-0.309993745,2.8685479464,0.8892694701
H,0,-1.6858781604,2.1169686221,0.009225693
H,0,-0.3190097728,2.8690336558,-0.884370256

N-Methyl Uracil Carbene – protonated at O4

E(RB+HF-LYP) = -454.068058911

Zero-point correction=	0.112733 (Hartree/Particle)
Thermal correction to Energy=	0.121064
Thermal correction to Enthalpy=	0.122008
Thermal correction to Gibbs Free Energy=	0.079782
Sum of electronic and zero-point Energies=	-453.955326
Sum of electronic and thermal Energies=	-453.946995
Sum of electronic and thermal Enthalpies=	-453.946051
Sum of electronic and thermal Free Energies=	-453.988277

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	75.969	30.516	88.873

N,0,-1.1185995982,-0.5097991368,-0.0000276993
C,0,-0.6939821991,0.8215509772,0.0000249913
N,0,0.6979856831,0.9627742876,-0.0001665179
C,0,1.566956709,-0.0930519193,-0.000016023
C,0,1.0693219385,-1.3698469979,0.0001465644
C,0,-0.3285817612,-1.6316082663,0.0001146068
C,0,-2.5855774626,-0.6672893683,-0.0000593243
O,0,-1.425185777,1.8007794605,0.0001099865
H,0,1.0097542143,1.9266551816,-0.000477873
O,0,2.8895160705,0.1677844522,-0.0001255638
H,0,1.7717424079,-2.1951161936,0.0003375263
H,0,-3.0154982864,-0.1942108647,0.8866216449
H,0,-3.0155518741,-0.1932581468,-0.8861988431
H,0,-2.7790713653,-1.7372254968,-0.0005973235
H,0,3.0894566129,1.1152916107,0.0005341155

5H N-Methyl Uracil Carbene – protonated at C5

E(RB+HF-LYP) = -454.083292315

Zero-point correction=	0.112662 (Hartree/Particle)
Thermal correction to Energy=	0.120801
Thermal correction to Enthalpy=	0.121746
Thermal correction to Gibbs Free Energy=	0.079224
Sum of electronic and zero-point Energies=	-453.970631
Sum of electronic and thermal Energies=	-453.962491
Sum of electronic and thermal Enthalpies=	-453.961547
Sum of electronic and thermal Free Energies=	-454.004068

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	75.804	29.501	89.494

C,0,1.4606716084,0.9320267395,-0.4107954012
C,0,1.560453718,-0.5312316135,-0.0964006596
C,0,0.1277969939,1.6499014852,-0.3871876431
O,0,-0.0426677691,2.8293358068,-0.6276352692
N,0,-0.9461925627,0.8251311299,-0.0540442381
C,0,-0.9020375612,-0.5233762472,0.2416244476
O,0,-1.8928909348,-1.164460562,0.5220121416
N,0,0.4086760616,-1.1266047768,0.195953438
C,0,0.3961639782,-2.5717240793,0.5216183724
H,0,1.9177536136,1.0879152332,-1.3979691212
H,0,2.1482321474,1.4610527723,0.2637890178
H,0,-1.8684946945,1.2492306859,-0.0216376623
H,0,-0.0000404857,-2.7242378202,1.5275833727
H,0,1.4280493178,-2.9074877857,0.4545119263
H,0,-0.2367071826,-3.1087372238,-0.1878116083

Transition state for rearrangement 5H N-Methyl Uracil Carbene – transfer of a proton from C5 to C6 to yield uracil

E(RB+HF-LYP) = -454.045218120

Zero-point correction= 0.109289 (Hartree/Particle)
Thermal correction to Energy= 0.117038
Thermal correction to Enthalpy= 0.117982
Thermal correction to Gibbs Free Energy= 0.076739
Sum of electronic and zero-point Energies= -453.935929
Sum of electronic and thermal Energies= -453.928180
Sum of electronic and thermal Enthalpies= -453.927236
Sum of electronic and thermal Free Energies= -453.968480

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	73.442	28.428	86.804

N,0,0.2729600777,-1.161631404,0.0502028854
C,0,1.5020403892,-0.5643569337,-0.0390692849
C,0,1.5197877499,0.8424700193,-0.0343204175
C,0,0.2881012216,1.6835827161,-0.0675435218
N,0,-0.8654138377,0.9065878086,-0.0762374421
C,0,-0.9565841749,-0.4867817155,-0.0349825928
O,0,0.2596611611,2.9019715177,-0.0791296994

O,0,-2.0323313794,-1.0566040059,-0.0556267235
H,0,2.4598453015,1.3622884218,-0.198340322
H,0,1.9508423196,0.1250803922,0.988948205
H,0,-1.7557812312,1.392544721,-0.1157522455
C,0,0.1789377476,-2.6264612754,0.1725195462
H,0,-0.3600866921,-2.8967832939,1.0840611089
H,0,-0.3576861822,-3.0439927793,-0.6825939378
H,0,1.19770695,-3.0074892523,0.2043480967

Protonation of 5H N-Methyl Uracil Carbene with Me_3NH^+

E(RB+HF-LYP) = -628.980138380

Zero-point correction= 0.244137 (Hartree/Particle)
Thermal correction to Energy= 0.259348
Thermal correction to Enthalpy= 0.260292
Thermal correction to Gibbs Free Energy= 0.199349
Sum of electronic and zero-point Energies= -628.736002
Sum of electronic and thermal Energies= -628.720790
Sum of electronic and thermal Enthalpies= -628.719846
Sum of electronic and thermal Free Energies= -628.780789

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.743	53.800	128.266

C,0,-2.242904846,-1.0016263566,0.005527877
N,0,-0.7670958551,-0.9845470413,0.0060743432
C,0,-0.0198579342,0.0902099045,-0.0003568135
C,0,-0.6999800625,1.4200277535,-0.008894612
C,0,-2.2159130395,1.4822719561,-0.0099912178
N,0,-2.8424971526,0.2319788003,-0.0024496168
C,0,-0.1879507863,-2.3500314461,0.0148930401
O,0,-2.8510298675,2.5090157038,-0.016712527
O,0,-2.8272501255,-2.0538383121,0.0118339751
N,0,2.7342966186,0.1817259756,-0.0003211284
C,0,3.2499931073,-0.4845917606,-1.2241401076
C,0,3.0546307103,1.6337746567,-0.0110233537
C,0,3.2492796372,-0.466357175,1.2335534656
H,0,-0.3379353821,1.9899538218,-0.876560494
H,0,-0.3387701232,2.0005547518,0.8520728448
H,0,-3.8604554998,0.2250473495,-0.002871539
H,0,-0.5264210987,-2.8833477483,0.9038553968
H,0,0.8943958985,-2.2531799798,0.0150855754
H,0,-0.5251438806,-2.8942708492,-0.8679178165

H,0,1.4764612521,0.0815135651,0.0001370183
H,0,4.3371679826,-0.3642350869,1.2973197622
H,0,2.7935714155,0.0053362908,2.1071069254
H,0,2.9928055608,-1.527729373,1.2236359514
H,0,4.3378594326,-0.3829643993,-1.289043604
H,0,2.9940068064,-1.5458140298,-1.1983846525
H,0,2.7943943673,-0.0262826859,-2.1048468691
H,0,4.1379857042,1.7884733949,-0.0116804091
H,0,2.6302232721,2.0930086749,-0.9065628131
H,0,2.6293882423,2.1063478323,0.8771482839

5H N-Methyl Uracil Cation

E(RB+HF-LYP) = -454.477463388

Zero-point correction= 0.125895 (Hartree/Particle)
Thermal correction to Energy= 0.134132
Thermal correction to Enthalpy= 0.135076
Thermal correction to Gibbs Free Energy= 0.092481
Sum of electronic and zero-point Energies= -454.351569
Sum of electronic and thermal Energies= -454.343331
Sum of electronic and thermal Enthalpies= -454.342387
Sum of electronic and thermal Free Energies= -454.384982

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	84.169	30.180	89.649

N,0,0.3825773428,-1.1294601475,0.200221442
C,0,1.4462232978,-0.4586952702,-0.0970836778
C,0,1.4432770017,0.9835200623,-0.4199547048
C,0,0.0891521753,1.6714405097,-0.3867131279
N,0,-0.9909492049,0.8347235083,-0.0501291706
C,0,-0.9742568704,-0.4993109667,0.2464180269
O,0,-0.068175746,2.8384585089,-0.6264025884
O,0,-1.9115674166,-1.1879280277,0.5301979383
C,0,0.3975130538,-2.5788448165,0.5230157996
H,0,1.8963596632,1.1269844827,-1.4129590529
H,0,2.1288992741,1.5035304029,0.2666419409
H,0,-1.910057686,1.2750737396,-0.021766683
H,0,-0.0039442623,-2.7162813144,1.5276008357
H,0,1.424164847,-2.936598578,0.461369892
H,0,-0.2412248861,-3.1012467326,-0.1899760698
H,0,2.3908994372,-1.0012064867,-0.1060134583

N-Methyl Uracil Anion

E(RB+HF-LYP) = -453.564821920

Zero-point correction= 0.100629 (Hartree/Particle)
Thermal correction to Energy= 0.108291
Thermal correction to Enthalpy= 0.109236
Thermal correction to Gibbs Free Energy= 0.068249
Sum of electronic and zero-point Energies= -453.464193
Sum of electronic and thermal Energies= -453.456531
Sum of electronic and thermal Enthalpies= -453.455586
Sum of electronic and thermal Free Energies= -453.496573

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	67.954	28.199	86.264

N,0,-1.0649266068,-0.5111032949,-0.0000634209
C,0,-0.6585076362,0.8114967784,-0.0000169035
N,0,0.7092470624,0.982810732,-0.000059395
C,0,1.6944268295,-0.0314598316,0.0000312742
C,0,1.1337261068,-1.3520786368,0.000073998
C,0,-0.2234042191,-1.6411889646,0.0000253307
C,0,-2.5133347457,-0.7106159882,-0.00006064
O,0,-1.4382750984,1.779813016,0.0000371453
H,0,1.0362619915,1.9401147736,-0.0000164286
O,0,2.8913319827,0.3159810273,0.0000332914
H,0,1.8532775955,-2.1667280306,0.0001512066
H,0,-2.9746069097,-0.2554196455,0.8848286754
H,0,-2.9746653699,-0.2549092776,-0.8846503912
H,0,-2.6724035836,-1.7882823693,-0.0003352006

N-Methyl Uracil Anion – 6-311++G

E(RB+HF-LYP) = -453.523191488

Zero-point correction= 0.100377 (Hartree/Particle)
Thermal correction to Energy= 0.107959
Thermal correction to Enthalpy= 0.108903
Thermal correction to Gibbs Free Energy= 0.068123
Sum of electronic and zero-point Energies= -453.422815
Sum of electronic and thermal Energies= -453.415232
Sum of electronic and thermal Enthalpies= -453.414288
Sum of electronic and thermal Free Energies= -453.455069

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	67.745	28.097	85.830

C,0,1.6100743714,0.2139350521,-0.3787259727
N,0,0.8604091574,0.019549238,0.8162180219
C,0,-0.513491762,-0.1404809634,0.8997107727
N,0,-1.1710126206,-0.1009927064,-0.3132638531
C,0,-0.5793634658,0.0829693786,-1.5858067186
C,0,0.8391981997,0.2362544129,-1.5389082834
C,0,1.5815341405,-0.0192080908,2.0937043466
O,0,-1.1413539662,-0.3109417007,1.9885139693
O,0,-1.3467144497,0.091909413,-2.6005537749
H,0,-2.173179951,-0.2146207147,-0.2861012347
H,0,1.330049364,0.3794276354,-2.4914369746
H,0,2.629789283,0.1193552162,1.8506594808
H,0,1.2354846582,0.7726352858,2.762388836
H,0,1.4289193135,-0.9752535787,2.6002842881

N-Methyl Uracil Anion – 6-311++G**

E(RB+HF-LYP) = -453.666862285

Zero-point correction= 0.099354 (Hartree/Particle)
Thermal correction to Energy= 0.106202
Thermal correction to Enthalpy= 0.107146
Thermal correction to Gibbs Free Energy= 0.068036
Sum of electronic and zero-point Energies= -453.567508
Sum of electronic and thermal Energies= -453.560660
Sum of electronic and thermal Enthalpies= -453.559716
Sum of electronic and thermal Free Energies= -453.598827

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	66.643	26.391	82.315

N,0,-0.7099488769,0.98793,0.0000027692
C,0,-1.6900798769,-0.03347,0.0000027692
C,0,-1.1411298769,-1.35117,-0.0000072308
C,0,0.2187101231,-1.65358,-0.0000072308
N,0,1.0699301231,-0.512001,-0.0000072308
C,0,0.6590711231,0.811539,0.0000027692
H,0,-1.0410588769,1.941,0.0000127692
O,0,-2.9127498769,0.31834,0.0000027692
H,0,-1.8579198769,-2.16053,-0.0000072308
O,0,1.4545211231,1.799569,0.0000127692

C,0,2.5219901231,-0.724261,-0.0000072308
H,0,2.6677801231,-1.799401,-0.0000572308
H,0,2.9829001231,-0.275041,-0.8829772308
H,0,2.9828901231,-0.275151,0.8830327692

N-Methyl Uracil

E(RB+HF-LYP) = -454.159086392

Zero-point correction= 0.114639 (Hartree/Particle)
Thermal correction to Energy= 0.122582
Thermal correction to Enthalpy= 0.123526
Thermal correction to Gibbs Free Energy= 0.081317
Sum of electronic and zero-point Energies= -454.044447
Sum of electronic and thermal Energies= -454.036505
Sum of electronic and thermal Enthalpies= -454.035560
Sum of electronic and thermal Free Energies= -454.077770

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	76.921	28.790	88.837

C,0,-0.1651765705,-1.5094989909,0.0000235068
N,0,-1.0760500334,-0.4768031949,-0.0000594467
C,0,-0.6575498955,0.8571839067,-0.0000719187
N,0,0.7156720323,1.0250202734,-0.0000471468
C,0,1.7158305659,0.0313470643,0.000042162
C,0,1.1753981342,-1.319162089,0.0000669943
C,0,-2.5228278067,-0.7132908063,-0.0000267084
O,0,-1.4486788669,1.7896346242,-0.0000398843
O,0,2.8991477039,0.3440038023,0.0000963995
H,0,1.0341145968,1.9877893553,-0.0000219824
H,0,1.8656329906,-2.1513286813,0.0001316347
H,0,-2.9782971828,-0.2651449576,0.8858325002
H,0,-2.9783782065,-0.264687233,-0.885607016
H,0,-2.6984197344,-1.7894733586,-0.0002959635
H,0,-0.5998037168,-2.5032565966,0.0000506436

N-Methyl Uracil – PCM acetone

E(RB+HF-LYP) = -454.182956703

Zero-point correction= 0.113382 (Hartree/Particle)
Thermal correction to Energy= 0.121155
Thermal correction to Enthalpy= 0.122099
Thermal correction to Gibbs Free Energy= 0.080791

Sum of electronic and zero-point Energies= -454.069574
Sum of electronic and thermal Energies= -454.061802
Sum of electronic and thermal Enthalpies= -454.060858
Sum of electronic and thermal Free Energies= -454.102165

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.026	28.704	86.939

C,0,-0.1708967865,-1.5082399319,0.0004385409
N,0,-1.0752450483,-0.4730885153,0.000306329
C,0,-0.6501801369,0.8502486047,0.0002298272
N,0,0.7185917462,1.0240626295,0.0005446743
C,0,1.7018742613,0.0292997321,0.0000431275
C,0,1.1724987894,-1.3152583624,0.0003398195
C,0,-2.5236245919,-0.715728591,-0.0001778814
O,0,-1.4407094607,1.7945494657,-0.0001880393
O,0,2.8994203863,0.3428189845,-0.0012114286
H,0,1.0409164752,2.0028358442,0.0001640696
H,0,1.8598196098,-2.1549687449,0.0002441136
H,0,-2.9784918699,-0.2735297046,0.8890405584
H,0,-2.9780174011,-0.2723246822,-0.8890356847
H,0,-2.691203341,-1.7929010371,-0.000943559
H,0,-0.6041669758,-2.5068067858,0.0005286204

N-Methyl Uracil – PCM water

E(RB+HF-LYP) = -454.184890808

Zero-point correction= 0.113233 (Hartree/Particle)
Thermal correction to Energy= 0.120994
Thermal correction to Enthalpy= 0.121938
Thermal correction to Gibbs Free Energy= 0.080682
Sum of electronic and zero-point Energies= -454.071658
Sum of electronic and thermal Energies= -454.063897
Sum of electronic and thermal Enthalpies= -454.062953
Sum of electronic and thermal Free Energies= -454.104209

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.925	28.716	86.830

C,0,-0.1713234993,-1.5084717413,0.0004997023
N,0,-1.0749885708,-0.4727763868,0.0003270051
C,0,-0.6495148698,0.8495899625,-0.000156617

N,0,0.7188356941,1.0239220381,0.000529068
C,0,1.7001019567,0.0294003178,0.0007902092
C,0,1.1723054309,-1.3151044172,0.0004947068
C,0,-2.5235405787,-0.71635272,0.0000584639
O,0,-1.4397402792,1.7953783691,-0.0011130543
O,0,2.8991758627,0.3430792107,-0.0009837732
H,0,1.0417824884,2.003357835,0.0001801356
H,0,1.8592401718,-2.1553270841,0.0000874053
H,0,-2.9781036914,-0.2749281201,0.8898319937
H,0,-2.9780808176,-0.2724734446,-0.8884883804
H,0,-2.6896240062,-1.7936783336,-0.0014147985
H,0,-0.6057993153,-2.50699946,0.0004669622

S_E2 Decarboxylation Transition State – C6 proton transfer from Water

E(RB+HF-LYP) = -718.621223657

Zero-point correction= 0.137131 (Hartree/Particle)
Thermal correction to Energy= 0.151262
Thermal correction to Enthalpy= 0.152207
Thermal correction to Gibbs Free Energy= 0.093902
Sum of electronic and zero-point Energies= -718.484092
Sum of electronic and thermal Energies= -718.469961
Sum of electronic and thermal Enthalpies= -718.469017
Sum of electronic and thermal Free Energies= -718.527321

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	94.919	47.542	122.712

C,0,-0.1722611858,1.4197092141,0.0370345298
C,0,0.374590662,0.1732395443,0.2517154254
N,0,-0.5205775424,-0.8906600761,0.4063936124
C,0,-1.9002062263,-0.7786256961,0.3534693378
N,0,-2.3605097042,0.5067019114,0.1424113803
C,0,-1.5879994616,1.6742729504,-0.027145796
C,0,-0.0106399507,-2.2442306488,0.6383002045
O,0,-2.6755580031,-1.7348574513,0.4862049679
O,0,-2.1726868649,2.7534167959,-0.2109807319
C,0,2.3319510696,-0.0543147373,-1.4152006057
O,0,2.9124604963,0.9449182003,-1.1785717927
O,0,1.9797535556,-1.0738289575,-1.8914852075
O,0,2.838345156,-0.1519253281,1.8285077859
H,0,3.4126325975,0.5521005619,1.5027549
H,0,-3.3661163667,0.6120537927,0.101680325

H,0,0.477643916,2.2786732214,-0.0983127442
H,0,1.0728848608,-2.1773497969,0.71254486
H,0,-0.4278477781,-2.6567884948,1.562301712
H,0,-0.2883956185,-2.9096535606,-0.1857302999
H,0,2.0156849523,-0.0534184057,1.264687549

S_E2 Decarboxylation Transition State – C6 proton transfer from Water – PCM Water

E(RB+HF-LYP) = -718.707918462

Zero-point correction= 0.135166 (Hartree/Particle)
Thermal correction to Energy= 0.149420
Thermal correction to Enthalpy= 0.150364
Thermal correction to Gibbs Free Energy= 0.090982
Sum of electronic and zero-point Energies= -718.572752
Sum of electronic and thermal Energies= -718.558498
Sum of electronic and thermal Enthalpies= -718.557554
Sum of electronic and thermal Free Energies= -718.616936

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	93.763	47.793	124.980

C,0,0.3042076649,-1.3669791966,0.2227758937
C,0,-0.3434383952,-0.1491391941,0.2344057669
N,0,0.4495009298,0.9855744855,0.0708134488
C,0,1.8218769391,0.9641225059,-0.1006881888
N,0,2.3935393392,-0.2894994251,-0.0951414106
C,0,1.7219098529,-1.5051754941,0.0622133047
C,0,-0.1666058932,2.3190229815,0.0863154505
O,0,2.507093191,1.9902933254,-0.2466159691
O,0,2.3846070481,-2.567752208,0.0469727743
C,0,-2.5011313254,-0.4055366356,-1.0098107861
O,0,-2.8502085974,-1.4487718711,-0.5812414524
O,0,-2.443413565,0.586147586,-1.6490249289
O,0,-2.4094397429,0.3214548562,2.2801011349
H,0,-2.8126087881,-0.5391083272,2.4934344575
H,0,3.4138793531,-0.3194483614,-0.2190385485
H,0,-0.2681095304,-2.2854923798,0.3330627656
H,0,-1.2359319478,2.1834878698,0.2281831458
H,0,0.2463372783,2.9222525108,0.9002268137
H,0,0.0180499458,2.840457404,-0.8572626382
H,0,-1.7929179229,0.1364625504,1.5188886197

S_E2 Decarboxylation Transition State – C6 proton transfer from Water – Onsager Water

E(RB+HF-LYP) = -718.622376500

Zero-point correction= 0.136930 (Hartree/Particle)
Thermal correction to Energy= 0.151158
Thermal correction to Enthalpy= 0.152103
Thermal correction to Gibbs Free Energy= 0.093281
Sum of electronic and zero-point Energies= -718.485446
Sum of electronic and thermal Energies= -718.471218
Sum of electronic and thermal Enthalpies= -718.470274
Sum of electronic and thermal Free Energies= -718.529096

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	94.853	47.782	123.800

C,0,-0.1673194919,1.4250133798,0.0427722886
C,0,0.3820519424,0.1735481851,0.2301196775
N,0,-0.5086847945,-0.8933734586,0.3722048731
C,0,-1.8885470342,-0.782282278,0.3247346409
N,0,-2.3507568924,0.5078989033,0.1380041997
C,0,-1.5821261572,1.6789501824,-0.0056336515
C,0,0.0043029351,-2.2523130385,0.5724281294
O,0,-2.6657818077,-1.7371174091,0.4468714534
O,0,-2.1718099525,2.7643363638,-0.1530799367
C,0,2.3046145304,-0.1667513534,-1.4116950278
O,0,3.0210978811,0.7269161351,-1.1213962828
O,0,1.8272698951,-1.1002421816,-1.95042147
O,0,2.8222781836,0.1540063113,1.9417931521
H,0,3.4896908488,0.524494846,1.350682553
H,0,-3.3565014594,0.6093209249,0.0958776195
H,0,0.4824259964,2.2871069321,-0.0734426764
H,0,1.0803857205,-2.1767308498,0.7151492914
H,0,-0.4635681141,-2.7085838332,1.449513727
H,0,-0.2120633842,-2.881673141,-0.2964972206
H,0,2.013428256,0.1242027881,1.3607615257

S_E2 Decarboxylation Transition State – C6 proton transfer from HF

E(RB+HF-LYP) = -742.652074250

Zero-point correction= 0.125242 (Hartree/Particle)
Thermal correction to Energy= 0.138266
Thermal correction to Enthalpy= 0.139211

Thermal correction to Gibbs Free Energy= 0.083682
Sum of electronic and zero-point Energies= -742.526833
Sum of electronic and thermal Energies= -742.513808
Sum of electronic and thermal Enthalpies= -742.512864
Sum of electronic and thermal Free Energies= -742.568392

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	86.764	44.195	116.870

C,0,-0.0551750959,1.4400430627,-0.0727308064
C,0,0.4644982467,0.1839188514,0.1026111255
N,0,-0.4148192096,-0.8702452886,0.3532681367
C,0,-1.7907717724,-0.7259395169,0.4182279287
N,0,-2.241295751,0.571009315,0.2456308753
C,0,-1.4687382045,1.7224431906,0.0051676409
C,0,0.091214308,-2.2296649677,0.5697282042
O,0,-2.5707491695,-1.6618226571,0.6231523293
O,0,-2.0373269619,2.8144368153,-0.1206091768
C,0,2.098878199,-0.1156512992,-1.3515146658
O,0,2.6881283375,0.9201830266,-1.3674066041
O,0,1.8753994869,-1.2200804205,-1.7525647324
F,0,2.5574132406,-0.1820161092,1.7545977213
H,0,-3.2444923984,0.6945641812,0.2977006297
H,0,0.6075723717,2.2681277043,-0.2960159771
H,0,1.1735266794,-2.1775878526,0.6535418378
H,0,-0.3412874363,-2.6420319807,1.4849438865
H,0,-0.1809759652,-2.8790908723,-0.2674166048
H,0,1.8786946785,-0.0038144227,1.0540625629

S_E2 Decarboxylation Transition State – C6 proton transfer from $HNMe_3^+$

E(RB+HF-LYP) = -817.182224350

Zero-point correction= 0.248185 (Hartree/Particle)
Thermal correction to Energy= 0.266075
Thermal correction to Enthalpy= 0.267019
Thermal correction to Gibbs Free Energy= 0.201124
Sum of electronic and zero-point Energies= -816.934039
Sum of electronic and thermal Energies= -816.916149
Sum of electronic and thermal Enthalpies= -816.915205
Sum of electronic and thermal Free Energies= -816.981100

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

TOTAL	166.965	62.531	138.688

C,0,2.0322968353,1.5862692324,0.4502675605
C,0,0.6779038904,1.141018156,0.7305141887
C,0,0.199317588,-0.0806462844,0.3355533704
N,0,1.0495465757,-0.9382970439,-0.3547330909
C,0,2.3795541265,-0.6350782705,-0.6473799524
N,0,2.7891675278,0.6221378312,-0.2365852579
C,0,0.6151798372,-2.2759132363,-0.7680629243
O,0,3.1249208463,-1.407864945,-1.2416569098
O,0,2.530149055,2.6713982154,0.7434724415
C,0,-1.0309680988,-0.9343825286,1.921933936
O,0,-0.4178869467,-1.9197953001,2.1806155248
O,0,-1.9370840598,-0.1656194203,2.0859337415
N,0,-2.2536516441,0.4955076132,-0.8551814509
H,0,3.7526775301,0.8566281229,-0.4460447698
H,0,0.0566107505,1.8161407321,1.3086982037
H,0,-0.4481579313,-2.3700132804,-0.5527736187
H,0,0.8082599445,-2.4242413972,-1.8340157503
H,0,1.1556863559,-3.0467124183,-0.212917865
H,0,-1.3613152811,0.1513134931,-0.2607929362
C,0,-2.7025412373,1.796569215,-0.2799518976
C,0,-1.7606185255,0.6616212655,-2.2508403221
C,0,-3.3172165184,-0.5420194208,-0.762695902
H,0,-4.1739612052,-0.2440587257,-1.3733605246
H,0,-2.9198060406,-1.4910256163,-1.1273124447
H,0,-3.6115616814,-0.6462082693,0.2812155015
H,0,-2.566540194,1.0387429953,-2.8854507073
H,0,-0.9270416202,1.365290805,-2.2447202816
H,0,-1.4142529734,-0.3031818922,-2.6243124617
H,0,-3.5467659814,2.178230587,-0.8610892461
H,0,-2.9872246595,1.6340994459,0.758468676
H,0,-1.8702827693,2.4999794434,-0.3230399042

S_E2 Decarboxylation Transition State – C6 proton transfer from $HNMe_3^+$ - PCM acetone radii=bondi

E(RB+HF-LYP) = -817.233331890

Zero-point correction=	0.249358 (Hartree/Particle)
Thermal correction to Energy=	0.266543
Thermal correction to Enthalpy=	0.267487
Thermal correction to Gibbs Free Energy=	0.203577
Sum of electronic and zero-point Energies=	-816.983974
Sum of electronic and thermal Energies=	-816.966789

Sum of electronic and thermal Enthalpies= -816.965845
Sum of electronic and thermal Free Energies= -817.029755

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.258	61.057	134.510

C,0,2.1023810246,1.515364041,0.6185621475
C,0,0.7565470246,1.062921041,0.8346971475
C,0,0.2545570246,-0.090903959,0.2752121475
N,0,1.1103640246,-0.838798959,-0.5278478525
C,0,2.4246920246,-0.495936959,-0.7836898525
N,0,2.8554730246,0.673527041,-0.1968748525
C,0,0.6415500246,-2.079311959,-1.1639898525
O,0,3.1789070246,-1.177289959,-1.4980348525
O,0,2.6310890246,2.549918041,1.0820291475
C,0,-0.9517249754,-1.243417959,1.9600001475
O,0,-0.3003399754,-2.232519959,1.9760411475
O,0,-1.7866539754,-0.461621959,2.2726101475
N,0,-2.4183779754,0.575621041,-0.7862938525
H,0,3.8188220246,0.934741041,-0.3825318525
H,0,0.1349980246,1.670358041,1.4851351475
H,0,-0.3976239754,-2.226829959,-0.8790378525
H,0,0.7231970246,-2.005862959,-2.2514838525
H,0,1.2333270246,-2.933394959,-0.8261828525
H,0,-1.5335649754,0.218236041,-0.3002768525
C,0,-2.8662079754,1.808840041,-0.0670508525
C,0,-2.0346739754,0.882735041,-2.1995258525
C,0,-3.4529959754,-0.502203959,-0.7238438525
H,0,-4.3483269754,-0.161540959,-1.2463298525
H,0,-3.0614859754,-1.397761959,-1.2077908525
H,0,-3.6844349754,-0.709624959,0.3204871475
H,0,-2.9088789754,1.264817041,-2.7287868525
H,0,-1.2428829754,1.632313041,-2.1937138525
H,0,-1.6818279754,-0.031398959,-2.6777678525
H,0,-3.7631759754,2.194723041,-0.5542848525
H,0,-3.0807589754,1.552061041,0.9693601475
H,0,-2.0683579754,2.550320041,-0.1130718525

S_E2 Decarboxylation Transition State – C6 proton transfer from $HNMe_3^+$ - Onsager acetone

E(RB+HF-LYP) = -817.198554238

Zero-point correction= 0.249704 (Hartree/Particle)

Thermal correction to Energy= 0.267807
Thermal correction to Enthalpy= 0.268751
Thermal correction to Gibbs Free Energy= 0.201751
Sum of electronic and zero-point Energies= -816.948851
Sum of electronic and thermal Energies= -816.930748
Sum of electronic and thermal Enthalpies= -816.929803
Sum of electronic and thermal Free Energies= -816.996804

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	168.051	62.730	141.014

C,0,2.1085164959,1.6645668397,0.1132319119
C,0,0.750739869,1.2696327436,0.418517421
C,0,0.2713176483,-0.001246152,0.2040892915
N,0,1.1307738925,-0.9389840225,-0.3667870561
C,0,2.4597052656,-0.6852081318,-0.6734761838
N,0,2.8626379307,0.61937307,-0.4470692277
C,0,0.6901732549,-2.319339842,-0.5969066323
O,0,3.2375658903,-1.5338324566,-1.1160673299
O,0,2.6471387194,2.7604944177,0.307114178
C,0,-0.7647486964,-0.6625938385,2.0700081343
O,0,0.0002777828,-1.5044734413,2.4167953853
O,0,-1.7237878099,0.0382103586,2.1832490921
N,0,-2.5571657982,0.3227576425,-0.7602021914
H,0,3.8262008653,0.8230428574,-0.6790354423
H,0,0.1276465417,2.0156636242,0.9006264482
H,0,-0.374960275,-2.3713375599,-0.3796291246
H,0,0.8803219128,-2.6107225936,-1.6328537269
H,0,1.2227627339,-3.01090264,0.0611024888
H,0,-1.6164303927,0.1188185973,-0.2910652806
C,0,-3.0309226198,1.6573676268,-0.271905525
C,0,-2.3037151275,0.345296724,-2.2343446169
C,0,-3.5200422532,-0.7629631361,-0.3884107635
H,0,-4.4764554648,-0.5771784333,-0.8810310875
H,0,-3.117222533,-1.721296005,-0.7190451741
H,0,-3.6439004494,-0.7632263307,0.6935200613
H,0,-3.232676904,0.5804057696,-2.7570862452
H,0,-1.5494888724,1.1031138013,-2.4487954806
H,0,-1.9415740419,-0.6344670808,-2.547752786
H,0,-3.9814127152,1.8952423788,-0.7536228615
H,0,-3.1497976772,1.6070940933,0.8091081631
H,0,-2.2824345858,2.4074546612,-0.5295794518

S_E2 Decarboxylation Transition State – C6 proton transfer from $HNMe_3^+$ - PCM water

E(RB+HF-LYP) = -817.221986351

Zero-point correction= 0.247644 (Hartree/Particle)
Thermal correction to Energy= 0.264848
Thermal correction to Enthalpy= 0.265792
Thermal correction to Gibbs Free Energy= 0.201840
Sum of electronic and zero-point Energies= -816.974342
Sum of electronic and thermal Energies= -816.957138
Sum of electronic and thermal Enthalpies= -816.956194
Sum of electronic and thermal Free Energies= -817.020146

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	166.195	60.866	134.598

C,0,2.0554761182,1.6709487055,0.0843478758
C,0,0.7359155357,1.256420532,0.4865913619
C,0,0.2551908921,-0.0150068409,0.2763153556
N,0,1.0986686181,-0.9284894181,-0.3484749685
C,0,2.3877865364,-0.633609145,-0.7617294517
N,0,2.8002292624,0.6608935043,-0.524799317
C,0,0.6521408266,-2.3036303813,-0.6067360496
O,0,3.1257476392,-1.461667738,-1.3133267332
O,0,2.5616147481,2.8005053615,0.2341946349
C,0,-0.8109412167,-0.7113326599,2.2296398467
O,0,-0.0851553368,-1.606352438,2.5080397303
O,0,-1.7086410922,0.0568815054,2.3543810885
N,0,-2.443406473,0.3008354268,-0.7594468455
H,0,3.7560620271,0.8899679632,-0.8307286676
H,0,0.1257487583,1.9992002408,0.9953424793
H,0,-0.3530778931,-2.4103187411,-0.2045319739
H,0,0.6509662876,-2.5117171665,-1.6807452878
H,0,1.3148057999,-3.0212133127,-0.1163775327
H,0,-1.5183465808,0.0863253889,-0.2417946788
C,0,-2.9085409477,1.6508472141,-0.3160534556
C,0,-2.1202899175,0.2931413989,-2.2190676049
C,0,-3.4348927039,-0.7609771822,-0.4120640183
H,0,-4.3659057584,-0.5683136595,-0.9504764723
H,0,-3.0334314387,-1.7325093774,-0.7064157476
H,0,-3.610603211,-0.739715181,0.6635469865
H,0,-3.020426263,0.540756986,-2.7862155432
H,0,-1.3409428294,1.0328927146,-2.4088172694

H,0,-1.7666403101,-0.7001923964,-2.4998925757
H,0,-3.8311789101,1.8999738697,-0.8457831097
H,0,-3.0815719893,1.6247591257,0.7593598341
H,0,-2.1334959458,2.3816835799,-0.5511954474

S_E2 Decarboxylation Transition State – C6 proton transfer from $HNMe_3^+$ - Onsager water

E(RB+HF-LYP) = -817.199968364

Zero-point correction= 0.249782 (Hartree/Particle)
Thermal correction to Energy= 0.267916
Thermal correction to Enthalpy= 0.268860
Thermal correction to Gibbs Free Energy= 0.201757
Sum of electronic and zero-point Energies= -816.950186
Sum of electronic and thermal Energies= -816.932052
Sum of electronic and thermal Enthalpies= -816.931108
Sum of electronic and thermal Free Energies= -816.998211

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	168.120	62.770	141.231

C,0,2.1285305273,1.6596474551,0.1262588438
C,0,0.7651423265,1.2724951278,0.412659195
C,0,0.280926436,0.0039094387,0.1917942276
N,0,1.142872281,-0.9371823138,-0.3710366257
C,0,2.4763140818,-0.6907715276,-0.6601516841
N,0,2.8833392584,0.6112657258,-0.4272812496
C,0,0.6966894363,-2.3146120471,-0.6087926014
O,0,3.2574335318,-1.5428236907,-1.092359033
O,0,2.6745870457,2.7507761668,0.3313527246
C,0,-0.7611492027,-0.655165215,2.0605709307
O,0,0.00727276,-1.4931179211,2.4094694079
O,0,-1.7209661644,0.0442849041,2.1694150567
N,0,-2.58789127,0.3234154268,-0.7687217753
H,0,3.8507252744,0.8098665504,-0.6466948497
H,0,0.1402082011,2.021170244,0.8882823197
H,0,-0.3711001768,-2.3601218177,-0.4038508297
H,0,0.8960532264,-2.6050373782,-1.6432520215
H,0,1.2177153141,-3.0105888641,0.0538511703
H,0,-1.6471235697,0.1236755831,-0.3077760788
C,0,-3.0608192499,1.658837976,-0.2799447061
C,0,-2.3483956938,0.3420941464,-2.2459060776
C,0,-3.5464369287,-0.7634848955,-0.3856476296

H,0,-4.5071716534,-0.5794081411,-0.8702351922
H,0,-3.145526725,-1.7218209549,-0.7184847038
H,0,-3.6608218337,-0.7614525361,0.6972779378
H,0,-3.2828772556,0.5747887875,-2.7596323461
H,0,-1.5973300424,1.1003181622,-2.469635106
H,0,-1.9889691086,-0.6384069941,-2.5600157126
H,0,-4.0165838134,1.8918351299,-0.7532624961
H,0,-3.1695939087,1.6116948242,0.8022737224
H,0,-2.3172735965,2.4103371084,-0.547636498

S_E2 Decarboxylation Transition State – C6 proton transfer from MeOH

E(RB+HF-LYP) = -757.921422618

Zero-point correction= 0.165565 (Hartree/Particle)
Thermal correction to Energy= 0.181256
Thermal correction to Enthalpy= 0.182200
Thermal correction to Gibbs Free Energy= 0.119126
Sum of electronic and zero-point Energies= -757.755857
Sum of electronic and thermal Energies= -757.740167
Sum of electronic and thermal Enthalpies= -757.739223
Sum of electronic and thermal Free Energies= -757.802297

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	113.740	51.246	132.751

C,0,0.1327831872,0.074857003,-0.015983311
N,0,-0.7622611575,-0.9782810245,0.2013158058
C,0,-2.140574631,-0.8477817023,0.2431432827
N,0,-2.598195302,0.4417419412,0.0520639713
C,0,-1.8245535534,1.5986123696,-0.1744367681
C,0,-0.4104937358,1.326721224,-0.2029759471
C,0,-0.2549058586,-2.3355323722,0.4195030488
O,0,-2.9168806232,-1.7922655648,0.438090386
O,0,-2.4062598342,2.6843856511,-0.3236682932
C,0,2.0829958748,-0.1761925946,-1.6357993126
O,0,1.8594507258,-1.2791105022,-1.9951311417
O,0,2.5507507963,0.9020194663,-1.5331753262
H,0,-3.6028363654,0.5598045571,0.0798685256
H,0,0.2406915025,2.1738965809,-0.3932635931
H,0,0.8298140923,-2.295723252,0.3529063491
H,0,-0.5588104959,-2.7045300638,1.4044571932
H,0,-0.6513474605,-3.0202472071,-0.3367235753
H,0,1.7463759155,-0.1728441921,0.9904058487

O,0,2.5074347174,-0.3060176377,1.6282872767
C,0,2.9805017714,0.9632316582,2.0275282037
H,0,3.7982463274,0.8089428471,2.7424154776
H,0,3.3692654941,1.5482968001,1.1796590332
H,0,2.2013116226,1.5625926975,2.5255179102

S_E2 Decarboxylation Transition State – C6 proton transfer from vinyl alcohol

E(RB+HF-LYP) = -796.020472683

Zero-point correction= 0.170526 (Hartree/Particle)
Thermal correction to Energy= 0.186592
Thermal correction to Enthalpy= 0.187537
Thermal correction to Gibbs Free Energy= 0.123130
Sum of electronic and zero-point Energies= -795.849946
Sum of electronic and thermal Energies= -795.833880
Sum of electronic and thermal Enthalpies= -795.832936
Sum of electronic and thermal Free Energies= -795.897343

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	117.089	53.987	135.556

C,0,-0.5269604957,1.2706205333,-0.4791230553
C,0,-0.0110375334,0.008706808,-0.3068338196
N,0,-0.8986661944,-1.013110305,0.0383386651
C,0,-2.260309061,-0.8348554105,0.2254625914
N,0,-2.6989414179,0.4630420887,0.0395626824
C,0,-1.9239850602,1.5873765133,-0.3058723235
C,0,-0.406347948,-2.3759574269,0.2601735448
O,0,-3.0353369752,-1.7456216807,0.5378540187
O,0,-2.4818429082,2.6863406849,-0.4275796713
C,0,1.657283603,-0.3351365585,-1.9632939797
O,0,2.1714061579,0.731669701,-2.002932585
O,0,1.4262545775,-1.4584332258,-2.2735705192
O,0,2.3166221502,-0.3254783035,1.2672384107
C,0,2.5368563087,0.8215103294,1.9352216427
H,0,-3.6906575145,0.6134099871,0.1746895322
H,0,0.1253720908,2.0833338161,-0.7800951208
H,0,0.6528249759,-2.3907080949,0.0162966494
H,0,-0.5582829835,-2.6726080735,1.302984641
H,0,-0.9443453217,-3.0821831078,-0.3781909321
H,0,1.5605105142,-0.2037601578,0.6014698425
C,0,3.476018592,0.9689219284,2.8849212773
H,0,1.8878304075,1.6531585525,1.6553093599

H,0,3.5961851399,1.9259379858,3.3797010423
H,0,4.1278815271,0.1489589002,3.1705130526

S_E2 Decarboxylation Transition State – C6 proton transfer from CFH_2OH

E(RB+HF-LYP) = -857.179632357

Zero-point correction= 0.158981 (Hartree/Particle)
Thermal correction to Energy= 0.174799
Thermal correction to Enthalpy= 0.175744
Thermal correction to Gibbs Free Energy= 0.112140
Sum of electronic and zero-point Energies= -857.020652
Sum of electronic and thermal Energies= -857.004833
Sum of electronic and thermal Enthalpies= -857.003889
Sum of electronic and thermal Free Energies= -857.067492

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	109.688	52.573	133.864

C,0,-0.864530736,-1.3723709178,-0.1906140975
C,0,-0.1842075623,-0.1900872283,-0.0169759204
N,0,-0.9352071977,0.9878804708,0.0057118904
C,0,-2.312969294,1.041085973,-0.1299436825
N,0,-2.9181893459,-0.1884433142,-0.3126788704
C,0,-2.2941694518,-1.4502616179,-0.3621600641
C,0,-0.2715144667,2.2819246683,0.1875511415
O,0,-2.9670559357,2.0900497808,-0.1000786966
O,0,-2.9935741215,-2.4588455506,-0.5336947003
C,0,1.4159384515,-0.5582286188,1.748630714
O,0,1.9207274597,-1.5750412157,1.4097878795
O,0,1.1530410322,0.3796607271,2.422090676
O,0,2.083658763,0.2559722933,-1.6636516658
C,0,3.2705155309,-0.3348565944,-1.3803806787
H,0,-3.9247629482,-0.1699058831,-0.4161922249
H,0,-0.3222394562,-2.3120791969,-0.1952435441
H,0,0.8007969827,2.1036647357,0.2189635274
H,0,-0.5181047364,2.9536592836,-0.6399643059
H,0,-0.5962860898,2.7530383551,1.1202483667
H,0,1.3893826801,0.0652505945,-0.9473163749
F,0,4.1117285162,0.5239860651,-0.5903922139
H,0,3.1755474413,-1.2488520569,-0.7853124914
H,0,3.8351328758,-0.4943127784,-2.3051565835

S_E2 Decarboxylation Transition State – developing C6 anion stabilized by K^+

E(RB+HF-LYP) = -1242.04652266

Zero-point correction= 0.114030 (Hartree/Particle)
Thermal correction to Energy= 0.127227
Thermal correction to Enthalpy= 0.128171
Thermal correction to Gibbs Free Energy= 0.071227
Sum of electronic and zero-point Energies= -1241.932492
Sum of electronic and thermal Energies= -1241.919296
Sum of electronic and thermal Enthalpies= -1241.918351
Sum of electronic and thermal Free Energies= -1241.975295

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	79.836	43.820	119.848

C,0,2.3146675037,0.4157837266,0.1880119686
N,0,2.4245029683,-0.8570096821,-0.3429308647
C,0,1.3772195843,-1.7370186738,-0.6636343872
C,0,0.0746486078,-1.1756121566,-0.3695152424
C,0,-0.1302891022,0.0803200911,0.1668616216
N,0,1.0053283348,0.8324566229,0.4378045331
O,0,1.6269133642,-2.8493950778,-1.1331457915
C,0,0.8926175647,2.1793810867,1.0052199232
O,0,3.2981112135,1.1121615347,0.4299736352
C,0,-2.2284099391,1.2984497602,-1.1170941128
O,0,-1.5573025455,2.0757521242,-1.670459719
O,0,-3.0959751916,0.6179306838,-0.6825602594
K,0,-2.3777529921,-0.9693732104,1.3841420693
H,0,3.3686940174,-1.1740901858,-0.5289162811
H,0,-0.7599376365,-1.804672131,-0.6815569196
H,0,-0.1659996384,2.3751330618,1.1701790179
H,0,1.4435232325,2.2491378279,1.9481298864
H,0,1.3055077129,2.9250367143,0.3197877524

S_E2 Decarboxylation Transition State – C6 proton transfer from MeOH and CO_2 H-bonded to a MeOH

E(RB+HF-LYP) = -873.665890807

Zero-point correction= 0.218108 (Hartree/Particle)
Thermal correction to Energy= 0.238910
Thermal correction to Enthalpy= 0.239854
Thermal correction to Gibbs Free Energy= 0.161746
Sum of electronic and zero-point Energies= -873.447782

Sum of electronic and thermal Energies= -873.426981
Sum of electronic and thermal Enthalpies= -873.426037
Sum of electronic and thermal Free Energies= -873.504144

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	149.918	65.321	164.391

C,0,-1.0894252324,1.1743091252,-0.2035971125
C,0,-0.5120300702,-0.0029975257,0.2170381404
N,0,-1.2632345984,-0.8011979861,1.0880394521
C,0,-2.5365511065,-0.4953223826,1.5412563834
N,0,-3.0330962899,0.7080861652,1.078674793
C,0,-2.3983684022,1.6168846752,0.207253551
C,0,-0.7158450706,-2.0727106839,1.568715528
O,0,-3.1897151195,-1.220880497,2.3016984526
O,0,-2.9958014677,2.6559988053,-0.1094643882
C,0,0.513528082,-1.1340623662,-1.8820169993
O,0,1.0531424077,-0.1984636131,-2.3571677891
O,0,0.0632473813,-2.2026212921,-1.6809629923
O,0,2.2931793784,-0.1156707918,0.8379332764
C,0,2.4013930127,0.7301569863,1.9623714923
H,0,-3.961830295,0.9519149319,1.3984784045
H,0,-0.5536602776,1.8238857901,-0.8885644202
H,0,0.314411586,-2.1377287662,1.2244071033
H,0,-0.7554426237,-2.1149398033,2.6614244079
H,0,-1.2923931329,-2.9169860744,1.1765174785
H,0,1.3361113623,-0.1028294722,0.517753902
H,0,3.4513836287,0.7429477158,2.2793725445
H,0,2.0974673123,1.7651997831,1.7399177814
H,0,1.7963487988,0.3780494724,2.8143369576
H,0,3.0373449701,0.2341283679,-2.8012362212
O,0,3.9907102514,0.3643789207,-2.9110740367
C,0,4.4952661392,0.9346539786,-1.7040885906
H,0,5.5765278321,0.7601917262,-1.6919800727
H,0,4.3213015973,2.0213532985,-1.6700196203
H,0,4.0408386936,0.479192681,-0.8167025

S_E2 Decarboxylation Transition State – Orientation A in a Cluster of 8 Waters

E(RB+HF-LYP) = -1253.78977686

Zero-point correction= 0.316804 (Hartree/Particle)
Thermal correction to Energy= 0.348676
Thermal correction to Enthalpy= 0.349620

Thermal correction to Gibbs Free Energy= 0.249966
Sum of electronic and zero-point Energies= -1253.472973
Sum of electronic and thermal Energies= -1253.441101
Sum of electronic and thermal Enthalpies= -1253.440157
Sum of electronic and thermal Free Energies= -1253.539811

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	218.797	107.230	209.738

C,0,-2.9327153525,0.8645543406,-0.3678114625
C,0,-1.5600333636,0.4907424625,-0.5196029877
C,0,-1.0832592347,-0.786935886,-0.3287396358
N,0,-2.0377384604,-1.7692622361,-0.0547435911
C,0,-3.4046917404,-1.544855442,0.0404404076
N,0,-3.7823284476,-0.2242780259,-0.1300015235
C,0,-1.6150859194,-3.153447561,0.1687876599
O,0,-4.2312912772,-2.4349551923,0.2663458212
O,0,-3.4177175703,2.0151999334,-0.4076386832
C,0,1.154012866,-1.15437634,-1.9281410223
O,0,1.546679198,-2.1842621278,-1.5090934699
O,0,0.9508477181,-0.1590477834,-2.5115353359
O,0,1.0702968778,0.0724854273,1.4306220819
H,0,0.5622130397,0.7917198415,1.8821701124
H,0,-4.768487119,-0.0296994733,-0.0099339201
H,0,-0.862489603,1.2929036748,-0.7253295175
H,0,-0.5341577319,-3.1825611679,0.0428604565
H,0,-1.8905184938,-3.4855264953,1.1754987324
H,0,-2.0976305572,-3.8258282427,-0.5479081336
H,0,0.4356976522,-0.3514969218,0.7830319304
H,0,2.2124649052,1.2587130453,0.5707029216
O,0,2.7349751429,1.9569070119,0.1219018565
H,0,3.5601072679,1.5224087475,-0.170707419
O,0,-0.1506247316,2.2947083768,2.5276171157
H,0,-0.6208295412,2.7950670181,1.8055620393
H,0,0.5528299534,2.8865274506,2.8211886122
H,0,3.343324398,-2.3329028428,-0.3290534827
O,0,4.1033950223,-2.1122244364,0.2295149822
H,0,3.717699061,-2.0025610226,1.1319738
H,0,5.2658287689,0.2632893233,-1.5180114525
O,0,5.0050935933,0.3602418728,-0.5951551411
H,0,4.7454882706,-0.5431483789,-0.2880569077
O,0,-1.2803439531,3.7064662209,0.4912932634
H,0,-2.0719008243,3.2450900933,0.1367214929

H,0,-0.5977997225,3.6578745361,-0.2107185518
O,0,0.8733601711,3.2987371854,-1.3806941262
H,0,0.6398085914,2.6541318798,-2.0610345506
H,0,1.6056246946,2.8684649383,-0.8730641262
H,0,2.2770846519,-2.3234747027,3.0356062933
O,0,2.7728249618,-1.6290742222,2.5871727853
H,0,2.0967859367,-0.9797570433,2.249310518

S_E2 Decarboxylation Transition State – Orientation A in a Cluster of 8 Waters

E(RB+HF-LYP) = -1253.78704952

Zero-point correction= 0.316228 (Hartree/Particle)
Thermal correction to Energy= 0.348196
Thermal correction to Enthalpy= 0.349140
Thermal correction to Gibbs Free Energy= 0.249018
Sum of electronic and zero-point Energies= -1253.470821
Sum of electronic and thermal Energies= -1253.438854
Sum of electronic and thermal Enthalpies= -1253.437910
Sum of electronic and thermal Free Energies= -1253.538032

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	218.496	107.516	210.725

C,0,-3.4201262257,1.0478522288,-0.4833278671
C,0,-1.9935913436,0.8592409987,-0.5735507531
C,0,-1.3522474505,-0.3096659474,-0.2388837848
N,0,-2.1554627889,-1.3732527149,0.1854323714
C,0,-3.5375283809,-1.3215653062,0.3049431443
N,0,-4.0960834721,-0.1063836721,-0.0404903632
C,0,-1.5457214709,-2.6495312976,0.5649202731
O,0,-4.2252786937,-2.2733707999,0.688903926
O,0,-4.0735136841,2.0677458765,-0.7393443439
C,0,0.5982994472,-0.662101599,-1.9735542507
O,0,0.7994046142,-1.8157223238,-1.8210437969
O,0,0.6163505711,0.4462187777,-2.3664514391
O,0,1.0382725148,-0.1282573159,1.2843237777
H,0,0.9029564637,0.63808654,1.8877995782
H,0,-5.1025322609,-0.0440302794,0.0485618565
H,0,-1.4211275634,1.7033807563,-0.9437948237
H,0,-0.4842348168,-2.5880942243,0.3355292063
H,0,-1.6932724082,-2.8471210996,1.632574839
H,0,-2.0016948998,-3.4721361679,0.0065693676
H,0,0.2274892208,-0.1966531459,0.6699265745

H,0,2.4888162302,0.7389122834,0.5803573695
O,0,3.1899853367,1.3844970814,0.3385968567
H,0,3.9345452468,0.8473356931,-0.003570857
O,0,1.310383647,2.2858402254,2.6488687146
H,0,0.8110937238,2.9455510245,2.1141648935
H,0,2.2161366496,2.3285300072,2.3055852338
H,0,2.6557837633,-2.6013091601,-0.987169293
O,0,3.438933645,-2.711948662,-0.4278382097
H,0,3.079676601,-2.7055062479,0.4919665328
H,0,5.3539731513,-0.4492950792,-1.5741287626
O,0,5.0532118338,-0.4989704453,-0.6597196613
H,0,4.5280499838,-1.3347801141,-0.5872660017
O,0,0.0321378147,3.9832290553,0.8366849387
H,0,-0.8650520923,3.686392974,0.6343320525
H,0,0.5775595655,3.7527200549,0.0458428846
O,0,1.7055212607,3.1151941768,-1.1918329014
H,0,1.2502646236,2.4968025205,-1.7802970786
H,0,2.339301729,2.5452484002,-0.6909174078
H,0,1.6224124419,-3.0101959909,2.4156540588
O,0,2.2514183515,-2.3934276715,2.0249821381
H,0,1.7515533269,-1.5499822965,1.8513651537

Decarboxylative Elimination ground state intermediate – gas phase

E(RB+HF-LYP) = -817.176100710

Zero-point correction= 0.255141 (Hartree/Particle)
Thermal correction to Energy= 0.271254
Thermal correction to Enthalpy= 0.272198
Thermal correction to Gibbs Free Energy= 0.211676
Sum of electronic and zero-point Energies= -816.920960
Sum of electronic and thermal Energies= -816.904847
Sum of electronic and thermal Enthalpies= -816.903903
Sum of electronic and thermal Free Energies= -816.964425

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	170.214	60.422	127.380

C,0,0.427722849,2.1606196755,0.8287433478
N,0,1.0607245193,0.9577173806,0.9237744623
C,0,0.2880418343,-0.2729123447,0.7724653346
C,0,-0.6479575561,-0.267244237,-0.4196243349
C,0,-1.3369715292,1.0902877662,-0.6085021224
N,0,-0.7988445841,2.1173685887,0.1067592133

C,0,2.2278999736,0.8896361821,1.8102471471
C,0,-0.6336506622,-0.6860545248,2.0634891599
O,0,-0.5281287215,0.063604788,3.0404217881
N,0,-0.0565534979,-0.753211708,-1.803670475
C,0,0.8067692752,0.3055114152,-2.4318789089
O,0,-2.3053830798,1.2418486275,-1.3484106224
O,0,0.8442565811,3.241856347,1.2167197578
O,0,-1.2728041812,-1.7360392442,1.8305379441
C,0,0.7606217666,-1.9994451446,-1.5894616525
C,0,-1.1915290428,-1.1110435534,-2.7378739691
H,0,-1.2710610329,3.0132654107,0.0432264171
H,0,2.900545879,0.1045133916,1.4502500688
H,0,2.7410911702,1.8500545383,1.78759764
H,0,1.9071236916,0.6653379655,2.832023743
H,0,-1.4105887734,-1.0189550591,-0.1908057122
H,0,1.001051613,-1.095345063,0.7234477995
H,0,1.2857207734,-0.1118692875,-3.319475706
H,0,0.180966663,1.1515329894,-2.7152611767
H,0,1.5553424841,0.6199264477,-1.7039930183
H,0,-0.7634159889,-1.3992293681,-3.6997615898
H,0,-1.7385944908,-1.9483926705,-2.3029440063
H,0,-1.8539634969,-0.2537562591,-2.8335902124
H,0,0.9521362068,-2.4492013944,-2.5647817572
H,0,1.7054541784,-1.7437991017,-1.1146418336
H,0,0.1976121425,-2.6864563596,-0.955931201

Decarboxylative Elimination ground state intermediate – PCM acetone

E(RB+HF-LYP) = -817.234185797

Zero-point correction= 0.254313 (Hartree/Particle)
Thermal correction to Energy= 0.270341
Thermal correction to Enthalpy= 0.271285
Thermal correction to Gibbs Free Energy= 0.210926
Sum of electronic and zero-point Energies= -816.979873
Sum of electronic and thermal Energies= -816.963845
Sum of electronic and thermal Enthalpies= -816.962901
Sum of electronic and thermal Free Energies= -817.023260

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	169.642	60.132	127.037

C,0,-0.0986534432,-0.4080417146,1.9768795999
N,0,0.9028140771,0.1689734706,1.2602761719

C,0,1.0224642092,-0.1456260392,-0.160763272
C,0,-0.3070421579,0.0144165842,-0.9008321885
C,0,-1.436904494,-0.6776226344,-0.117508035
N,0,-1.1923411958,-0.8707254725,1.2104274834
C,0,2.1222922117,0.5605186951,1.9722581186
C,0,1.5609901032,-1.6246935921,-0.4454361187
O,0,1.8328601753,-2.3237901043,0.5536978604
N,0,-0.7320457082,1.4640181419,-1.2869688166
C,0,-1.2509611433,2.2535828449,-0.1091911898
O,0,-2.4772528532,-1.0424911423,-0.6552915865
O,0,-0.1450420209,-0.4984329029,3.2025998699
O,0,1.6667825129,-1.8940545179,-1.6685424967
C,0,0.4383600736,2.2030454233,-1.8900510886
C,0,-1.8175302008,1.3975671149,-2.3435773307
H,0,-1.9322066801,-1.3412782086,1.7546975197
H,0,2.5913148146,1.3921345579,1.4398460143
H,0,1.8578605444,0.8798117403,2.9793716237
H,0,2.8226454877,-0.279487849,2.0293770008
H,0,-0.204940072,-0.5020631849,-1.8572626285
H,0,1.7908257598,0.5045883649,-0.5834003668
H,0,-1.4479850452,3.2721906978,-0.4471506974
H,0,-2.1779761679,1.8023527609,0.2466468843
H,0,-0.49880341,2.257510323,0.6778636981
H,0,-2.115888466,2.4200606288,-2.5794099264
H,0,-1.4081757022,0.90950974,-3.2296138069
H,0,-2.6583006634,0.8261274946,-1.9579727091
H,0,0.056233422,3.119621462,-2.3417663028
H,0,1.1579895743,2.4579879016,-1.1137442763
H,0,0.9015429294,1.5763398387,-2.6540060446

Decarboxylative Elimination ground state intermediate – PCM water

E(RB+HF-LYP) = -817.240283428

Zero-point correction= 0.253947 (Hartree/Particle)
Thermal correction to Energy= 0.269997
Thermal correction to Enthalpy= 0.270941
Thermal correction to Gibbs Free Energy= 0.210843
Sum of electronic and zero-point Energies= -816.986336
Sum of electronic and thermal Energies= -816.970286
Sum of electronic and thermal Enthalpies= -816.969342
Sum of electronic and thermal Free Energies= -817.029441

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	169.426	60.200	126.488

C,0,-0.1509053686,-0.4090266187,1.9620994868
N,0,0.8684986884,0.1705357877,1.2759530022
C,0,1.0306549875,-0.1270706592,-0.1455130757
C,0,-0.2831346974,0.0202999332,-0.9176819226
C,0,-1.4093256732,-0.721541398,-0.174734619
N,0,-1.227181176,-0.8660084439,1.1700629631
C,0,2.061826971,0.5747521005,2.02460897
C,0,1.5943117796,-1.5947805264,-0.4234459068
O,0,1.7649115252,-2.3311497167,0.5732673057
N,0,-0.7249011999,1.4719178824,-1.2751745809
C,0,-1.1545554307,2.2764925218,-0.071608753
O,0,-2.3940578993,-1.1643630177,-0.7563299496
O,0,-0.2227248966,-0.5117564818,3.187294834
O,0,1.8179720656,-1.8303280421,-1.6378544216
C,0,0.4102746226,2.1916714302,-1.9638005901
C,0,-1.8812639292,1.4175670678,-2.2546576322
H,0,-1.969631486,-1.3626081106,1.6894860417
H,0,2.5734516444,1.3643995234,1.4687999515
H,0,1.7588807022,0.9568275072,2.9987898677
H,0,2.7404272393,-0.2740080002,2.1624356001
H,0,-0.1562925757,-0.4682226747,-1.8891902287
H,0,1.8007272105,0.5401642377,-0.5421743189
H,0,-1.4336808285,3.2730147867,-0.4177289272
H,0,-2.0169999017,1.7966984886,0.3929335821
H,0,-0.3271274803,2.34100168,0.6324149188
H,0,-2.1321345207,2.4433223233,-2.5282239268
H,0,-1.5642915892,0.8563287635,-3.1347686663
H,0,-2.7301261706,0.9268701084,-1.7855546901
H,0,0.0209732373,3.1341009245,-2.3514021408
H,0,1.2075688631,2.3962369081,-1.2509705201
H,0,0.7772355409,1.571351909,-2.7833541257

Decarboxylative Elimination transition state – gas phase

E(RB+HF-LYP) = -817.170764947

Zero-point correction=	0.251829 (Hartree/Particle)
Thermal correction to Energy=	0.268313
Thermal correction to Enthalpy=	0.269257
Thermal correction to Gibbs Free Energy=	0.208197
Sum of electronic and zero-point Energies=	-816.918936
Sum of electronic and thermal Energies=	-816.902452
Sum of electronic and thermal Enthalpies=	-816.901508

Sum of electronic and thermal Free Energies= -816.962568

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
TOTAL	168.369	60.913	128.511

C,0,-1.4521590169,-0.5413216877,0.0321757756
N,0,-1.1265752587,-0.7861167944,1.3402221819
C,0,0.0974496372,-0.545429444,2.0125462483
N,0,1.0900482316,-0.0552213543,1.2119524974
C,0,0.9903790225,-0.1717385016,-0.2198998042
C,0,-0.321572405,0.0118371946,-0.7991458382
O,0,0.164024749,-0.7229978123,3.2218028449
C,0,2.4354361812,0.0310500106,1.7840255647
C,0,1.4373661154,-1.8637919518,-0.8374051684
O,0,1.4768752389,-1.8268478875,-2.0591037341
N,0,-0.8460439405,1.7489146792,-1.1359907837
C,0,0.3468472337,2.450635041,-1.6637643634
O,0,-2.5830421546,-0.723996264,-0.4103607339
O,0,1.6312129694,-2.6032686945,0.10907786
C,0,-1.9182003986,1.7122379564,-2.169515207
C,0,-1.3298311988,2.4093423221,0.104314991
H,0,-1.8511554262,-1.1853904319,1.9273519576
H,0,2.9664896539,0.8708846111,1.3259452337
H,0,2.3478208698,0.1935422559,2.8571496572
H,0,2.9846911778,-0.8983044216,1.6008391326
H,0,-0.3618875373,-0.3177665234,-1.8346147156
H,0,1.8068397662,0.3547240976,-0.707578009
H,0,-1.5592364977,3.4602588955,-0.1024042218
H,0,-2.2335765755,1.908777557,0.452644318
H,0,-0.5546829462,2.3463179937,0.869428335
H,0,-2.2461949967,2.7335231041,-2.3920363002
H,0,-1.5208803879,1.254130277,-3.0773130704
H,0,-2.7487044976,1.1118570557,-1.8001490502
H,0,0.0650674378,3.4566156196,-1.9905501162
H,0,1.10428594,2.5255842359,-0.8832565834
H,0,0.7522633483,1.8921695888,-2.510066921

Decarboxylative Elimination transition state – PCM acetone

E(RB+HF-LYP) = -817.208564907

Zero-point correction= 0.248602 (Hartree/Particle)
Thermal correction to Energy= 0.265765
Thermal correction to Enthalpy= 0.266709

Thermal correction to Gibbs Free Energy= 0.203577
Sum of electronic and zero-point Energies= -816.959963
Sum of electronic and thermal Energies= -816.942800
Sum of electronic and thermal Enthalpies= -816.941855
Sum of electronic and thermal Free Energies= -817.004988

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	166.770	62.076	132.874

C,0,-1.3978459758,-0.5931937967,-0.0311825256
N,0,-1.1183567429,-0.7200736406,1.3073514846
C,0,0.096964417,-0.4698808576,1.9626575717
N,0,1.1191574904,-0.0579260969,1.1577668928
C,0,1.0241017195,-0.1797635478,-0.2587727689
C,0,-0.2630678759,-0.0741761329,-0.8487878962
O,0,0.1745171859,-0.5959219821,3.1871155274
C,0,2.4482698902,0.0877238651,1.7566405394
C,0,1.4376800268,-2.0438021348,-0.7701934831
O,0,1.7277838496,-2.0655587663,-1.9492955225
N,0,-0.9010456802,1.8606340734,-1.1263256507
C,0,0.2923866484,2.5734391109,-1.615548827
O,0,-2.5032249368,-0.8655938763,-0.498268295
O,0,1.3602029211,-2.7256769459,0.2292795576
C,0,-1.9639729092,1.8371878253,-2.1541888297
C,0,-1.3940760568,2.4553486987,0.1340860917
H,0,-1.8757127222,-1.0701610343,1.9133001026
H,0,3.0320774328,0.7845634298,1.1516840312
H,0,2.3424590212,0.4828341736,2.7659121691
H,0,2.963207037,-0.8787107924,1.8005185062
H,0,-0.3321936392,-0.2814658806,-1.9115751836
H,0,1.871023584,0.2621094765,-0.780379686
H,0,-1.6879778217,3.4996474714,-0.0336286418
H,0,-2.264252433,1.9007134812,0.4904024377
H,0,-0.6049712773,2.426162381,0.8876372904
H,0,-2.2923393872,2.8606759546,-2.3769029441
H,0,-1.5760496665,1.3816625218,-3.0687485186
H,0,-2.8079893454,1.2502060477,-1.7910025207
H,0,0.0363615296,3.611153205,-1.8629151723
H,0,1.0642172934,2.5781227906,-0.8434841013
H,0,0.6769834597,2.0787608067,-2.5112762279

Decarboxylative Elimination transition state – PCM water

E(RB+HF-LYP) = -817.212913209

Zero-point correction= 0.248327 (Hartree/Particle)
Thermal correction to Energy= 0.265431
Thermal correction to Enthalpy= 0.266375
Thermal correction to Gibbs Free Energy= 0.203884
Sum of electronic and zero-point Energies= -816.964586
Sum of electronic and thermal Energies= -816.947483
Sum of electronic and thermal Enthalpies= -816.946538
Sum of electronic and thermal Free Energies= -817.009029

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	166.560	62.082	131.523

C,0,-1.397410196,-0.5814472364,-0.002664528
N,0,-1.1039955173,-0.7022043624,1.3338134318
C,0,0.1224927857,-0.466527815,1.9708265858
N,0,1.1391228645,-0.0701242943,1.1522661121
C,0,1.023181478,-0.1855508913,-0.2617367392
C,0,-0.2683902034,-0.0825236863,-0.836922517
O,0,0.2181025533,-0.5960688402,3.1948482127
C,0,2.476204039,0.0705971403,1.7349545469
C,0,1.4168258844,-2.0559199591,-0.791312806
O,0,1.6685584263,-2.0793721371,-1.9788941462
N,0,-0.911974285,1.870313079,-1.1269964469
C,0,0.2944923535,2.5905165723,-1.5699565278
O,0,-2.5126446879,-0.8448570469,-0.4531294204
O,0,1.3693251144,-2.7378458965,0.2103260743
C,0,-1.9347435414,1.8311839492,-2.193862944
C,0,-1.4568604323,2.4611380158,0.1125178548
H,0,-1.860663696,-1.0345434293,1.9526847174
H,0,3.0625438663,0.7436837805,1.1062868196
H,0,2.3870017921,0.4927583973,2.7349731477
H,0,2.9780149207,-0.9016244409,1.7973627311
H,0,-0.3484167868,-0.2868616899,-1.9018389613
H,0,1.8678142209,0.2487712312,-0.7956681182
H,0,-1.7533635419,3.5030532195,-0.0668449927
H,0,-2.3351196927,1.8992809226,0.4364422982
H,0,-0.696513333,2.4395211407,0.8958140228
H,0,-2.2721682629,2.8492243072,-2.4288251767
H,0,-1.5049578923,1.3826831893,-3.0930249634
H,0,-2.7821370989,1.230560731,-1.8612288465
H,0,0.041713625,3.6265507281,-1.8288261885
H,0,1.0355893496,2.6004399667,-0.7681036243

H,0,0.7171068411,2.0969658169,-2.4490478609

3-carboxybenzisoxazole – PCM acetone 6-31+G*

E(RB+HF-LYP) = -587.840581254

Zero-point correction= 0.106190 (Hartree/Particle)
Thermal correction to Energy= 0.114773
Thermal correction to Enthalpy= 0.115717
Thermal correction to Gibbs Free Energy= 0.071638
Sum of electronic and zero-point Energies= -587.734392
Sum of electronic and thermal Energies= -587.725808
Sum of electronic and thermal Enthalpies= -587.724864
Sum of electronic and thermal Free Energies= -587.768943

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.021	32.970	92.772

C,0,-3.0589097878,-0.442487386,-0.0445175175
C,0,-2.5090961764,0.8370454331,0.0168973741
C,0,-1.1145154643,0.8989608661,0.0311507852
C,0,-0.2845328946,-0.226948032,-0.010389621
C,0,-0.857491433,-1.5101060252,-0.0713384348
C,0,-2.2463870016,-1.5997455491,-0.0885751887
O,0,-0.3541114322,2.027380087,0.0858007755
C,0,1.0482149544,0.3292924941,0.0163990866
N,0,1.0108433804,1.6383800014,0.0711794886
C,0,2.3859048154,-0.4144910427,0.0007452016
O,0,3.4234129269,0.2650822779,-0.2124806865
O,0,2.3011065677,-1.6555242214,0.2071868083
H,0,-4.1426716345,-0.5534868299,-0.0590056669
H,0,-3.1252172119,1.7337408197,0.0505538296
H,0,-0.2287634619,-2.3950317661,-0.1005819863
H,0,-2.7216379261,-2.5785119321,-0.135507889

3-carboxybenzisoxazole – PCM water 6-31+G*

E(RB+HF-LYP) = -587.845017782

Zero-point correction= 0.105911 (Hartree/Particle)
Thermal correction to Energy= 0.114606
Thermal correction to Enthalpy= 0.115551
Thermal correction to Gibbs Free Energy= 0.071024
Sum of electronic and zero-point Energies= -587.739107
Sum of electronic and thermal Energies= -587.730411

Sum of electronic and thermal Enthalpies= -587.729467
Sum of electronic and thermal Free Energies= -587.773994

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	71.917	33.071	93.714

C,0,3.0405817743,-0.5046057663,0.0647554465
C,0,2.5219816949,0.7867643046,-0.0252887038
C,0,1.1291712932,0.8849569972,-0.0450038208
C,0,0.2795255531,-0.2257143311,0.0190353167
C,0,0.8178229163,-1.5208251986,0.1095003752
C,0,2.2039789785,-1.643555938,0.1311030926
O,0,0.3945442981,2.0259791825,-0.1272568069
C,0,-1.0405074029,0.3532985963,-0.0210166329
N,0,-0.9890076237,1.6570636844,-0.1038173143
C,0,-2.3837156308,-0.3744489479,-0.0023104122
O,0,-3.1222166982,-0.1761141573,0.9963446388
O,0,-2.5976599833,-1.1165182257,-0.996962902
H,0,4.1217324902,-0.6396632216,0.084298284
H,0,3.1614663971,1.6664116748,-0.0758864166
H,0,0.1722802455,-2.3966737371,0.1574561721
H,0,2.6571982408,-2.6315131995,0.1992057544

Transition State for decarboxylation of 3-carboxybenzisoxazole – PCM acetone 6-31+G*

E(RB+HF-LYP) = -587.806833813

Zero-point correction= 0.101501 (Hartree/Particle)
Thermal correction to Energy= 0.110950
Thermal correction to Enthalpy= 0.111894
Thermal correction to Gibbs Free Energy= 0.065769
Sum of electronic and zero-point Energies= -587.705333
Sum of electronic and thermal Energies= -587.695884
Sum of electronic and thermal Enthalpies= -587.694940
Sum of electronic and thermal Free Energies= -587.741065

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.622	34.919	97.078

C,0,-2.9510897967,-0.7954887536,0.1574871304
C,0,-2.643555513,0.5524384556,0.011702594
C,0,-1.2851839476,0.9747627607,-0.0666069086

C,0,-0.2868187413,-0.0640021245,0.014130758
C,0,-0.6135679601,-1.4183823976,0.1609576837
C,0,-1.9526790355,-1.789424583,0.2333561015
O,0,-0.8979782575,2.1988386065,-0.2020358048
C,0,0.9991988284,0.5776107632,-0.0843216001
N,0,1.1975694897,1.7747036424,-0.2115477506
C,0,2.5396024609,-0.4476260648,-0.0199668684
O,0,2.8110219787,-0.788789815,-1.1511061406
O,0,2.8700205388,-0.556235688,1.1413341758
H,0,-3.9995670747,-1.0901316504,0.2146781895
H,0,-3.4295258057,1.3036241791,-0.0448641045
H,0,0.1732007703,-2.1699886459,0.2176356972
H,0,-2.2270461699,-2.8362625431,0.3474132849

Transition State for decarboxylation of 3-carboxybenzisoxazole – PCM acetone 6-31+G*

E(RB+HF-LYP) = -587.810757002

Zero-point correction= 0.101414 (Hartree/Particle)
Thermal correction to Energy= 0.110865
Thermal correction to Enthalpy= 0.111810
Thermal correction to Gibbs Free Energy= 0.065692
Sum of electronic and zero-point Energies= -587.709343
Sum of electronic and thermal Energies= -587.699892
Sum of electronic and thermal Enthalpies= -587.698947
Sum of electronic and thermal Free Energies= -587.745065

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	69.569	34.934	97.063

C,0,-2.9505988251,-0.795418431,0.1573237821
C,0,-2.6431195982,0.5526624277,0.0111913593
C,0,-1.2848456921,0.9740018291,-0.066342382
C,0,-0.286573829,-0.0642680318,0.0143698685
C,0,-0.6130330426,-1.4190327621,0.1616005224
C,0,-1.9521453384,-1.7894013143,0.2338387941
O,0,-0.896985314,2.1990897595,-0.2015316965
C,0,0.9991948894,0.5773816878,-0.0840249632
N,0,1.1984509618,1.7745601547,-0.2113247546
C,0,2.5377794378,-0.4471319753,-0.0204597754
O,0,2.8105010078,-0.786656806,-1.1519349573
O,0,2.8680825811,-0.5575527799,1.1408218111
H,0,-3.9992259163,-1.0901319862,0.2142710449

H,0,-3.4295613893,1.3036163929,-0.0457871383
H,0,0.1737444928,-2.1709193477,0.218636717
H,0,-2.2268481306,-2.8362881114,0.3483281647

Epoxidation of Enones with t-Butyl hydroperoxide

B3LYP//6-311G+** on all atoms unless otherwise noted

Cyclohexenone

E(RB+HF-LYP) = -308.755175957

Zero-point correction= 0.126814 (Hartree/Particle)
Thermal correction to Energy= 0.132924
Thermal correction to Enthalpy= 0.133869
Thermal correction to Gibbs Free Energy= 0.096882
Sum of electronic and zero-point Energies= -308.628362
Sum of electronic and thermal Energies= -308.622252
Sum of electronic and thermal Enthalpies= -308.621307
Sum of electronic and thermal Free Energies= -308.658294

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.411	23.295	77.844

C,0,0.8693989519,-0.5285247445,-0.5189583684
C,0,1.0111716363,-0.077893738,0.8830383662
O,0,1.8117936197,-0.986399998,-1.1403422332
C,0,-0.0097670518,0.4571194981,1.5693444565
H,0,1.9866122999,-0.2266515525,1.3339697295
C,0,-1.3689915247,0.7047328657,0.9774429879
H,0,0.1353363661,0.7278149069,2.6125371985
C,0,-1.32881352,0.7433369607,-0.5553036023
H,0,-2.0509515842,-0.0867754448,1.3222825972
H,0,-1.7786146896,1.6381723575,1.3771834704
C,0,-0.5265470737,-0.4351154727,-1.1209285753
H,0,-2.3432079299,0.7439248374,-0.9636713114
H,0,-0.8593890349,1.6811175638,-0.8730144215
H,0,-1.0346703945,-1.3811469163,-0.8872433457
H,0,-0.4281724988,-0.3871879845,-2.2071176384

Cyclohexenone – PCM Toluene

E(RB+HF-LYP) = -308.760486621

Zero-point correction= 0.126465 (Hartree/Particle)
Thermal correction to Energy= 0.132576
Thermal correction to Enthalpy= 0.133520
Thermal correction to Gibbs Free Energy= 0.096535
Sum of electronic and zero-point Energies= -308.634021
Sum of electronic and thermal Energies= -308.627911
Sum of electronic and thermal Enthalpies= -308.626967
Sum of electronic and thermal Free Energies= -308.663952

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.193	23.312	77.841

C,0,0.8669570058,-0.5272284246,-0.5162922379
C,0,1.0122824862,-0.0770931532,0.8812797099
O,0,1.8111206629,-0.9928522427,-1.1391593009
C,0,-0.0103822939,0.4578425925,1.5679138399
H,0,1.9879385568,-0.2262471742,1.3352248815
C,0,-1.3683053394,0.7060095685,0.9767202991
H,0,0.1352110663,0.726701954,2.6127746479
C,0,-1.3293972565,0.7444686499,-0.5556400804
H,0,-2.0484943714,-0.0866154931,1.3238051709
H,0,-1.7771661115,1.6390359957,1.3784706144
C,0,-0.5247004588,-0.4324041382,-1.1210512678
H,0,-2.3438337563,0.7397656977,-0.9637822522
H,0,-0.86292668,1.683449413,-0.8749370045
H,0,-1.0320307281,-1.3797476143,-0.8881440995
H,0,-0.4263881391,-0.3830954067,-2.207719128

Cyclohexenone – 6-31G*

E(RB+HF-LYP) = -308.701464004

Zero-point correction= 0.127949 (Hartree/Particle)
Thermal correction to Energy= 0.134033
Thermal correction to Enthalpy= 0.134977
Thermal correction to Gibbs Free Energy= 0.098046
Sum of electronic and zero-point Energies= -308.538183
Sum of electronic and thermal Energies= -308.532099
Sum of electronic and thermal Enthalpies= -308.531155
Sum of electronic and thermal Free Energies= -308.568086

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total	84.107	23.132	77.729

C,0,0.8708466997,-0.5288422935,-0.5196205762
C,0,1.0124466372,-0.0760027397,0.8829988402
O,0,1.816330977,-0.98870742,-1.1426269112
C,0,-0.0100588159,0.4588958475,1.572071204
H,0,1.9914400115,-0.2230833423,1.3320121427
C,0,-1.3722539208,0.7030131125,0.9789290195
H,0,0.1349273641,0.7340270057,2.6164555651
C,0,-1.3285643516,0.7450560069,-0.5555545179
H,0,-2.0552720062,-0.0927047033,1.3195251711
H,0,-1.7877856292,1.6367312192,1.3792727763
C,0,-0.5290477215,-0.4368434435,-1.1210719416
H,0,-2.3446792725,0.7518687794,-0.9664363125
H,0,-0.8527392544,1.6834186525,-0.8697032776
H,0,-1.0445367031,-1.3814643354,-0.8865215298
H,0,-0.4322134881,-0.3907928565,-2.2101014145

Cyclohexenone – 6-31+G - PCM Dichloroethane**

E(RB+HF-LYP) = -308.701464004

Zero-point correction=	0.126464 (Hartree/Particle)
Thermal correction to Energy=	0.132570
Thermal correction to Enthalpy=	0.133514
Thermal correction to Gibbs Free Energy=	0.096559
Sum of electronic and zero-point Energies=	-308.575000
Sum of electronic and thermal Energies=	-308.568894
Sum of electronic and thermal Enthalpies=	-308.567950
Sum of electronic and thermal Free Energies=	-308.604905

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.189	23.331	77.780

C,0,0.8636677704,-0.5273862026,-0.5121933653
C,0,1.0172569278,-0.0738445916,0.8795792693
O,0,1.8120635641,-1.0117463208,-1.1386250137
C,0,-0.0106786424,0.4640271769,1.56887479
H,0,1.9951351289,-0.221482417,1.3366230651
C,0,-1.3700602963,0.7082240283,0.9774071295
H,0,0.1373911019,0.73490935,2.6160745163
C,0,-1.3315747902,0.7483494988,-0.5565166171
H,0,-2.0464762114,-0.0905589538,1.3248701252
H,0,-1.7831469249,1.6402934119,1.3826349413

C,0,-0.5232632516,-0.4274279256,-1.1238389479
H,0,-2.3479315193,0.7378892127,-0.96507092
H,0,-0.8677405295,1.6908920775,-0.8765341978
H,0,-1.0344005611,-1.3770070801,-0.8970031808
H,0,-0.4214253033,-0.3726169393,-2.2124677904

t-Butyl Hydroperoxide – 6-31G*

E(RB+HF-LYP) = -308.844828851

Zero-point correction= 0.139541 (Hartree/Particle)
Thermal correction to Energy= 0.147519
Thermal correction to Enthalpy= 0.148464
Thermal correction to Gibbs Free Energy= 0.108623
Sum of electronic and zero-point Energies= -308.662614
Sum of electronic and thermal Energies= -308.654635
Sum of electronic and thermal Enthalpies= -308.653691
Sum of electronic and thermal Free Energies= -308.693531

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.570	28.888	83.851

C,0,1.0054098095,-1.4491964527,0.4998789743
C,0,0.3564293,-0.1553038646,-0.0060246468
O,0,-1.0043670839,-0.306092839,0.4710581157
O,0,-1.7769892579,0.8720116109,0.0971905635
C,0,1.0030698891,1.0786874629,0.6315238378
C,0,0.3782940102,-0.0831582328,-1.537132013
H,0,2.065398675,-1.4671591457,0.225613265
H,0,0.9273801776,-1.5172220599,1.5894446744
H,0,0.5186745049,-2.3265737817,0.0616000974
H,0,2.0515090917,1.165730337,0.3244184116
H,0,0.4770576385,1.9879512293,0.3287606124
H,0,0.9653967387,1.0054671145,1.7233615003
H,0,1.4083808716,-0.0401380237,-1.9074661385
H,0,-0.1035445462,-0.9673701836,-1.9702311188
H,0,-0.1453899668,0.8106576841,-1.8887327165
H,0,-2.3732305036,0.4751331774,-0.5622349344

t-Butyl Hydroperoxide

E(RB+HF-LYP) = -308.904150268

Zero-point correction= 0.137675 (Hartree/Particle)
Thermal correction to Energy= 0.145265

Thermal correction to Enthalpy= 0.146209
Thermal correction to Gibbs Free Energy= 0.106948
Sum of electronic and zero-point Energies= -308.766476
Sum of electronic and thermal Energies= -308.758885
Sum of electronic and thermal Enthalpies= -308.757941
Sum of electronic and thermal Free Energies= -308.797202

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.155	27.435	82.633

C,0,1.0673301667,-1.4204285457,0.4496014283
C,0,0.3625529671,-0.147672653,-0.0306071437
C,0,0.9923338789,1.1034814429,0.5895959343
C,0,0.3313388845,-0.0737225798,-1.5603847415
O,0,-0.9740198828,-0.3431212179,0.4873281368
O,0,-1.7859081187,0.8195559211,0.1003228935
H,0,2.1093783039,-1.4061150696,0.121394685
H,0,1.0483244353,-1.4867231257,1.5396104689
H,0,0.5862241124,-2.3097044552,0.0365624242
H,0,2.0282539362,1.2086208697,0.2559334412
H,0,0.4437545934,1.9995676222,0.2970167739
H,0,0.9842595296,1.0331988692,1.679923653
H,0,1.3485647052,-0.0018768953,-1.9548529282
H,0,-0.1394956895,-0.968161279,-1.9752504898
H,0,-0.2302094013,0.7992662739,-1.8951476715
H,0,-2.6209658973,0.550503577,0.5043685357

t-Butyl Hydroperoxide

E(RB+HF-LYP) = -308.904150268

Zero-point correction= 0.137675 (Hartree/Particle)
Thermal correction to Energy= 0.145265
Thermal correction to Enthalpy= 0.146209
Thermal correction to Gibbs Free Energy= 0.106948
Sum of electronic and zero-point Energies= -308.766476
Sum of electronic and thermal Energies= -308.758885
Sum of electronic and thermal Enthalpies= -308.757941
Sum of electronic and thermal Free Energies= -308.797202

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.155	27.435	82.633

C,0,1.0673301667,-1.4204285457,0.4496014283
C,0,0.3625529671,-0.147672653,-0.0306071437
C,0,0.9923338789,1.1034814429,0.5895959343
C,0,0.3313388845,-0.0737225798,-1.5603847415
O,0,-0.9740198828,-0.3431212179,0.4873281368
O,0,-1.7859081187,0.8195559211,0.1003228935
H,0,2.1093783039,-1.4061150696,0.121394685
H,0,1.0483244353,-1.4867231257,1.5396104689
H,0,0.5862241124,-2.3097044552,0.0365624242
H,0,2.0282539362,1.2086208697,0.2559334412
H,0,0.4437545934,1.9995676222,0.2970167739
H,0,0.9842595296,1.0331988692,1.679923653
H,0,1.3485647052,-0.0018768953,-1.9548529282
H,0,-0.1394956895,-0.968161279,-1.9752504898
H,0,-0.2302094013,0.7992662739,-1.8951476715

t-Butyl Hydroperoxide – PCM toluene

E(RB+HF-LYP) = -308.909960945

Zero-point correction= 0.137769 (Hartree/Particle)
Thermal correction to Energy= 0.145767
Thermal correction to Enthalpy= 0.146712
Thermal correction to Gibbs Free Energy= 0.106853
Sum of electronic and zero-point Energies= -308.772192
Sum of electronic and thermal Energies= -308.764194
Sum of electronic and thermal Enthalpies= -308.763249
Sum of electronic and thermal Free Energies= -308.803108

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	91.470	29.140	83.890

C,0,1.103390433,-1.3839082618,0.47377355
C,0,0.3695171295,-0.1351619865,-0.022440704
C,0,0.9233262875,1.1330912488,0.631088003
C,0,0.39181307,-0.0462135161,-1.5500158983
O,0,-0.9876205776,-0.3917358883,0.4387329394
O,0,-1.8645469706,0.6898638177,0.0075086439
H,0,2.1542027292,-1.3323324271,0.1786766806
H,0,1.0535702798,-1.4584855089,1.5625853627
H,0,0.6660834362,-2.2860384063,0.0404839483
H,0,1.9680045202,1.2803392878,0.3443138049
H,0,0.3589128571,2.0121258077,0.3145864181
H,0,0.8750015891,1.0562350132,1.7207375596

H,0,1.4189236208,0.0727444395,-1.9056434082
H,0,-0.0246830185,-0.9551276008,-1.9908624311
H,0,-0.1926988438,0.8073461846,-1.8965882313
H,0,-2.1882583047,1.0113248681,0.8673479253

t-Butyl peroxide anion

E(RB+HF-LYP) = -308.305631528

Zero-point correction= 0.123958 (Hartree/Particle)
Thermal correction to Energy= 0.131586
Thermal correction to Enthalpy= 0.132531
Thermal correction to Gibbs Free Energy= 0.093337
Sum of electronic and zero-point Energies= -308.181673
Sum of electronic and thermal Energies= -308.174045
Sum of electronic and thermal Enthalpies= -308.173101
Sum of electronic and thermal Free Energies= -308.212294

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.572	27.692	82.489

C,0,1.0323040568,-1.4241769411,0.4624225651
C,0,0.2918662253,-0.1608125962,-0.0016803189
C,0,0.2850507605,-0.0728728639,-1.5412445861
O,0,-1.0266103897,-0.3076430315,0.4840705838
O,0,-1.846390413,0.8710380135,0.0907282801
C,0,0.943675238,1.1001102527,0.6010273734
H,0,2.0789909131,-1.4140492936,0.13508191
H,0,1.0073105376,-1.4935884235,1.5547071449
H,0,0.5457715252,-2.3155708317,0.0534833682
H,0,1.9393181836,1.2928739898,0.1806213967
H,0,0.2730430494,1.9376876899,0.3975734761
H,0,1.034081283,0.9898107825,1.6874351741
H,0,1.2845556599,0.1267683588,-1.9490892363
H,0,-0.0892641116,-1.0108204097,-1.96640797
H,0,-0.407178303,0.7262411707,-1.8149463793

t-Butyl peroxide anion – PCM toluene

E(RB+HF-LYP) = -308.365046091

Zero-point correction= 0.124629 (Hartree/Particle)
Thermal correction to Energy= 0.132203
Thermal correction to Enthalpy= 0.133147
Thermal correction to Gibbs Free Energy= 0.094048

Sum of electronic and zero-point Energies= -308.240418
Sum of electronic and thermal Energies= -308.232843
Sum of electronic and thermal Enthalpies= -308.231899
Sum of electronic and thermal Free Energies= -308.270999

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	82.959	27.514	82.292

C,0,-0.2644007915,0.4365575728,-1.064975646
C,0,0.5299643642,0.3205574013,0.2430606659
C,0,-0.0622460144,-0.7852984864,1.1333464841
O,0,1.8476776022,-0.0222543319,-0.1685304122
O,0,2.7465898421,-0.1721867383,1.0040445463
C,0,0.5307279759,1.665028841,0.9905202056
H,0,-1.3085524889,0.7012701387,-0.8668496683
H,0,0.173439972,1.2061656386,-1.7077977344
H,0,-0.2434176007,-0.5135446503,-1.6072566084
H,0,-0.4718343855,1.9295393324,1.3461924527
H,0,1.2156200179,1.5887973518,1.8365050555
H,0,0.8897888732,2.461564203,0.3306609439
H,0,-1.0651969702,-0.5227046613,1.4893705471
H,0,-0.1237950877,-1.7248836722,0.5745968213
H,0,0.6044752269,-0.9375034283,1.9835638114

$HNMe_3$ cation

E(RB+HF-LYP) = -174.901199608

Zero-point correction= 0.135581 (Hartree/Particle)
Thermal correction to Energy= 0.141188
Thermal correction to Enthalpy= 0.142132
Thermal correction to Gibbs Free Energy= 0.107969
Sum of electronic and zero-point Energies= -174.765618
Sum of electronic and thermal Energies= -174.760012
Sum of electronic and thermal Enthalpies= -174.759068
Sum of electronic and thermal Free Energies= -174.793231

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.597	19.511	71.902

C,0,0.2471511036,-0.0344963566,1.4218073912
N,0,0.3279580078,0.0087805953,-0.0812789315
C,0,-0.2985742965,1.2595025352,-0.6391701373

C,0,-0.2488084097,-1.2331075047,-0.7082955764
H,0,1.3206199585,0.0355090614,-0.3273436835
H,0,-0.8028878838,-0.0559566968,1.7096416869
H,0,0.7520843143,-0.9313024531,1.776668818
H,0,0.7291221499,0.8537844886,1.8265905597
H,0,-0.1249902097,-1.1731916168,-1.788181836
H,0,0.276555963,-2.1024716914,-0.3166517836
H,0,-1.3062669703,-1.2873006518,-0.4539870385
H,0,-0.1663233478,1.2685393428,-1.7197306481
H,0,-1.3587870449,1.2533916164,-0.3907116134
H,0,0.1865566318,2.1261423901,-0.1933920064

$HNMe_3$ cation – PCM toluene

E(RB+HF-LYP) = -174.947121815

Zero-point correction= 0.135789 (Hartree/Particle)
Thermal correction to Energy= 0.141381
Thermal correction to Enthalpy= 0.142325
Thermal correction to Gibbs Free Energy= 0.108180
Sum of electronic and zero-point Energies= -174.812649
Sum of electronic and thermal Energies= -174.807057
Sum of electronic and thermal Enthalpies= -174.806112
Sum of electronic and thermal Free Energies= -174.840258

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	88.718	19.416	71.865

C,0,0.2440260639,-0.0361538148,1.4158391098
N,0,0.3329075682,0.0089466918,-0.0825663223
C,0,-0.2981827538,1.2546421608,-0.6345687031
C,0,-0.2490599349,-1.2268011129,-0.7062633862
H,0,1.327082529,0.0359543548,-0.3283928644
H,0,-0.8074601488,-0.0657445405,1.6974355334
H,0,0.7539948969,-0.9288738289,1.7731677287
H,0,0.7167173378,0.8553368941,1.8241892879
H,0,-0.1217148687,-1.1704736127,-1.7857526965
H,0,0.2691178927,-2.0987290342,-0.311469666
H,0,-1.3075458726,-1.2727120774,-0.4545134399
H,0,-0.1726543294,1.2640263143,-1.7156460911
H,0,-1.3566653485,1.2463499646,-0.3790259116
H,0,0.1880746825,2.1221153243,-0.1920697473

***t*-butanol**

E(RB+HF-LYP) = -233.752389705

Zero-point correction= 0.134805 (Hartree/Particle)
Thermal correction to Energy= 0.141607
Thermal correction to Enthalpy= 0.142551
Thermal correction to Gibbs Free Energy= 0.105737
Sum of electronic and zero-point Energies= -233.617585
Sum of electronic and thermal Energies= -233.610783
Sum of electronic and thermal Enthalpies= -233.609839
Sum of electronic and thermal Free Energies= -233.646653

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	88.860	25.084	77.482

C,0,-0.0064337278,-0.0111435475,0.002497412
C,0,-0.0351465985,-0.0608758696,1.5303492307
C,0,1.4360000294,-0.0409430161,-0.5213706903
O,0,-0.6965966252,-1.2065409177,-0.4190298275
C,0,-0.753457945,1.2231409031,-0.5213705623
H,0,-0.7094168116,-1.2287459963,-1.3820980926
H,0,-0.7664052878,1.2345270774,-1.616692287
H,0,-1.7871014436,1.2182427654,-0.1677551961
H,0,-0.274830053,2.1475941106,-0.1856575271
H,0,1.4523343294,-0.0464625492,-1.6166924172
H,0,1.9972859448,0.8357875522,-0.1856576185
H,0,1.9485800255,-0.9385535722,-0.1677554517
H,0,-1.0670528033,-0.0783636784,1.8884589546
H,0,0.4656616881,-0.9632767617,1.888458851
H,0,0.4679468655,0.8105075736,1.9569970635

***t*-butanol – PCM toluene**

E(RB+HF-LYP) = -233.756202402

Zero-point correction= 0.134462 (Hartree/Particle)
Thermal correction to Energy= 0.141249
Thermal correction to Enthalpy= 0.142193
Thermal correction to Gibbs Free Energy= 0.105415
Sum of electronic and zero-point Energies= -233.621740
Sum of electronic and thermal Energies= -233.614953
Sum of electronic and thermal Enthalpies= -233.614009
Sum of electronic and thermal Free Energies= -233.650788

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	88.635	25.080	77.407

C,0,-0.0063265832,-0.0109901365,0.0027948281
C,0,-0.0345273146,-0.059966769,1.5303746349
C,0,1.435670214,-0.0404071697,-0.5202024257
O,0,-0.6976527596,-1.2081238451,-0.4217252439
C,0,-0.7528101455,1.2230411124,-0.5203262
H,0,-0.713731146,-1.2353480036,-1.3894249546
H,0,-0.7644432992,1.2350034636,-1.6154575155
H,0,-1.786786217,1.2190243289,-0.1668505768
H,0,-0.2736255907,2.1463571685,-0.1820901325
H,0,1.4520003614,-0.0445798933,-1.615324167
H,0,1.9955340274,0.8363382249,-0.1819470874
H,0,1.9492383534,-0.9377637814,-0.166558017
H,0,-1.0660495351,-0.0754021921,1.8906465179
H,0,0.4679555596,-0.9610172107,1.8905048776
H,0,0.4690925387,0.812316433,1.9544579833

_t_-butoxide anion

E(RB+HF-LYP) = -233.143749887

Zero-point correction= 0.119466 (Hartree/Particle)
Thermal correction to Energy= 0.125888
Thermal correction to Enthalpy= 0.126833
Thermal correction to Gibbs Free Energy= 0.090745
Sum of electronic and zero-point Energies= -233.024283
Sum of electronic and thermal Energies= -233.017861
Sum of electronic and thermal Enthalpies= -233.016917
Sum of electronic and thermal Free Energies= -233.053005

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	78.996	23.906	75.952

C,0,0.0148527329,0.0258351627,-1.5220530401
C,0,-0.0715286077,-0.1239532754,0.0395496999
C,0,1.4010346467,-0.0998559213,0.587237565
C,0,-0.7869671174,1.1635543804,0.5869741559
O,0,-0.7176715397,-1.2432317977,0.3968620156
H,0,1.3693221081,-0.1808768633,1.6793937022
H,0,1.9317409488,-0.9777759285,0.2025815741
H,0,1.9682746,0.8052866268,0.3148002158

H,0,-0.8410587873,1.095677681,1.679143194
H,0,-0.2862735976,2.1071873986,0.3146906137
H,0,-1.8126370346,1.1847667966,0.2023944046
H,0,0.5312741308,-0.8503682315,-1.9294052621
H,0,-1.00228588,0.033254204,-1.9292830525
H,0,0.5386659021,0.9352206189,-1.8594617978

_t_-butoxide anion – PCM toluene

E(RB+HF-LYP) = -233.198827449

Zero-point correction= 0.120218 (Hartree/Particle)
Thermal correction to Energy= 0.126536
Thermal correction to Enthalpy= 0.127480
Thermal correction to Gibbs Free Energy= 0.091591
Sum of electronic and zero-point Energies= -233.078610
Sum of electronic and thermal Energies= -233.072291
Sum of electronic and thermal Enthalpies= -233.071347
Sum of electronic and thermal Free Energies= -233.107236

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.403	23.592	75.535

C,0,0.0158583866,0.0273813426,-1.5164337404
C,0,-0.067686536,-0.1176497899,0.037549751
C,0,1.3961225314,-0.0989310794,0.5844836304
C,0,-0.782770732,1.1602454738,0.5833196083
O,0,-0.7224437941,-1.2502039654,0.4003266848
H,0,1.3699963004,-0.1768768979,1.6768304779
H,0,1.9329705142,-0.9729022264,0.1996662587
H,0,1.958405785,0.8063741924,0.3108765168
H,0,-0.8352923534,1.1013046398,1.676055677
H,0,-0.2812457778,2.0996000877,0.3065828008
H,0,-1.8090977379,1.1861735593,0.201053809
H,0,0.5350249648,-0.8439432345,-1.9304976585
H,0,-0.9989760715,0.0385858164,-1.9288513199
H,0,0.5386228294,0.9370401033,-1.8478455354

Cyclhexenone oxide – chair conformation

E(RB+HF-LYP) = -383.970105530

Zero-point correction= 0.131882 (Hartree/Particle)
Thermal correction to Energy= 0.138586
Thermal correction to Enthalpy= 0.139530

Thermal correction to Gibbs Free Energy= 0.100917
Sum of electronic and zero-point Energies= -383.838224
Sum of electronic and thermal Energies= -383.831519
Sum of electronic and thermal Enthalpies= -383.830575
Sum of electronic and thermal Free Energies= -383.869189

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.964	25.771	81.269

C,0,-0.6036564995,-0.516622837,-1.2415943617
C,0,0.8376137149,-0.4351074963,-0.783405183
C,0,1.0251861181,-0.1338029022,0.6774037182
C,0,-0.0681631346,0.5623607175,1.405141084
C,0,-1.3626782345,0.9609913187,0.7183928679
C,0,-1.3471073088,0.7650523359,-0.8083341694
O,0,1.7932642053,-0.537902252,-1.5225945866
H,0,2.0565144057,-0.0460379164,1.0073639364
H,0,0.2214666401,1.1450467422,2.2776350786
H,0,-2.1632162803,0.3655955658,1.1712157462
H,0,-1.5804334851,2.00709176,0.9533587432
H,0,-2.3708903551,0.7446520642,-1.1913132381
H,0,-0.8574003986,1.6245637793,-1.2791034497
H,0,-1.0731775067,-1.3945368837,-0.7849665815
H,0,-0.6130496838,-0.6390549582,-2.3253394923
O,0,0.1433631361,-0.8401661195,1.5682852768

Cyclhexenone oxide – chair conformation – PCM toluene

E(RB+HF-LYP) = -383.974068295

Zero-point correction= 0.132258 (Hartree/Particle)
Thermal correction to Energy= 0.138958
Thermal correction to Enthalpy= 0.139902
Thermal correction to Gibbs Free Energy= 0.101279
Sum of electronic and zero-point Energies= -383.842474
Sum of electronic and thermal Energies= -383.835774
Sum of electronic and thermal Enthalpies= -383.834830
Sum of electronic and thermal Free Energies= -383.873453

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	87.198	25.735	81.290

C,0,-0.601384555,-0.5144542354,-1.2405113815

C,0,0.8358842685,-0.4331105607,-0.7803726108
C,0,1.0258494283,-0.13207006,0.6769694058
C,0,-0.0682180294,0.5625334639,1.4044244768
C,0,-1.3607128531,0.9614189382,0.717485056
C,0,-1.3473666445,0.7641719669,-0.8072958235
O,0,1.7930295141,-0.5398921945,-1.5203558466
H,0,2.0546876156,-0.0463598028,1.0072245756
H,0,0.2218057229,1.1413034594,2.2768116861
H,0,-2.1627549059,0.3701440226,1.1714712601
H,0,-1.575662924,2.0074995741,0.9512493806
H,0,-2.3706885214,0.7381896491,-1.188744276
H,0,-0.8629983418,1.6245352714,-1.2802917623
H,0,-1.0707382521,-1.3931319599,-0.7861628063
H,0,-0.6112408185,-0.6366137537,-2.3238539073
O,0,0.141130578,-0.8421707476,1.5638684856

Cyclhexenone oxide – boat conformation

E(RB+HF-LYP) = -383.970730979

Zero-point correction=	0.131714 (Hartree/Particle)
Thermal correction to Energy=	0.138430
Thermal correction to Enthalpy=	0.139375
Thermal correction to Gibbs Free Energy=	0.100593
Sum of electronic and zero-point Energies=	-383.839017
Sum of electronic and thermal Energies=	-383.832301
Sum of electronic and thermal Enthalpies=	-383.831356
Sum of electronic and thermal Free Energies=	-383.870138

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.866	25.828	81.622

C,0,-1.4831477517,0.3238839531,0.8067666369
C,0,-0.2597202078,-0.3196062396,1.4735821316
C,0,0.8820294736,-0.6978030674,0.5403830904
C,0,0.872823742,-0.1271264948,-0.8533864418
C,0,-0.0987426837,0.9320317986,-1.2034872199
C,0,-1.086667629,1.4352410368,-0.1745162914
O,0,1.8186421177,-1.3723096035,0.9111373136
O,0,-0.2961919815,-0.4100732348,-1.6509091795
H,0,1.8171297675,-0.2164851389,-1.3831774648
H,0,0.1879076075,1.6246569925,-1.9928359276
H,0,-0.633317244,2.2818193232,0.3564677971
H,0,-1.9738712603,1.8227312834,-0.6857508042

H,0,-2.1453627077,0.7300003849,1.5759179121
H,0,-2.05061503,-0.4377158124,0.2675934766
H,0,0.1888143873,0.3809843935,2.1918121378
H,0,-0.5297362706,-1.2066546397,2.0520963655

Cyclhexenone oxide – boat conformation- PCM toluene

E(RB+HF-LYP) = -383.976584578

Zero-point correction= 0.131352 (Hartree/Particle)
Thermal correction to Energy= 0.138078
Thermal correction to Enthalpy= 0.139022
Thermal correction to Gibbs Free Energy= 0.100215
Sum of electronic and zero-point Energies= -383.845232
Sum of electronic and thermal Energies= -383.838507
Sum of electronic and thermal Enthalpies= -383.837562
Sum of electronic and thermal Free Energies= -383.876369

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.645	25.877	81.676

C,0,-1.4872831326,0.539384157,-0.67586703
C,0,-0.6808913111,-0.6556821195,-1.202341337
C,0,0.6965369932,-0.8444359233,-0.5911703773
C,0,1.0186502296,-0.1013053164,0.6772722391
C,0,-0.056733782,0.6194107199,1.3927400347
C,0,-1.4698444246,0.617022953,0.8563582008
O,0,1.5040423525,-1.6279821072,-1.0523985069
O,0,0.906113441,1.3375897799,0.6117865331
H,0,1.8959646885,-0.465908873,1.2070262814
H,0,0.0664736878,0.7446528175,2.4677013113
H,0,-2.0027450709,-0.2352395618,1.2969382054
H,0,-1.9854845898,1.5212895921,1.195924197
H,0,-2.5188717815,0.4632519751,-1.0293897852
H,0,-1.0786995123,1.466554199,-1.0845300377
H,0,-1.2117553952,-1.5929680314,-0.9811124038

DBU Model – 6-31G*

E(RB+HF-LYP) = -345.393699812

Zero-point correction= 0.178755 (Hartree/Particle)
Thermal correction to Energy= 0.187104
Thermal correction to Enthalpy= 0.188048
Thermal correction to Gibbs Free Energy= 0.146084

Sum of electronic and zero-point Energies= -345.214945
Sum of electronic and thermal Energies= -345.206596
Sum of electronic and thermal Enthalpies= -345.205652
Sum of electronic and thermal Free Energies= -345.247616

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.409	31.080	88.321

N,0,-0.4497629139,-0.6436122481,0.3219127112
C,0,0.719857511,-0.6921150291,1.203481563
C,0,1.954082416,-0.1899201448,0.4625885179
C,0,1.6479474434,1.1816429909,-0.1408739993
N,0,0.398133485,1.2195956769,-0.9063185814
C,0,-0.5351134622,0.3646995908,-0.6247594771
C,0,-1.814120679,0.4418990924,-1.4302962211
C,0,-1.6257460872,-1.3404791301,0.8297578806
H,0,2.4614120361,1.4957475005,-0.8061334339
H,0,1.5975551558,1.9380531209,0.6578610845
H,0,-1.3213161516,-2.3257007021,1.1971289564
H,0,-2.1016836338,-0.7988587239,1.6625025811
H,0,-2.3675417271,-1.4925178426,0.0464932528
H,0,0.5411639899,-0.0858640617,2.1074633975
H,0,2.2130241027,-0.8982166053,-0.3347409035
H,0,2.8073876232,-0.136870455,1.1483197214
H,0,0.8541770143,-1.7299150018,1.5307053819
H,0,-2.0333945683,-0.5051915305,-1.9359502592
H,0,-2.6760666608,0.6902114762,-0.800801183
H,0,-1.6947540294,1.2228746027,-2.1813970897

dbuHOOtBuB3 complex – 6-31G*

E(RB+HF-LYP) = -654.181398974

Zero-point correction= 0.322020 (Hartree/Particle)
Thermal correction to Energy= 0.339778
Thermal correction to Enthalpy= 0.340722
Thermal correction to Gibbs Free Energy= 0.274558
Sum of electronic and zero-point Energies= -653.859379
Sum of electronic and thermal Energies= -653.841621
Sum of electronic and thermal Enthalpies= -653.840677
Sum of electronic and thermal Free Energies= -653.906841

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total	213.214	64.015	139.255

C,0,-3.5027746004,1.2722240777,0.889972451
C,0,-2.3994189,2.324753604,0.934000631
C,0,-1.4083667747,2.053185247,-0.1979249749
N,0,-0.9501773191,0.6668823699,-0.2333709861
C,0,-1.6972426838,-0.2692743072,0.2545645372
N,0,-2.9218704255,-0.0698914588,0.867909991
C,0,-1.1726620309,-1.6859776496,0.1831842384
C,0,-3.8682443572,-1.146950417,1.1094492914
O,0,1.3778904737,0.2644213503,-1.7392212725
O,0,1.935529294,-0.9322989605,-1.1269194239
C,0,3.1435129707,-0.5874370415,-0.4116506928
C,0,3.5860116417,-1.9426028065,0.1532826042
C,0,4.1835124769,-0.0308607464,-1.3916690196
C,0,2.8395317573,0.4102229134,0.7120188924
H,0,3.7415220174,0.6199027646,1.298465989
H,0,2.4708449454,1.3504204727,0.293950454
H,0,2.0737102356,0.0080830059,1.3843220274
H,0,5.1229281263,0.1968221214,-0.8741532142
H,0,4.3893758685,-0.7611086364,-2.1816139637
H,0,3.8094997342,0.8836666745,-1.858684925
H,0,4.5311683058,-1.8366484879,0.6967314107
H,0,2.8341342832,-2.3415132533,0.842803458
H,0,3.7306993286,-2.6657227274,-0.6560297513
H,0,0.5568822279,0.3794799234,-1.1797578789
H,0,-0.5263623924,2.6969404622,-0.0999544918
H,0,-1.864287558,2.3034346517,-1.1681838727
H,0,-4.4504929318,-0.920066631,2.0101809482
H,0,-4.5753446986,-1.2740919221,0.2739351253
H,0,-3.3553166698,-2.093943257,1.2719603668
H,0,-4.1462328894,1.4264270881,0.0076197646
H,0,-1.8817918493,2.2666999623,1.8992164731
H,0,-2.8331783149,3.3276303583,0.8507047082
H,0,-4.1489373361,1.3464424271,1.7736348582
H,0,-1.1595399143,-2.1569483637,1.1732070397
H,0,-1.7904969885,-2.3104398594,-0.4733687722
H,0,-0.154964456,-1.6650795124,-0.2090009664

dbuHOOtBuB3 complex – 6-31+G**

E(RB+HF-LYP) = -654.237108355

Zero-point correction=	0.319533 (Hartree/Particle)
Thermal correction to Energy=	0.337504

Thermal correction to Enthalpy= 0.338448
Thermal correction to Gibbs Free Energy= 0.270655
Sum of electronic and zero-point Energies= -653.917576
Sum of electronic and thermal Energies= -653.899604
Sum of electronic and thermal Enthalpies= -653.898660
Sum of electronic and thermal Free Energies= -653.966453

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	211.787	64.380	142.682

C,0,-3.324463523,0.7616961321,1.6224688223
C,0,-2.1938428749,0.2871502151,2.5303070437
C,0,-0.8653350282,0.4147514032,1.7849630824
N,0,-0.9032637345,-0.1870076321,0.4522987112
C,0,-2.0295112628,-0.3023513703,-0.1739448882
N,0,-3.2624404359,0.071990377,0.3318795529
C,0,-2.0009862651,-0.9330372497,-1.5480128189
C,0,-4.4402999051,0.2333193385,-0.5090806541
O,0,1.5184749843,-1.2865559511,-0.2515011101
O,0,2.4355213764,-0.2861434892,0.2857942853
C,0,3.3313031356,0.1553985301,-0.7597855775
C,0,4.2292043082,1.1527920549,-0.0170807062
C,0,4.1457360586,-1.0324724816,-1.2886365126
C,0,2.5507519504,0.8475759582,-1.8843486071
H,0,3.2377624531,1.238710836,-2.6430138074
H,0,1.8694308709,0.1419795821,-2.3661973436
H,0,1.9632223228,1.6808010391,-1.4846214828
H,0,4.8691153109,-0.6977510062,-2.040670088
H,0,4.6908345796,-1.5132428196,-0.4700649972
H,0,3.4858052947,-1.774587326,-1.7443102886
H,0,4.9800557798,1.5602569031,-0.7018728398
H,0,3.6385435225,1.9824544103,0.384024142
H,0,4.7458279167,0.6611737719,0.8128538178
H,0,0.6373014059,-0.8602315228,-0.0315232495
H,0,-0.0560408098,-0.0653201549,2.3446425136
H,0,-0.582760407,1.4729223752,1.684937578
H,0,-5.3360464847,0.0607056524,0.0963544955
H,0,-4.5101542689,1.2456626331,-0.9378417266
H,0,-4.4474947677,-0.4884457807,-1.3247693357
H,0,-3.2664345505,1.8530145857,1.47485853
H,0,-2.3650225452,-0.7604511179,2.8054815827
H,0,-2.185002833,0.8742655658,3.4550581626
H,0,-4.3018215284,0.5485848929,2.0710913503

H,0,-2.6443159316,-1.8182729887,-1.5976768002
H,0,-2.3331754202,-0.2321098499,-2.3217558004
H,0,-0.9770111645,-1.2323385545,-1.7696727656

dbuHOOtBuB3 complex – PCM Dichloroethane - 6-31G*

E(RB+HF-LYP) = -654.189415415

Zero-point correction= 0.320935 (Hartree/Particle)
Thermal correction to Energy= 0.337944
Thermal correction to Enthalpy= 0.338889
Thermal correction to Gibbs Free Energy= 0.274644
Sum of electronic and zero-point Energies= -653.868481
Sum of electronic and thermal Energies= -653.851471
Sum of electronic and thermal Enthalpies= -653.850527
Sum of electronic and thermal Free Energies= -653.914771

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.063	62.153	135.214

C,0,3.4236333543,1.0122284472,0.5296635944
C,0,2.6680301725,1.9996320876,-0.3545850047
C,0,1.1732078182,1.687880046,-0.2895070686
N,0,0.8781779659,0.276652807,-0.5343840074
C,0,1.7758362288,-0.6215129338,-0.2711534047
N,0,3.0448118745,-0.3629472465,0.1926459001
C,0,1.4026083075,-2.065364973,-0.5271390774
C,0,3.9167035778,-1.3977493311,0.7319855758
O,0,-1.6313900196,-0.2988373999,-1.4729924112
O,0,-2.4344472565,0.6634175261,-0.7302226218
C,0,-3.1615368145,-0.0035613829,0.3298522773
C,0,-3.9420327987,1.1561672065,0.9608914556
C,0,-4.1122662015,-1.0520508543,-0.259100094
C,0,-2.1942973488,-0.6285412821,1.3411434292
H,0,-2.7465012449,-1.0581782029,2.184936441
H,0,-1.6085411231,-1.423408087,0.8724166459
H,0,-1.5024006618,0.1278706111,1.7266047437
H,0,-4.7031461897,-1.5271658937,0.5325125494
H,0,-4.8010516568,-0.5850892159,-0.9720388176
H,0,-3.5448706874,-1.8265429666,-0.7820361996
H,0,-4.5616925228,0.7890072679,1.7860059715
H,0,-3.2572585212,1.9155712398,1.353580992
H,0,-4.5968743402,1.6287944055,0.2209204749
H,0,-0.7102281871,-0.0879776718,-1.1150585994

H,0,0.6215432991,2.2813185836,-1.0283153024
H,0,0.7701887362,1.9698224522,0.6951591991
H,0,4.958972577,-1.1041331486,0.5676906261
H,0,3.7704187694,-1.5404857898,1.8137633475
H,0,3.7564850977,-2.352482004,0.2312445731
H,0,3.2208133482,1.2122890701,1.5941741966
H,0,3.0205863021,1.9044161814,-1.3893260474
H,0,2.8721662692,3.0254658958,-0.0275792133
H,0,4.506255478,1.1085582973,0.3835036819
H,0,2.0799735314,-2.5355053618,-1.2495065169
H,0,1.4335332869,-2.6603615158,0.3929216057
H,0,0.3880799914,-2.0971262603,-0.9259974341

dbuHOOtBuB3 complex – PCM Dichloroethane - 6-31+G**

E(RB+HF-LYP) = -654.247510760

Zero-point correction= 0.318764 (Hartree/Particle)
Thermal correction to Energy= 0.336621
Thermal correction to Enthalpy= 0.337565
Thermal correction to Gibbs Free Energy= 0.270910
Sum of electronic and zero-point Energies= -653.928747
Sum of electronic and thermal Energies= -653.910890
Sum of electronic and thermal Enthalpies= -653.909946
Sum of electronic and thermal Free Energies= -653.976601

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	211.233	64.268	140.287

N,0,3.025753471,-0.3611033532,0.3257832003
C,0,3.5233209625,1.0175924102,0.455963292
C,0,2.7047177998,1.9790762696,-0.3993250914
C,0,1.2181970457,1.6895832361,-0.1929331533
N,0,0.8929074854,0.2900803939,-0.4676207538
C,0,1.7852330067,-0.6184573895,-0.195923335
C,0,1.4185173279,-2.0602407871,-0.4652941182
C,0,4.003957734,-1.3944448606,0.6458790243
O,0,-1.5840460104,-0.1150856891,-1.4343931908
O,0,-2.4024279345,0.7534958416,-0.5971451985
C,0,-3.2340880421,-0.0391997932,0.2941065411
C,0,-2.3665382464,-0.8706191973,1.245353042
C,0,-4.0074087411,1.0421032197,1.0586563515
C,0,-4.1830944077,-0.9245928772,-0.5213613505
H,0,-2.9986834445,-1.397043144,1.9688804542

H,0,-1.7869314985,-1.6134939762,0.6917979552
H,0,-1.6715319226,-0.2264950582,1.793322871
H,0,-4.8454587386,-1.4884120174,0.1446043225
H,0,-4.8006540274,-0.312583818,-1.1871718284
H,0,-3.615939098,-1.6345823915,-1.1288527477
H,0,-4.6984603066,0.5727345069,1.7660237785
H,0,-3.3233113817,1.6870440315,1.6192770409
H,0,-4.5884771128,1.6637696235,0.3699578771
H,0,-0.6546971069,0.0200371471,-1.0354019456
H,0,0.602942917,2.3168736983,-0.8467771331
H,0,0.9294880561,1.9354386025,0.8412221792
H,0,4.7459069148,-1.5128876835,-0.1570458339
H,0,4.5349775821,-1.1096757904,1.5607571894
H,0,3.5263384438,-2.3560136288,0.8263996437
H,0,3.4952262247,1.3147377071,1.5145194798
H,0,2.9580646151,1.842520184,-1.4582338775
H,0,2.9492188072,3.012423264,-0.1303183972
H,0,4.5751461519,1.0275219462,0.1435738924
H,0,2.1426445306,-2.5455019448,-1.1281839843
H,0,1.3723971496,-2.6422552651,0.4621109276
H,0,0.4360714742,-2.0890778825,-0.9360190908

TS addition of t-BuOO$^-$ to cyclohexenone – chair conformation

E(RB+HF-LYP) = -617.086656472

Zero-point correction= 0.251999 (Hartree/Particle)
Thermal correction to Energy= 0.266629
Thermal correction to Enthalpy= 0.267573
Thermal correction to Gibbs Free Energy= 0.209175
Sum of electronic and zero-point Energies= -616.834657
Sum of electronic and thermal Energies= -616.820028
Sum of electronic and thermal Enthalpies= -616.819083
Sum of electronic and thermal Free Energies= -616.877481

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.312	54.413	122.908

C,0,1.2664422207,1.9206865225,0.0000132603
C,0,2.7637794174,2.1489058705,0.2354732518
C,0,3.5301979086,0.8231834291,0.1666467527
C,0,2.9635993209,-0.2236258409,1.127242542
C,0,1.5380999759,-0.1625059128,1.3744708437
C,0,0.7257594544,0.7748207903,0.8099024454

O,0,3.7103649364,-1.0709308374,1.628433462
O,0,-0.7138726005,0.180449347,-1.1456462569
O,0,-2.0634128003,0.3811304139,-0.6179626791
C,0,-2.8127265988,-0.8295096168,-0.7008566497
H,0,1.1265425089,-0.9487997282,1.999936691
H,0,-0.3335098219,0.7776473046,1.0217363501
H,0,1.0489425222,1.6928206144,-1.0494410229
H,0,0.6916502427,2.8267910005,0.2239300674
H,0,3.1625597623,2.8610134801,-0.4971218226
H,0,2.9185308941,2.5947063561,1.2270928932
H,0,3.4519369959,0.4053640268,-0.8466967895
H,0,4.5947893741,0.9427973862,0.387367912
C,0,-4.186725179,-0.4687036026,-0.1217004224
C,0,-2.9391968281,-1.2649673764,-2.1705944313
C,0,-2.1413732492,-1.9332783205,0.1327797699
H,0,-4.8582469175,-1.3339659566,-0.1418495297
H,0,-4.0842333855,-0.1311280222,0.9140112466
H,0,-4.6411151745,0.3401479297,-0.7016808535
H,0,-3.4847519671,-2.211446129,-2.2657075938
H,0,-3.4651863029,-0.495452815,-2.7449411121
H,0,-1.9351607467,-1.3717354369,-2.5839975378
H,0,-2.668130987,-2.889887795,0.034543832
H,0,-1.1103622657,-2.0425032487,-0.2068269992
H,0,-2.1260296729,-1.6515960096,1.190783887

TS addition of t-BuOO$^-$ to cyclohexenone – boat conformation

E(RB+HF-LYP) = -617.088776322

Zero-point correction= 0.252068 (Hartree/Particle)
Thermal correction to Energy= 0.266597
Thermal correction to Enthalpy= 0.267542
Thermal correction to Gibbs Free Energy= 0.209416
Sum of electronic and zero-point Energies= -616.836709
Sum of electronic and thermal Energies= -616.822179
Sum of electronic and thermal Enthalpies= -616.821235
Sum of electronic and thermal Free Energies= -616.879360

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	167.292	54.337	122.335

C,0,-1.3779176296,-2.8376852339,-1.641322765
C,0,-0.0117114432,-3.1945411865,-1.044498207
C,0,0.4634754157,-2.3728377541,0.043878314

C,0,-0.2466285091,-1.3177629699,0.5410432022
C,0,-1.6328128288,-0.9951619936,0.0650015001
C,0,-1.7905552511,-1.3800836688,-1.4080191403
O,0,0.60130155,-4.1786753547,-1.477365059
O,0,0.5498899058,0.7516375664,-0.3771832597
O,0,-0.2085749173,1.8275697336,0.2638824448
C,0,0.6710353817,2.715182693,0.949949758
H,0,1.4419083887,-2.6224588417,0.4426881294
H,0,0.1074139932,-0.7984227585,1.4211075048
H,0,-2.3610722274,-1.5534274068,0.6799336335
H,0,-1.817449334,0.0690851113,0.2148863316
H,0,-2.8215552585,-1.216098832,-1.7456901847
H,0,-1.1411340843,-0.7112239375,-1.9808064892
H,0,-2.1078559617,-3.518644359,-1.1779835397
H,0,-1.3478866464,-3.093927037,-2.7047038285
C,0,-0.2564271668,3.7688823242,1.5684035037
C,0,1.4492482915,1.9658193581,2.0445060024
C,0,1.6422556904,3.3633622216,-0.0514285396
H,0,2.359474932,4.0233329022,0.4510003082
H,0,2.174211557,2.5688466596,-0.5769288729
H,0,1.0835201606,3.9469826817,-0.7899079128
H,0,2.1617413552,2.625192611,2.553845563
H,0,0.7567309707,1.5603098214,2.7896005418
H,0,1.9846968509,1.1355874529,1.5812267503
H,0,0.3186896837,4.5219616205,2.1180778555
H,0,-0.8310181938,4.2718024736,0.7850546815
H,0,-0.9611201977,3.2958035355,2.258844748

TS addition of t-BuOO^{-} to cyclohexenone – boat conformation – PCM toluene

E(RB+HF-LYP) = -617.132417329

Zero-point correction=	0.252024 (Hartree/Particle)
Thermal correction to Energy=	0.266662
Thermal correction to Enthalpy=	0.267606
Thermal correction to Gibbs Free Energy=	0.209674
Sum of electronic and zero-point Energies=	-616.880394
Sum of electronic and thermal Energies=	-616.865756
Sum of electronic and thermal Enthalpies=	-616.864811
Sum of electronic and thermal Free Energies=	-616.922744

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.333	54.554	121.928

C,0,2.1927384778,1.5195945634,-0.1084954738
C,0,3.5196645868,0.8716724733,-0.5186943352
C,0,3.515498222,-0.6456895799,-0.3582962144
C,0,2.2297912604,-1.31609614,-0.4525696088
C,0,1.0729111214,-0.6444553203,-0.6768646679
C,0,1.0065778597,0.845690396,-0.8057662794
O,0,4.5786553561,-1.2576862988,-0.206883479
O,0,-0.8987214257,-0.5449159761,1.2376214297
O,0,-1.7479967043,0.583457369,0.8289100268
C,0,-3.0190378947,0.1338461031,0.3556847028
C,0,-3.783145031,-0.5763295438,1.4840909201
C,0,-3.7439807891,1.4199972059,-0.061124105
C,0,-2.8544226459,-0.8041413698,-0.8519821972
H,0,2.2407402642,-2.3981663323,-0.3527023813
H,0,0.1412573427,-1.1836526832,-0.781408107
H,0,0.9990126365,1.1084709237,-1.8769432306
H,0,0.0536419454,1.1744101287,-0.3835767035
H,0,2.2109882292,2.5932209712,-0.3246837552
H,0,2.0560214465,1.4122003082,0.9731446117
H,0,3.7254378138,1.0729037886,-1.5806343503
H,0,4.3689306066,1.2678898219,0.0450767276
H,0,-4.7484148709,-0.960659183,1.1358715719
H,0,-3.1725177644,-1.4014626175,1.8539887174
H,0,-3.9606276278,0.1164410792,2.3125764136
H,0,-3.8269503576,-1.1430515265,-1.2257747853
H,0,-2.3313256089,-0.2888551952,-1.6636506196
H,0,-2.2625321343,-1.6703517723,-0.5527211271
H,0,-4.7530222484,1.1983651464,-0.4234235634
H,0,-3.8228854918,2.1028852484,0.7896441951
H,0,-3.1928229931,1.9280384124,-0.8578638808

TS addition of t-BuOO$^-$ to cyclohexenone solvated HNMe$_3^+$ – chair conformation

E(RB+HF-LYP) = -792.157626655

Zero-point correction= 0.391038 (Hartree/Particle)
Thermal correction to Energy= 0.411666
Thermal correction to Enthalpy= 0.412610
Thermal correction to Gibbs Free Energy= 0.342363
Sum of electronic and zero-point Energies= -791.766589
Sum of electronic and thermal Energies= -791.745961
Sum of electronic and thermal Enthalpies= -791.745017
Sum of electronic and thermal Free Energies= -791.815264

E (Thermal) CV S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	258.324	77.624	147.847

C,0,2.4732090423,0.2578483446,-1.2135177604
C,0,1.2608351757,-0.4285052087,-1.389421532
C,0,0.715749841,-1.3305317859,-0.4178572948
C,0,1.6665870703,-1.8526130481,0.6612453662
C,0,3.1333603305,-1.7388488513,0.2339119876
C,0,3.4500716067,-0.2964064798,-0.167257301
O,0,-0.4094453968,-0.5143626334,0.5610313311
O,0,-1.7055802947,-0.476461417,-0.0989668007
C,0,-2.6792700992,-1.2741417863,0.6285606417
C,0,-2.2606596522,-2.7464505272,0.6707735067
O,0,2.8157143252,1.2920089094,-1.8511697496
C,0,-2.8668131903,-0.7148421529,2.0428706211
C,0,-3.9453365963,-1.0915285877,-0.2137284774
H,0,0.6483069217,-0.1678357736,-2.2472558006
H,0,0.027094233,-2.0748894911,-0.8100798674
H,0,1.5194765979,-1.2618686333,1.5738031393
H,0,1.4064048305,-2.882909339,0.9207507686
H,0,3.7864929734,-2.0716228016,1.0485916722
H,0,3.3203006502,-2.4003385707,-0.6185825529
H,0,3.4296242155,0.3526279432,0.7209031943
H,0,4.4546540195,-0.2002330497,-0.5888582052
H,0,-3.6087377452,-1.3010751405,2.5920179287
H,0,-1.9237693664,-0.7496997087,2.5903341494
H,0,-3.2144056971,0.3213383499,2.006129944
H,0,-3.02937321,-3.3415613986,1.1718402353
H,0,-2.1290357165,-3.1396676607,-0.3399798838
H,0,-1.3255320441,-2.8663872319,1.2192109891
H,0,-4.7748001578,-1.6448295623,0.2338280561
H,0,-4.2281569052,-0.0372798416,-0.2695914913
H,0,-3.7896663729,-1.4625142836,-1.2291699712
H,0,0.0000205114,1.174321761,0.0553952045
N,0,-0.0400221102,2.2260937931,-0.0306549751
C,0,1.196786375,2.7824168363,0.5994604705
C,0,-0.0995879918,2.5791338985,-1.4851888602
C,0,-1.2668739017,2.6531722009,0.6987178718
H,0,-0.220937311,3.6608789053,-1.5697328466
H,0,0.8336694595,2.2520520033,-1.9517795452
H,0,-0.9527510166,2.0678010218,-1.9274226006
H,0,-1.3551815681,3.7389762033,0.645190254
H,0,-2.126296807,2.1716876604,0.2389169473
H,0,-1.188348351,2.3335415883,1.7366965478

H,0,1.114344437,3.8701343021,0.6275702623
H,0,1.2797081018,2.3903039293,1.6125810927
H,0,2.0531929591,2.4846962807,-0.0052964802

TS addition of t-BuOO$^-$ to cyclohexenone solvated HNMe$_3^+$ – boat conformation

E(RB+HF-LYP) = -792.158698043

Zero-point correction= 0.389575 (Hartree/Particle)
Thermal correction to Energy= 0.410536
Thermal correction to Enthalpy= 0.411481
Thermal correction to Gibbs Free Energy= 0.340531
Sum of electronic and zero-point Energies= -791.769123
Sum of electronic and thermal Energies= -791.748162
Sum of electronic and thermal Enthalpies= -791.747217
Sum of electronic and thermal Free Energies= -791.818168

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.615	78.264	149.327

C,0,-0.2344543639,-1.6417243369,0.6172851444
C,0,-0.1168587891,-2.5007787535,-0.6339883888
C,0,1.1426914434,-2.1712474397,-1.4380090983
C,0,2.4028361915,-2.2198899148,-0.5640747191
C,0,2.2826790632,-1.4657511336,0.7650902094
C,0,0.9978130702,-1.4067762334,1.375797298
O,0,3.3122039844,-0.9762063024,1.2775871989
O,0,-0.3789668505,-0.2162529839,0.3191021219
O,0,-1.6514291293,0.3716726854,-0.8324493538
C,0,-2.9188214282,0.5588298261,-0.2391155418
C,0,-3.5843163111,-0.778523639,0.1348438094
C,0,-2.8484185721,1.475654417,0.9950148369
C,0,-3.7467454216,1.2423510483,-1.3520387795
N,0,1.3562785577,1.7833838584,0.0277291672
C,0,2.0135623372,2.0365059198,1.3460223825
C,0,0.4437562818,2.8913372537,-0.3732113388
C,0,2.3677612813,1.5039570657,-1.0324555097
H,0,0.9277500431,-1.0201280097,2.385516762
H,0,-1.0807809395,-1.955884509,1.2322501642
H,0,-0.0981210496,-3.5502502367,-0.3143262915
H,0,-1.0095577258,-2.3580040896,-1.2476721879
H,0,1.2425918943,-2.8625182086,-2.2810713038
H,0,1.026058587,-1.1731138455,-1.871694609
H,0,2.6350309704,-3.2614565281,-0.3039810527

H,0,3.2803211377,-1.8392682136,-1.0943326775
H,0,-4.7631482482,1.4485215053,-1.0005825852
H,0,-3.2827840147,2.1866555846,-1.647030376
H,0,-3.8054116288,0.5975720183,-2.2316388503
H,0,-3.8336581012,1.595280874,1.4558552878
H,0,-2.1678829423,1.0502634259,1.7355740653
H,0,-2.4864363889,2.4693744716,0.7156146875
H,0,-4.6270369187,-0.6304332891,0.4330099641
H,0,-3.5627304668,-1.4592916308,-0.719622508
H,0,-3.0648733766,-1.2544173893,0.9688908487
H,0,0.7439575313,0.9113541845,0.1366157067
H,0,1.0336027615,3.7824152124,-0.5953340271
H,0,-0.1312788494,2.5673114728,-1.2384989152
H,0,-0.2427984485,3.0903325034,0.4463514818
H,0,2.6221384972,1.1676397012,1.6037771589
H,0,2.6302921232,2.934002044,1.2684136128
H,0,1.2371831253,2.1827978689,2.0953955792
H,0,3.0159470437,0.6985277036,-0.6932304798
H,0,1.8477420566,1.2157244907,-1.9447122946
H,0,2.9565606915,2.4059342088,-1.2085228964

TS addition of t-BuOO$^-$ to cyclohexenone solvated HNMe$_3^+$ – chair conformation-PCM toluene

E(RB+HF-LYP) = -792.167859304

Zero-point correction=	0.390166 (Hartree/Particle)
Thermal correction to Energy=	0.411084
Thermal correction to Enthalpy=	0.412029
Thermal correction to Gibbs Free Energy=	0.340428
Sum of electronic and zero-point Energies=	-791.777693
Sum of electronic and thermal Energies=	-791.756775
Sum of electronic and thermal Enthalpies=	-791.755831
Sum of electronic and thermal Free Energies=	-791.827431

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.959	77.925	150.696

C,0,2.6751757888,-0.1376195382,-0.9619797873
C,0,1.3909162092,-0.5816669129,-1.3188602951
C,0,0.5795514228,-1.4003616551,-0.4780126378
C,0,1.2620809825,-2.1255211124,0.6804072285
C,0,2.7752351156,-2.2446078451,0.4726141295
C,0,3.3773455186,-0.8659712548,0.1906994266

O,0,-0.5364714515,-0.4050832466,0.4269090697
O,0,-1.7463146701,-0.1764171165,-0.345058712
C,0,-2.8870689453,-0.8458633431,0.2628810617
C,0,-2.6806776928,-2.3627930592,0.2880036396
O,0,3.2906414142,0.8095250164,-1.5284849551
C,0,-3.1300539689,-0.2997114061,1.673311269
C,0,-4.0294069758,-0.4654040521,-0.6834332409
H,0,0.9489068471,-0.1764574273,-2.2248582596
H,0,-0.1953914409,-1.9691447117,-0.984309574
H,0,1.0757395981,-1.5641823231,1.6037458053
H,0,0.8048145946,-3.1087483855,0.8246381493
H,0,3.2384727118,-2.6994280439,1.3554920086
H,0,2.9800669256,-2.9080120256,-0.3748091381
H,0,3.3199565877,-0.2404896151,1.0936587508
H,0,4.4386178397,-0.9306513871,-0.0673575315
H,0,-3.993031487,-0.7920567865,2.1300034005
H,0,-2.2571498405,-0.4776712654,2.3032719831
H,0,-3.3300901078,0.7747193385,1.6429829402
H,0,-3.5686320006,-2.8557139543,0.6937568737
H,0,-2.507809726,-2.7464267562,-0.720478233
H,0,-1.828162462,-2.6262789864,0.9154393594
H,0,-4.9654917029,-0.9091671077,-0.3349259051
H,0,-4.1577594972,0.6192702439,-0.7221211053
H,0,-3.8302494674,-0.8279673011,-1.6945053995
H,0,0.0523891175,1.1690064014,0.1942942266
N,0,0.2260183124,2.2201792598,0.1587836115
C,0,1.4604852488,2.5049795021,0.9496263084
C,0,0.4006663446,2.628219368,-1.2696408635
C,0,-0.9724049942,2.8604514684,0.7721666168
H,0,0.4871299373,3.7155887531,-1.3115120512
H,0,1.3043569515,2.1566820562,-1.6567541076
H,0,-0.4710902813,2.2980546781,-1.8320268032
H,0,-0.8371310029,3.9428697106,0.7796119089
H,0,-1.847741162,2.5889268108,0.1868784045
H,0,-1.0868040368,2.4915003342,1.7903986922
H,0,1.5971387035,3.5856060949,1.0143393597
H,0,1.3423801528,2.0863660836,1.9487429555
H,0,2.3105293968,2.0535725706,0.4412976543

TS addition of t-BuOO$^-$ to cyclohexenone solvated HNMe$_3^+$ – boat conformation-PCM toluene

E(RB+HF-LYP) = -792.160667807

Zero-point correction= 0.390104 (Hartree/Particle)

Thermal correction to Energy= 0.410816
Thermal correction to Enthalpy= 0.411761
Thermal correction to Gibbs Free Energy= 0.341588
Sum of electronic and zero-point Energies= -791.770564
Sum of electronic and thermal Energies= -791.749851
Sum of electronic and thermal Enthalpies= -791.748907
Sum of electronic and thermal Free Energies= -791.819080

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.791	77.966	147.691

C,0,-0.2361308205,-1.5278657702,-0.8210088269
C,0,-0.2799888044,-2.4581634733,0.3708891137
C,0,-1.3274044058,-2.0273665051,1.3997781002
C,0,-2.6924435517,-1.7877204073,0.7448284713
C,0,-2.6330839915,-0.9116892289,-0.5153773064
C,0,-1.4618357142,-0.9765978571,-1.3016042111
O,0,-3.6342287924,-0.2052552682,-0.7931836789
O,0,0.5806509684,-0.1146102372,-0.3141914295
O,0,1.7383955279,-0.2156359022,0.6090544519
C,0,3.0052117043,-0.1123184069,-0.0841906072
C,0,4.0122576641,-0.2354175049,1.0660624309
C,0,3.1887085322,-1.2554518778,-1.0879797658
C,0,3.1345776607,1.2462761143,-0.7813994646
N,0,-0.9853270199,2.0326216626,0.2193562087
C,0,0.0746031889,3.0242651368,0.5491097089
C,0,-1.7484740946,2.4163141369,-1.0092176127
C,0,-1.9079143582,1.8206751698,1.3736306309
H,0,-1.4786412076,-0.4935473423,-2.2735403646
H,0,0.4654714423,-1.8528965651,-1.585110365
H,0,-0.5204729734,-3.4590463938,-0.0114084243
H,0,0.7090354071,-2.5189830759,0.8315986608
H,0,-1.408917811,-2.7787222714,2.1927129983
H,0,-0.9795840553,-1.1075091166,1.8828095715
H,0,-3.1351032277,-2.745634054,0.4411384259
H,0,-3.4008703857,-1.3337118977,1.4438794554
H,0,4.0986657279,1.3270454589,-1.2913072855
H,0,2.3444721221,1.364403915,-1.5254001774
H,0,3.0674477777,2.0598409892,-0.0539936942
H,0,4.202824449,-1.2399423378,-1.4976370383
H,0,3.0294310603,-2.2216255202,-0.6038386756
H,0,2.4883067862,-1.1591306597,-1.9187159443
H,0,5.0330863162,-0.1516245273,0.6836616652

H,0,3.8538191671,0.554448757,1.8042409013
H,0,3.9076316733,-1.2003762632,1.5669263658
H,0,-0.4729213082,1.1085894888,0.0171105859
H,0,0.6409992722,2.6627446353,1.4058928517
H,0,0.741314264,3.1240488574,-0.3047935621
H,0,-0.3865603202,3.9862211585,0.7780946534
H,0,-1.3398420972,1.4092622159,2.2069253507
H,0,-2.3437427736,2.7803227079,1.6578735793
H,0,-2.6939937032,1.1335165745,1.0672262743
H,0,-2.214642909,3.3891429767,-0.8396054275
H,0,-1.0512575437,2.4771654029,-1.8434590896
H,0,-2.5057056964,1.6520193512,-1.2013334673

Intermediate t-butyl peroxy enolate – boat conformation

E(RB+HF-LYP) = -617.101546121

Zero-point correction= 0.253537 (Hartree/Particle)
Thermal correction to Energy= 0.267930
Thermal correction to Enthalpy= 0.268874
Thermal correction to Gibbs Free Energy= 0.212163
Sum of electronic and zero-point Energies= -616.848009
Sum of electronic and thermal Energies= -616.833616
Sum of electronic and thermal Enthalpies= -616.832672
Sum of electronic and thermal Free Energies= -616.889383

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	168.129	55.016	119.359

C,0,-1.875224564,-1.3658733996,-1.4518631745
C,0,-1.1493521971,-2.6877572593,-1.7231624199
C,0,0.2381875117,-2.8192701633,-1.0590867555
C,0,0.5384306351,-1.9550296979,0.001354944
C,0,-0.3417580939,-0.8786986918,0.4829739675
C,0,-1.7986598996,-0.9979472022,0.0314398377
O,0,0.9792999487,-3.7457296581,-1.487196726
O,0,0.2516367054,0.3586090007,-0.0897806348
O,0,-0.405989793,1.5926807312,0.5470956295
C,0,0.6336280599,2.4853139259,0.9495765381
H,0,1.5098680015,-2.0665259926,0.4749995756
H,0,-0.2962979601,-0.7346663973,1.5719004745
H,0,-2.283151458,-1.7762700544,0.6369434467
H,0,-2.3168446328,-0.0542906913,0.2310093815
H,0,-2.9224201558,-1.4220206371,-1.7805335087

H,0,-1.4022965701,-0.5628037912,-2.0273551948
H,0,-1.7534942575,-3.5320575605,-1.3596796388
H,0,-1.0107562279,-2.8533276324,-2.7968675574
C,0,-0.1344043724,3.677379866,1.5392805606
C,0,1.5302423518,1.837796673,2.0158826875
C,0,1.462141258,2.9247772463,-0.2680249747
H,0,0.5628030929,4.4476663901,1.8852296695
H,0,-0.793439968,4.1161193169,0.7855512453
H,0,-0.7462429789,3.3552786801,2.3861096833
H,0,2.3104951199,2.5326700786,2.3453888599
H,0,0.9336958071,1.5464634836,2.8850444499
H,0,2.0025143169,0.9438928161,1.6066037108
H,0,2.2364860179,3.6431166576,0.0235332308
H,0,1.9368073131,2.0557280507,-0.7250403435
H,0,0.8133155151,3.3923989106,-1.0140108973

Intermediate t-butyl peroxy enolate – boat conformation – PCM toluene

E(RB+HF-LYP) = -617.150164081

Zero-point correction= 0.254385 (Hartree/Particle)
Thermal correction to Energy= 0.268517
Thermal correction to Enthalpy= 0.269461
Thermal correction to Gibbs Free Energy= 0.213768
Sum of electronic and zero-point Energies= -616.895779
Sum of electronic and thermal Energies= -616.881647
Sum of electronic and thermal Enthalpies= -616.880703
Sum of electronic and thermal Free Energies= -616.936396

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	168.497	54.465	117.217

C,0,2.1640280633,1.6548978002,0.4684888465
C,0,3.3252287756,0.6600206889,0.3729459261
C,0,2.9158116835,-0.7830954584,0.031067428
C,0,1.6510890688,-1.0003602269,-0.5043352181
C,0,0.6391061429,0.052160316,-0.732908217
C,0,1.1992188912,1.4752762376,-0.7044465852
O,0,3.8032618095,-1.6789108233,0.2217109131
O,0,-0.3551295251,-0.1152003479,0.3604053786
O,0,-1.564627772,0.7177035834,0.0575827239
C,0,-2.730530785,-0.1266424673,0.0920733533
H,0,1.3774072589,-2.0236227502,-0.7511622312
H,0,0.0671848847,-0.1045984684,-1.6568920642

H,0,1.7237789579,1.6570006318,-1.6520849378
H,0,0.3705338578,2.1877083849,-0.6477482666
H,0,2.5402141029,2.685371573,0.5038517802
H,0,1.6116147672,1.4855033377,1.3992987688
H,0,4.035615759,0.982580837,-0.4022455531
H,0,3.8942893952,0.6255251692,1.3082974536
C,0,-3.8704106299,0.8548183136,-0.2073517155
C,0,-2.6508367733,-1.2142565733,-0.9867536505
C,0,-2.8962942405,-0.745171279,1.4864339589
H,0,-4.8277796614,0.3258518685,-0.2250012701
H,0,-3.91862386,1.6335529905,0.5580250104
H,0,-3.7202043733,1.3327577597,-1.1788122085
H,0,-3.5522513785,-1.834950413,-0.9739747904
H,0,-2.5558868484,-0.7634941927,-1.978315903
H,0,-1.7854909278,-1.8547830191,-0.811199275
H,0,-3.8063713814,-1.3515407458,1.5349275445
H,0,-2.0395981861,-1.3784863165,1.7205249074
H,0,-2.9609296461,0.0409999476,2.2436341518

Intermediate t-butyl peroxy enolate – chair conformation

E(RB+HF-LYP) = -617.093994188

Zero-point correction= 0.253430 (Hartree/Particle)
Thermal correction to Energy= 0.267950
Thermal correction to Enthalpy= 0.268894
Thermal correction to Gibbs Free Energy= 0.211747
Sum of electronic and zero-point Energies= -616.840564
Sum of electronic and thermal Energies= -616.826044
Sum of electronic and thermal Enthalpies= -616.825100
Sum of electronic and thermal Free Energies= -616.882247

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	168.141	55.138	120.277

C,0,0.6481784528,1.4136706411,-0.2987748684
C,0,2.021388348,2.0850756502,-0.3547076915
C,0,3.1114019358,1.0210482568,-0.5060485384
C,0,3.0319614143,-0.0843817318,0.5700448484
C,0,1.8044281811,-0.2623805546,1.2146378257
C,0,0.5397466234,0.430329358,0.8776564341
O,0,4.1022148265,-0.7062552575,0.8222067076
O,0,-0.3742303846,-0.6781702275,0.5433042426
O,0,-1.786209788,-0.0346202274,0.5267625107

C,0,-2.6232284449,-0.6511368462,-0.4456288348
H,0,1.7728312889,-0.9604747919,2.0460332538
H,0,0.0646630632,0.9200434906,1.7423654549
H,0,0.5034993726,0.8429387501,-1.2220495857
H,0,-0.1584331748,2.1522017589,-0.2470177169
H,0,2.054687176,2.808125741,-1.1827325002
H,0,2.19461467,2.6539987895,0.5682124337
H,0,3.0399797493,0.5518075552,-1.4982343503
H,0,4.1142269302,1.4552035558,-0.4372057337
C,0,-3.8964722263,0.2097630796,-0.3881638764
C,0,-2.005771416,-0.6005233402,-1.8514408054
C,0,-2.9441648029,-2.0975544813,-0.0454254719
H,0,-4.6478643723,-0.1748178137,-1.0856215008
H,0,-4.3177072778,0.197866983,0.6204526028
H,0,-3.6680278093,1.2447908574,-0.6540888319
H,0,-2.6853977107,-1.0483499206,-2.5846940676
H,0,-1.8091921837,0.4338738495,-2.1436569365
H,0,-1.0609775535,-1.1452268758,-1.8646947012
H,0,-3.6701215848,-2.5470719054,-0.7319698719
H,0,-2.0334664899,-2.690854207,-0.06453531
H,0,-3.3523197166,-2.1251503066,0.9683555468

Intermediate t-butyl peroxy enolate – chair conformation – PCM toluene

E(RB+HF-LYP) = -617.145304636

Zero-point correction= 0.254192 (Hartree/Particle)
Thermal correction to Energy= 0.268490
Thermal correction to Enthalpy= 0.269435
Thermal correction to Gibbs Free Energy= 0.212789
Sum of electronic and zero-point Energies= -616.891113
Sum of electronic and thermal Energies= -616.876814
Sum of electronic and thermal Enthalpies= -616.875870
Sum of electronic and thermal Free Energies= -616.932516

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	168.480	54.502	119.221

C,0,-0.9550655025,1.342345598,-0.2345696242
C,0,-2.4354442654,1.7231980539,-0.2708699233
C,0,-3.2543505119,0.7160712681,0.540684782
C,0,-2.9799623773,-0.7487306591,0.1544954751
C,0,-1.7966102904,-1.034213282,-0.511250771
C,0,-0.7178779201,-0.0583928576,-0.8164834507

O,0,-3.894605405,-1.5920764007,0.445900799
O,0,0.4934354018,-0.6524765515,-0.2307507292
O,0,1.6690748025,0.1163708367,-0.7631356129
C,0,2.7625094934,-0.0418088454,0.154492095
H,0,-1.6482032987,-2.0509669783,-0.8672391402
H,0,-0.4954950715,0.0120203123,-1.8941473553
H,0,-0.6178288946,1.3277724545,0.8079180862
H,0,-0.3388174551,2.0772464276,-0.7611306296
H,0,-2.5736476282,2.7419607802,0.1149862018
H,0,-2.7912224297,1.7301169852,-1.3094712146
H,0,-3.0435798529,0.839495109,1.6127976594
H,0,-4.3296401009,0.8828647767,0.4164244225
C,0,3.8897454321,0.7450707294,-0.5265426704
C,0,2.4228146262,0.5703200888,1.5202792421
C,0,3.1409039946,-1.5230221497,0.2905452531
H,0,4.7971583002,0.7023194439,0.0825282464
H,0,4.1117019635,0.3248637245,-1.5106832587
H,0,3.6058554291,1.7929589402,-0.6526545471
H,0,3.2794768932,0.4947007865,2.1973657152
H,0,2.1613365431,1.6258419548,1.4082315323
H,0,1.5754170603,0.0503933853,1.9682885248
H,0,4.0185950632,-1.6362891405,0.9346508229
H,0,2.3143318033,-2.0886987421,0.7222382526
H,0,3.3713472083,-1.9461709622,-0.6909014198

TS for formation of cyclohexenone oxide – boat conformation

E(RB+HF-LYP) = -617.100637964

Zero-point correction= 0.252442 (Hartree/Particle)
Thermal correction to Energy= 0.266567
Thermal correction to Enthalpy= 0.267512
Thermal correction to Gibbs Free Energy= 0.210842
Sum of electronic and zero-point Energies= -616.848196
Sum of electronic and thermal Energies= -616.834071
Sum of electronic and thermal Enthalpies= -616.833126
Sum of electronic and thermal Free Energies= -616.889795

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.274	53.614	119.270

C,0,-2.1867497306,-1.0717564048,-0.9723928623
C,0,-1.7376765688,-2.5255678936,-1.1624355026
C,0,-0.4007020885,-2.8956387045,-0.4961390899

C,0,0.07775711,-2.0588889166,0.5395366591
C,0,-0.5561946329,-0.7742971604,0.9190525661
C,0,-2.0141451207,-0.6201736287,0.480261423
O,0,0.1472760472,-3.9646562055,-0.8497237068
O,0,0.3256874318,0.0026009027,0.1388104153
O,0,-0.0286072525,1.7358996896,0.467745684
C,0,1.1709509578,2.4299925587,0.2734548532
H,0,1.0124907114,-2.3312065642,1.0159937548
H,0,-0.4447208283,-0.5199405335,1.9832569928
H,0,-2.644677897,-1.2249184195,1.1474978633
H,0,-2.3043787381,0.4279051001,0.5981826756
H,0,-3.2302746823,-0.9506344747,-1.2915196357
H,0,-1.5798409418,-0.4152571781,-1.6028660943
H,0,-2.4873931228,-3.21122033,-0.7411203313
H,0,-1.6541084831,-2.7833282468,-2.2231935943
C,0,0.8218132346,3.9143552832,0.5227743602
C,0,2.2482719048,1.9763260779,1.2811117483
C,0,1.686236978,2.2558960645,-1.1705281605
H,0,1.7047768449,4.5526871797,0.3951110226
H,0,0.0488066894,4.2404096538,-0.1784410019
H,0,0.4397760392,4.0445193099,1.5391618022
H,0,2.5998240608,2.8369809573,-1.3468026678
H,0,1.892007331,1.2017095175,-1.3621433493
H,0,0.9191513858,2.5854414556,-1.8777415684
H,0,3.183046616,2.5370383673,1.1578308976
H,0,1.88465787,2.124655558,2.3027414977
H,0,2.4486350708,0.9129198993,1.1412166294

TS for formation of cyclohexenone oxide – chair conformation

E(RB+HF-LYP) = -617.096207800

Zero-point correction=	0.252592 (Hartree/Particle)
Thermal correction to Energy=	0.266735
Thermal correction to Enthalpy=	0.267680
Thermal correction to Gibbs Free Energy=	0.210855
Sum of electronic and zero-point Energies=	-616.843616
Sum of electronic and thermal Energies=	-616.829472
Sum of electronic and thermal Enthalpies=	-616.828528
Sum of electronic and thermal Free Energies=	-616.885353

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.379	53.565	119.599

C,0,-0.7301978973,1.064554322,-1.7126265893
C,0,-2.0776936984,1.7778071078,-1.5253889206
C,0,-2.6444156256,1.5614209443,-0.1171269752
C,0,-2.8598262697,0.0645477466,0.1690383554
C,0,-1.9044830259,-0.8054021304,-0.3918730679
C,0,-0.657803397,-0.3180688265,-1.0201420847
O,0,-3.8705858437,-0.2811405006,0.8280682866
O,0,0.1532615415,-0.2656647633,0.1691119149
O,0,1.727380055,0.1232733227,-0.2428910054
C,0,2.5644488259,-0.5541068391,0.6702704751
C,0,2.273671598,-0.107973349,2.1154243052
C,0,2.411882559,-2.0807270691,0.5352367926
C,0,3.9883345436,-0.1290103866,0.263262578
H,0,-1.9995605449,-1.8680318612,-0.1947426798
H,0,-0.2075215931,-1.0584111338,-1.6951511875
H,0,0.0816441025,1.6714858789,-1.3018166897
H,0,-0.5200931004,0.9460600664,-2.7824909208
H,0,-1.9660626581,2.8488489314,-1.744880251
H,0,-2.8035748323,1.383712744,-2.2473891911
H,0,-1.9580563147,1.9746407259,0.6334254105
H,0,-3.6103349424,2.0600287114,0.0086178559
H,0,3.0890809491,-2.6114194416,1.214650402
H,0,1.3837786629,-2.3660975017,0.7620807538
H,0,2.6359812946,-2.3883275967,-0.4906642769
H,0,2.9540794294,-0.5921491099,2.8258418275
H,0,2.3920845884,0.97621084,2.2000155765
H,0,1.2454974372,-0.3583923729,2.3794962886
H,0,4.7337200349,-0.6017459326,0.9132617052
H,0,4.189792288,-0.4226802519,-0.7705649835
H,0,4.0955935003,0.9562737149,0.3395475803

TS for formation of cyclohexenone oxide – boat conformation – PCM toluene

E(RB+HF-LYP) = -617.142856576

Zero-point correction= 0.252203 (Hartree/Particle)
Thermal correction to Energy= 0.266407
Thermal correction to Enthalpy= 0.267351
Thermal correction to Gibbs Free Energy= 0.210829
Sum of electronic and zero-point Energies= -616.890653
Sum of electronic and thermal Energies= -616.876450
Sum of electronic and thermal Enthalpies= -616.875506
Sum of electronic and thermal Free Energies= -616.932027

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	167.173	53.770	118.960

C,0,-2.927350823,0.4544742814,0.8946549817
C,0,-2.786173018,-0.7271386676,-0.0692282845
C,0,-1.8280553679,-0.6335066004,-1.1161256287
C,0,-0.856851405,0.48369483,-1.2217918453
C,0,-1.2271088195,1.7580676848,-0.4665708459
C,0,-1.736691321,1.4218241421,0.9375119955
O,0,-3.5796053556,-1.6888821793,0.0480227748
O,0,0.031138506,-0.3433006414,-0.5411884781
O,0,1.7440540832,0.6257241472,-0.5189173287
C,0,2.6296949426,-0.1682056099,0.2020990057
C,0,3.9831534368,0.5847619643,0.2319495989
C,0,2.1415419443,-0.3768487233,1.6547750579
C,0,2.8342614994,-1.5411779391,-0.47828195
H,0,-1.76267702,-1.4514691217,-1.8235797656
H,0,-0.5240952215,0.7020795669,-2.245667322
H,0,-0.3396924572,2.3939006861,-0.4092446612
H,0,-1.9947889684,2.2956162142,-1.0405975435
H,0,-0.9146497337,0.9642661186,1.4936168655
H,0,-2.0189126644,2.336456702,1.4718865234
H,0,-3.1468288872,0.0472629417,1.8867280389
H,0,-3.8358501787,0.988083188,0.5793540447
H,0,3.5556992495,-2.1657332773,0.0629437573
H,0,1.8790632692,-2.0666852935,-0.5323969916
H,0,3.1984297932,-1.3947366482,-1.5001478396
H,0,2.8488627079,-0.973388788,2.2439907931
H,0,2.0146712682,0.5944278409,2.1432198306
H,0,1.1734654552,-0.8809506268,1.6453597615
H,0,4.7417957201,0.0202824297,0.7880238229
H,0,4.3449703185,0.7446540435,-0.7878700493
H,0,3.8573130685,1.5619312376,0.70709248

TS for formation of cyclohexenone oxide – chair conformation – PCM toluene

E(RB+HF-LYP) = -617.139286938

Zero-point correction= 0.252207 (Hartree/Particle)
Thermal correction to Energy= 0.266490
Thermal correction to Enthalpy= 0.267434
Thermal correction to Gibbs Free Energy= 0.210462
Sum of electronic and zero-point Energies= -616.887080
Sum of electronic and thermal Energies= -616.872797
Sum of electronic and thermal Enthalpies= -616.871853

Sum of electronic and thermal Free Energies= -616.928825

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	167.225	53.801	119.909

C,0,-0.9826389058,1.6872432137,-0.95655016
C,0,-2.222815158,1.9433186105,-0.0861806565
C,0,-2.4833385317,0.7976831909,0.9025044558
C,0,-2.6898783795,-0.5272086965,0.1670141917
C,0,-1.8873119379,-0.734206891,-0.9839008784
C,0,-0.7969332013,0.2079682424,-1.347140201
O,0,-3.5596512746,-1.3338560643,0.5737921065
O,0,0.0464984005,-0.5028655804,-0.4847392884
O,0,1.7815494966,0.2609731466,-0.6442242472
C,0,2.5669793754,-0.3362837445,0.3432798847
C,0,2.0210998336,-0.028679255,1.755219209
C,0,2.6581749775,-1.8645288255,0.1387587868
C,0,3.9796829435,0.2782126104,0.2017459538
H,0,-1.9686907322,-1.67506385,-1.5159222853
H,0,-0.4667308564,0.1101320812,-2.3898885344
H,0,-0.0673525925,1.9746748277,-0.4327722227
H,0,-1.0372396975,2.2989884426,-1.8644422248
H,0,-2.1174347921,2.8942906208,0.4498474017
H,0,-3.1065381094,2.0450230313,-0.7283067347
H,0,-1.633466976,0.6914123028,1.5867063864
H,0,-3.3752026384,0.9854776933,1.507265302
H,0,3.3008555254,-2.3385178441,0.8903831349
H,0,1.6603905809,-2.3024922844,0.197397005
H,0,3.0659403618,-2.0803257431,-0.8537918509
H,0,2.65313512,-0.4623345916,2.5394496948
H,0,1.9746119425,1.0544320913,1.9058897142
H,0,1.0109310264,-0.4295623594,1.8522199364
H,0,4.6692591648,-0.1416488152,0.9439470258
H,0,4.378118016,0.0783627259,-0.7970083211
H,0,3.9341155825,1.3620289236,0.3418944897

TS for formation of cyclohexenone oxide solvated $HNMe_3^+$ – chair conformation

E(RB+HF-LYP) = -792.149110819

Zero-point correction= 0.388919 (Hartree/Particle)
Thermal correction to Energy= 0.410105
Thermal correction to Enthalpy= 0.411050
Thermal correction to Gibbs Free Energy= 0.338871

Sum of electronic and zero-point Energies= -791.760192
Sum of electronic and thermal Energies= -791.739005
Sum of electronic and thermal Enthalpies= -791.738061
Sum of electronic and thermal Free Energies= -791.810239

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.345	78.514	151.912

C,0,1.8664800107,-0.3646474274,-0.9696628928
C,0,0.6245112412,-1.1205767878,-1.0470127648
C,0,0.6333480516,-2.4850987783,-0.3281293591
C,0,2.0301568963,-2.9120721035,0.1423470246
C,0,2.7211704498,-1.7826571965,0.9127097421
C,0,2.8163964872,-0.5085633409,0.0723400867
O,0,-0.2218231593,-0.1120733829,-0.2948881519
O,0,-1.8754571463,0.1213860921,-0.6359862428
C,0,-2.8025530286,-0.6465041257,0.127945465
C,0,-2.4539505668,-0.6466228055,1.6224407349
O,0,3.7164475822,0.3262246584,0.3079767837
C,0,-4.1332191503,0.1026654652,-0.1018526616
C,0,-2.9297202529,-2.0774900179,-0.4169120915
N,0,0.3352791994,2.4517625694,0.0149465634
C,0,0.5968245682,3.0562671628,-1.3198014561
C,0,-0.917247399,2.9920625121,0.6113527964
C,0,1.5069960964,2.6076115245,0.9302502804
H,0,2.0118688431,0.4558514728,-1.6647860782
H,0,0.1808332162,-1.1731366624,-2.0439827248
H,0,-0.0221353939,-2.4153952654,0.5432009453
H,0,0.2078008152,-3.2507912353,-0.9836178391
H,0,1.9493712126,-3.8124588496,0.761443943
H,0,2.6451527031,-3.1781376925,-0.7244267821
H,0,2.171061514,-1.558178451,1.8364311721
H,0,3.7375992906,-2.0526675841,1.2108926736
H,0,-3.1953130336,-1.2139775174,2.1925380417
H,0,-1.472090009,-1.0906181402,1.7896936369
H,0,-2.4358308024,0.3750004988,2.0121499236
H,0,-3.7439686445,-2.6144618932,0.0797135542
H,0,-3.1390100835,-2.0486755489,-1.4891269532
H,0,-2.0122704725,-2.6439288453,-0.2627316012
H,0,-4.9506891058,-0.4140946978,0.4105763153
H,0,-4.0737978385,1.1233394026,0.2833243077
H,0,-4.3666883025,0.1464040248,-1.1680291157
H,0,0.1800423855,1.3934883236,-0.1438404655

H,0,-1.7468872731,2.7545190635,-0.0509786014
H,0,-1.0822680493,2.5091463191,1.5726497233
H,0,-0.8188710103,4.070673859,0.7487585802
H,0,-0.2325730995,2.8125143935,-1.9825539891
H,0,0.6913340353,4.1386136074,-1.2159367828
H,0,1.5203381452,2.6415290798,-1.7176693497
H,0,1.7070693069,3.6713545239,1.0745385573
H,0,1.2593347984,2.1456588201,1.8849819404
H,0,2.3751338214,2.0955475816,0.5092524864

TS for formation of cyclohexenone oxide solvated $HNMe_3^+$ – boat conformation

E(RB+HF-LYP) = -792.158698043

Zero-point correction= 0.389575 (Hartree/Particle)
Thermal correction to Energy= 0.410536
Thermal correction to Enthalpy= 0.411481
Thermal correction to Gibbs Free Energy= 0.340531
Sum of electronic and zero-point Energies= -791.769123
Sum of electronic and thermal Energies= -791.748162
Sum of electronic and thermal Enthalpies= -791.747217
Sum of electronic and thermal Free Energies= -791.818168

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.615	78.264	149.327

C,0,-0.2344543639,-1.6417243369,0.6172851444
C,0,-0.1168587891,-2.5007787535,-0.6339883888
C,0,1.1426914434,-2.1712474397,-1.4380090983
C,0,2.4028361915,-2.2198899148,-0.5640747191
C,0,2.2826790632,-1.4657511336,0.7650902094
C,0,0.9978130702,-1.4067762334,1.375797298
O,0,3.3122039844,-0.9762063024,1.2775871989
O,0,-0.3789668505,-0.2162529839,0.3191021219
O,0,-1.6514291293,0.3716726854,-0.8324493538
C,0,-2.9188214282,0.5588298261,-0.2391155418
C,0,-3.5843163111,-0.778523639,0.1348438094
C,0,-2.8484185721,1.475654417,0.9950148369
C,0,-3.7467454216,1.2423510483,-1.3520387795
N,0,1.3562785577,1.7833838584,0.0277291672
C,0,2.0135623372,2.0365059198,1.3460223825
C,0,0.4437562818,2.8913372537,-0.3732113388
C,0,2.3677612813,1.5039570657,-1.0324555097
H,0,0.9277500431,-1.0201280097,2.385516762

H,0,-1.0807809395,-1.955884509,1.2322501642
H,0,-0.0981210496,-3.5502502367,-0.3143262915
H,0,-1.0095577258,-2.3580040896,-1.2476721879
H,0,1.2425918943,-2.8625182086,-2.2810713038
H,0,1.026058587,-1.1731138455,-1.871694609
H,0,2.6350309704,-3.2614565281,-0.3039810527
H,0,3.2803211377,-1.8392682136,-1.0943326775
H,0,-4.7631482482,1.4485215053,-1.0005825852
H,0,-3.2827840147,2.1866555846,-1.647030376
H,0,-3.8054116288,0.5975720183,-2.2316388503
H,0,-3.8336581012,1.595280874,1.4558552878
H,0,-2.1678829423,1.0502634259,1.7355740653
H,0,-2.4864363889,2.4693744716,0.7156146875
H,0,-4.6270369187,-0.6304332891,0.4330099641
H,0,-3.5627304668,-1.4592916308,-0.719622508
H,0,-3.0648733766,-1.2544173893,0.9688908487
H,0,0.7439575313,0.9113541845,0.1366157067
H,0,1.0336027615,3.7824152124,-0.5953340271
H,0,-0.1312788494,2.5673114728,-1.2384989152
H,0,-0.2427984485,3.0903325034,0.4463514818
H,0,2.6221384972,1.1676397012,1.6037771589
H,0,2.6302921232,2.934002044,1.2684136128
H,0,1.2371831253,2.1827978689,2.0953955792
H,0,3.0159470437,0.6985277036,-0.6932304798
H,0,1.8477420566,1.2157244907,-1.9447122946
H,0,2.9565606915,2.4059342088,-1.2085228964

TS for formation cyclohexenone oxide solvated $HNMe_3^+$ – chair conformation – PCM toluene

E(RB+HF-LYP) = -792.159199465

Zero-point correction=	0.388790 (Hartree/Particle)
Thermal correction to Energy=	0.410074
Thermal correction to Enthalpy=	0.411018
Thermal correction to Gibbs Free Energy=	0.338549
Sum of electronic and zero-point Energies=	-791.770409
Sum of electronic and thermal Energies=	-791.749126
Sum of electronic and thermal Enthalpies=	-791.748182
Sum of electronic and thermal Free Energies=	-791.820650

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	257.325	78.576	152.524

C,0,1.9368699625,-0.2346554739,-0.9287237105
C,0,0.7278373341,-1.0451010309,-1.0971203824
C,0,0.779155368,-2.4542866121,-0.4705695507
C,0,2.1639383886,-2.8297476365,0.0728936908
C,0,2.7455468889,-1.702104077,0.9329426604
C,0,2.8510987039,-0.4011493458,0.1387141314
O,0,-0.1321531587,-0.1221146801,-0.3198882567
O,0,-1.8545240474,-0.014200008,-0.6524424781
C,0,-2.7219241107,-0.8041999103,0.1517689404
C,0,-2.2947538093,-0.8138008761,1.6269364202
O,0,3.7414934471,0.4347789811,0.4233466453
C,0,-4.0856764641,-0.08952796,0.0127661347
C,0,-2.8487176934,-2.234775925,-0.3985080319
N,0,0.1249155083,2.5125626664,-0.0113457939
C,0,0.3690961541,3.1515170055,-1.3353170972
C,0,-1.1677569785,2.9696709664,0.5730601312
C,0,1.2685979874,2.7307768845,0.92632209
H,0,2.0697727059,0.6275005583,-1.5743349587
H,0,0.3341840293,-1.0583517436,-2.1174601362
H,0,0.0613455274,-2.4829705323,0.3516055423
H,0,0.449509962,-3.1964029743,-1.204045669
H,0,2.0937144047,-3.7591829857,0.6487087297
H,0,2.8477232111,-3.0252773042,-0.7608946831
H,0,2.1149132082,-1.5314960895,1.8155546111
H,0,3.746079089,-1.9458519756,1.3007053581
H,0,-3.0023213113,-1.391454632,2.2289785021
H,0,-1.3021872954,-1.250936269,1.7397732499
H,0,-2.2627829976,0.20458596,2.0236220465
H,0,-3.6107508886,-2.8003324809,0.1472476846
H,0,-3.1337169772,-2.2019065662,-1.4533691596
H,0,-1.9064114954,-2.7759055151,-0.3174148775
H,0,-4.8580726781,-0.6384516895,0.5609774229
H,0,-4.0316101483,0.9257125928,0.4127176505
H,0,-4.381912293,-0.0342445278,-1.0375251378
H,0,0.0500992486,1.4575890853,-0.1808923105
H,0,-1.9716438983,2.6891867213,-0.1036655993
H,0,-1.3147932003,2.4723980255,1.5298845927
H,0,-1.1356028543,4.0511215207,0.7168732961
H,0,-0.4420693442,2.8800675551,-2.0098330206
H,0,0.4093303993,4.2347226096,-1.2115487775
H,0,1.3154798676,2.7900573282,-1.7327022333
H,0,1.4056906744,3.8029007547,1.0779086279
H,0,1.0333172052,2.2498087723,1.8747244114
H,0,2.1699069747,2.2757647404,0.5147055525

TS for formation cyclohexenone oxide solvated $HNMe_3^+$ – boat conformation – PCM toluene

E(RB+HF-LYP) = -792.130485118

Zero-point correction=	0.390742 (Hartree/Particle)
Thermal correction to Energy=	0.411920
Thermal correction to Enthalpy=	0.412864
Thermal correction to Gibbs Free Energy=	0.339080
Sum of electronic and zero-point Energies=	-791.739743
Sum of electronic and thermal Energies=	-791.718565
Sum of electronic and thermal Enthalpies=	-791.717621
Sum of electronic and thermal Free Energies=	-791.791405

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	258.484	78.117	155.292

C,0,-3.062775385,-1.2321907158,0.680475729
C,0,-2.7533320876,-0.7982942604,-0.7564803
C,0,-1.4906131444,-1.1538003832,-1.3032394315
C,0,-0.3822015315,-1.6730840151,-0.4875160581
C,0,-0.754108067,-2.2605818473,0.8671595879
C,0,-1.8338325074,-1.4393284875,1.5736057234
O,0,-3.6475657146,-0.2178489306,-1.4121683208
O,0,0.2275343731,-0.3634984058,-0.4043957481
O,0,1.7352514097,-0.2008486986,0.638292393
C,0,2.9339525212,-0.3782091574,-0.083520812
C,0,4.0418322196,-0.1678350986,0.9737048334
C,0,3.0591345931,-1.7954383623,-0.6697821171
C,0,3.0854074451,0.6639010648,-1.2052242097
N,0,-0.5820449037,2.1152693044,0.2518991413
C,0,0.227133834,2.5425753841,1.4308756904
C,0,-0.1422868783,2.8022093693,-0.9975590926
C,0,-2.0441113838,2.3111600873,0.4801484378
H,0,-1.3133836548,-0.9490899391,-2.3540534378
H,0,0.2919519791,-2.3411166448,-1.0290454646
H,0,-1.1119146872,-3.284996961,0.7007436101
H,0,0.1465570759,-2.3266529716,1.4832503404
H,0,-2.1269670389,-1.9262472129,2.5100106341
H,0,-1.4091347881,-0.4707417358,1.8621864059
H,0,-3.6243501901,-2.1734664693,0.5997863711
H,0,-3.7623877235,-0.5100053347,1.1129710344
H,0,4.0204267425,0.5285152759,-1.7581642258
H,0,2.2572594223,0.5774786529,-1.9123758307

H,0,3.0898332237,1.6778592704,-0.7916272947
H,0,4.0632419424,-1.9725705696,-1.0684537767
H,0,2.8607788713,-2.5445150734,0.1012381349
H,0,2.3495084811,-1.9451748518,-1.4861292858
H,0,5.0335105885,-0.260784558,0.5182095496
H,0,3.9627454274,0.8254527278,1.4230246497
H,0,3.9562556407,-0.9106484577,1.7701963026
H,0,-0.3892465453,1.0846090306,0.0943477429
H,0,-0.1484421189,2.0339586592,2.3171090279
H,0,1.2573820559,2.2389414178,1.2667697037
H,0,0.1402869764,3.6226176293,1.5561195452
H,0,-2.3352822518,1.7839297655,1.3864089707
H,0,-2.2457470909,3.3767907132,0.5960154916
H,0,-2.5997698311,1.9092038802,-0.3648627911
H,0,-0.3197087623,3.8739494752,-0.9017371864
H,0,0.9155156918,2.6062406437,-1.1510629669
H,0,-0.7115634238,2.4006453204,-1.8338837219

Int axAB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.827702437

Zero-point correction= 0.454296 (Hartree/Particle)
Thermal correction to Energy= 0.478235
Thermal correction to Enthalpy= 0.479179
Thermal correction to Gibbs Free Energy= 0.400711
Sum of electronic and zero-point Energies= -962.373406
Sum of electronic and thermal Energies= -962.349467
Sum of electronic and thermal Enthalpies= -962.348523
Sum of electronic and thermal Free Energies= -962.426991

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	300.097	90.765	165.151

C,0,-1.4206363323,2.4546982925,1.1473376434
C,0,-0.1227263744,2.2183812991,1.9253824503
C,0,1.1125726508,2.5952318564,1.0956916452
C,0,1.0884391421,2.1112076017,-0.3659298622
C,0,-0.154798348,1.8637645068,-0.9577603902
C,0,-1.4080938875,1.7377020934,-0.2006262174
O,0,2.2102109366,2.015469041,-0.9575486919
O,0,-1.5068216326,0.2449635562,0.0050508937
O,0,-2.7881115725,-0.1440113165,0.6985761463
C,0,-3.5850726499,-0.9746341532,-0.1645078802

C,0,-3.947991866,-0.249521605,-1.4661423143
C,0,-2.860933017,-2.2983535173,-0.4529145707
C,0,-4.8364489885,-1.2209406912,0.6916294782
H,0,-0.1830635543,1.6515774448,-2.025058952
H,0,-2.3014071251,2.0000476588,-0.77979941
H,0,-1.5459406389,3.5281172861,0.946789862
H,0,-2.2894605061,2.1281180453,1.7298582057
H,0,-0.1389389331,2.7798415542,2.8695637422
H,0,-0.0761509575,1.1570907642,2.1998421344
H,0,1.2185758808,3.6903628688,1.0637479573
H,0,2.034998381,2.2230397333,1.5614921136
H,0,-3.5002327971,-2.9769681387,-1.0295768432
H,0,-1.9477137972,-2.1236432626,-1.0298718369
H,0,-2.5903663896,-2.7948942868,0.4857544245
H,0,-4.6034898593,-0.8730781984,-2.0855138157
H,0,-4.4695262413,0.6887369911,-1.2497992241
H,0,-3.0469794491,-0.0197946526,-2.0417141522
H,0,-5.5413965696,-1.8683727542,0.1581239326
H,0,-4.567505383,-1.7044535562,1.6365278764
H,0,-5.3368705181,-0.2744688218,0.9194335905
H,0,0.1173214904,-0.6754868366,-0.6459951309
N,0,1.0794474142,-1.0288274897,-0.7485720637
C,0,1.7377642992,-0.7202387207,-2.0269589645
C,0,3.1613303641,-1.262797555,-2.0148250854
H,0,1.1358042342,-1.165644741,-2.8248939178
H,0,1.7668662481,0.3742588883,-2.1211518919
C,0,1.7205066168,-1.255065291,0.3851881955
N,0,3.0587904854,-1.3031641073,0.4343695162
C,0,3.7918466902,-1.5056718541,1.679593428
C,0,3.8345234094,-0.8071519404,-0.7225192335
H,0,4.7190997136,-2.0412879715,1.4575620898
H,0,4.0469016064,-0.5470964855,2.149896682
H,0,3.2137291549,-2.1050501705,2.3825356437
H,0,3.8522137681,0.2900504709,-0.6770592616
C,0,0.8870974484,-1.4952476306,1.6139519691
H,0,3.1793261397,-2.357792817,-2.0823381562
H,0,3.7083479379,-0.8637997893,-2.8744143176
H,0,4.8487183701,-1.2058178015,-0.6336605895
H,0,0.9354025543,-2.5505448485,1.9075775135
H,0,1.2393514289,-0.8894102556,2.4526729355
H,0,-0.1517762823,-1.2292415319,1.4107180951

Int axAB3 DBU model – PCM Dichloroethane - 6-31G*

E(RB+HF-LYP) = -962.849221182

Zero-point correction= 0.453209 (Hartree/Particle)
Thermal correction to Energy= 0.477490
Thermal correction to Enthalpy= 0.478434
Thermal correction to Gibbs Free Energy= 0.397738
Sum of electronic and zero-point Energies= -962.396013
Sum of electronic and thermal Energies= -962.371731
Sum of electronic and thermal Enthalpies= -962.370787
Sum of electronic and thermal Free Energies= -962.451483

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.630	90.957	169.840

C,0,-1.7487249329,2.277775,1.1812809146
C,0,-0.3723269329,2.284246,1.8506309146
C,0,0.6539310671,3.036556,0.9964679146
C,0,0.6357970671,2.67255,-0.5000670854
C,0,-0.5338649329,2.126398,-1.0325430854
C,0,-1.6852469329,1.682136,-0.2240540854
O,0,1.6880570671,2.945929,-1.1658130854
O,0,-1.4821769329,0.195797,-0.1503290854
O,0,-2.5643729329,-0.495811,0.6225569146
C,0,-3.2893679329,-1.397773,-0.2440600854
C,0,-3.9747729329,-0.638692,-1.3858430854
C,0,-2.3548009329,-2.486558,-0.7876250854
C,0,-4.3275089329,-2.000043,0.7138559146
H,0,-0.5601479329,1.925133,-2.1037610854
H,0,-2.6513519329,1.806819,-0.7303190854
H,0,-2.1253569329,3.307155,1.0912269146
H,0,-2.4760109329,1.718654,1.7803149146
H,0,-0.4371329329,2.722677,2.8558949146
H,0,-0.0453319329,1.245229,1.9853169146
H,0,0.4775420671,4.121743,1.0740659146
H,0,1.6745030671,2.872278,1.3657899146
H,0,-2.9148479329,-3.211071,-1.3896870854
H,0,-1.5780649329,-2.046698,-1.4199050854
H,0,-1.8725599329,-3.025284,0.0358009146
H,0,-4.5803519329,-1.323474,-1.9908120854
H,0,-4.6317919329,0.142498,-0.9885310854
H,0,-3.2318459329,-0.171189,-2.0381970854
H,0,-4.9470929329,-2.732008,0.1841599146
H,0,-3.8338219329,-2.505638,1.5505689146
H,0,-4.9809339329,-1.219172,1.1166759146

H,0,0.2439190671,-0.378083,-0.4094470854
N,0,1.2268910671,-0.667037,-0.5231220854
C,0,1.8896850671,-0.252399,-1.7671870854
C,0,3.2346140671,-0.960515,-1.8850690854
H,0,1.2291610671,-0.537232,-2.5928470854
H,0,1.9774990671,0.843321,-1.7690530854
C,0,1.8326740671,-1.188247,0.5285689146
N,0,3.1571660671,-1.371327,0.5487569146
C,0,3.8851750671,-1.932226,1.6856429146
C,0,3.9904410671,-0.87011,-0.5622730854
H,0,4.5099390671,-2.763056,1.3413149146
H,0,4.5324910671,-1.166722,2.1297429146
H,0,3.2043520671,-2.302473,2.4494439146
H,0,4.2812950671,0.166466,-0.3446700854
C,0,0.9710440671,-1.578795,1.7004449146
H,0,3.0897590671,-2.015683,-2.1468280854
H,0,3.8306260671,-0.499128,-2.6786480854
H,0,4.9000000671,-1.477316,-0.5886190854
H,0,1.0279550671,-2.658963,1.8746889146
H,0,1.2959760671,-1.069579,2.6132339146
H,o,-0.0693139329,-1.313794,1.5032999146

Int axAB3 DBU model – 6-31+G**

E(RB+HF-LYP) = -962.903855215

Zero-point correction= 0.450992 (Hartree/Particle)
Thermal correction to Energy= 0.475214
Thermal correction to Enthalpy= 0.476159
Thermal correction to Gibbs Free Energy= 0.396692
Sum of electronic and zero-point Energies= -962.452864
Sum of electronic and thermal Energies= -962.428641
Sum of electronic and thermal Enthalpies= -962.427697
Sum of electronic and thermal Free Energies= -962.507163

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.202	91.600	167.251

C,0,-1.4582449036,2.4567701651,1.144188616
C,0,-0.1940555279,2.2001517827,1.9701795662
C,0,1.0820338396,2.5489416419,1.189051888
C,0,1.1011869844,2.0860728707,-0.2775048721
C,0,-0.1215522588,1.8719131649,-0.9216642196
C,0,-1.4019423315,1.7487319552,-0.2073481077

O,0,2.2464978037,1.9688847742,-0.8286752888
O,0,-1.5177639768,0.2487289513,-0.0158225888
O,0,-2.8130152534,-0.1351844247,0.649374237
C,0,-3.6137132952,-0.9474717739,-0.2356858915
C,0,-3.9725746036,-0.1887535338,-1.5197511431
C,0,-2.8934927969,-2.2659298481,-0.5560136309
C,0,-4.8671876108,-1.2108806222,0.6121226402
H,0,-0.1142986061,1.669901427,-1.9904669454
H,0,-2.2705164409,2.0187483474,-0.8181681186
H,0,-1.5638202321,3.5316553992,0.9426622822
H,0,-2.3513699517,2.1374992125,1.6920873943
H,0,-0.2344460978,2.7678415345,2.9092148801
H,0,-0.180235288,1.1403635406,2.2513714247
H,0,1.221991022,3.639769506,1.1677902038
H,0,1.9748678972,2.1459617216,1.6845039638
H,0,-3.5417655423,-2.9270607029,-1.1418092837
H,0,-1.9863111865,-2.08216237,-1.1383126245
H,0,-2.6185671884,-2.7842575093,0.3687194077
H,0,-4.6263990737,-0.7989368738,-2.1528874247
H,0,-4.4950566946,0.7432102733,-1.2826583898
H,0,-3.0718427512,0.053089214,-2.0899907715
H,0,-5.5701900427,-1.8409227469,0.0567939959
H,0,-4.603131523,-1.7216383154,1.5432504403
H,0,-5.3662423267,-0.2701458154,0.8627228287
H,0,0.1040109096,-0.7648035386,-0.5399136296
N,0,1.0718404662,-1.0845375857,-0.6760402151
C,0,1.6573224871,-0.8201778821,-1.997717022
C,0,3.0814747063,-1.3589469955,-2.045158221
H,0,1.0164674269,-1.2961096324,-2.7454168751
H,0,1.6655281432,0.2661754485,-2.1400321581
C,0,1.779269095,-1.244871127,0.4308939211
N,0,3.1175501111,-1.2765296596,0.4098883346
C,0,3.919380343,-1.3656249532,1.6282903143
C,0,3.8323925701,-0.856335814,-0.8153237949
H,0,4.8415052073,-1.9062638936,1.4011666468
H,0,4.1803871281,-0.3661507489,1.9975810404
H,0,3.3908417595,-1.9103319204,2.4090053867
H,0,3.8779609781,0.2407610996,-0.8213609679
C,0,1.017858089,-1.4301475019,1.7139493699
H,0,3.0932699774,-2.4554773143,-2.0731879216
H,0,3.5771514743,-0.9944788104,-2.9493681208
H,0,4.8405489828,-1.275592098,-0.7651121293
H,0,1.1344824126,-2.45522988,2.0820590016
H,0,1.3762830327,-0.7442235576,2.4847598485

H,0,-0.0415147526,-1.2338038609,1.5439924266

Int axAB3 DBU model – PCM Dichloroethane - 6-31+G**

E(RB+HF-LYP) = -962.932821155

Zero-point correction=	0.450061 (Hartree/Particle)
Thermal correction to Energy=	0.474516
Thermal correction to Enthalpy=	0.475460
Thermal correction to Gibbs Free Energy=	0.394258
Sum of electronic and zero-point Energies=	-962.482760
Sum of electronic and thermal Energies=	-962.458305
Sum of electronic and thermal Enthalpies=	-962.457361
Sum of electronic and thermal Free Energies=	-962.538563

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	297.763	91.577	170.904

C,0,-1.7285224066,2.2514444949,1.2362915408
C,0,-0.3060877187,2.334185592,1.7964241962
C,0,0.5993325053,3.170632243,0.8837861176
C,0,0.4621671227,2.8639884112,-0.6135980609
C,0,-0.6736870996,2.2005676627,-1.0646743775
C,0,-1.7407826471,1.6778156158,-0.1807554687
O,0,1.4097341533,3.2924638835,-1.3727976158
O,0,-1.4777461051,0.2020372387,-0.149067645
O,0,-2.5373797149,-0.5215252184,0.6099304879
C,0,-3.2319523715,-1.4487411299,-0.2662917077
C,0,-3.9254190641,-0.7083300973,-1.4153587427
C,0,-2.260541874,-2.5112302213,-0.7967425273
C,0,-4.2612402529,-2.0767641016,0.6832105216
H,0,-0.7710389425,2.0192318785,-2.1349727487
H,0,-2.7424148922,1.771282707,-0.6178873949
H,0,-2.170839739,3.2569256264,1.1928090922
H,0,-2.372671772,1.6437689051,1.8810358849
H,0,-0.3187493389,2.7516646355,2.8116322041
H,0,0.0980392037,1.3177613467,1.8833598423
H,0,0.3775699662,4.2411639212,1.0160525757
H,0,1.6554212243,3.047560026,1.1559296897
H,0,-2.7987801915,-3.255806507,-1.3931424239
H,0,-1.4965021898,-2.0555462484,-1.4323624279
H,0,-1.7673067666,-3.0289367361,0.0326799739
H,0,-4.4943394531,-1.4154041588,-2.029008321
H,0,-4.6179559082,0.0456057831,-1.027811174

H,0,-3.1904008888,-0.214303354,-2.0563712345
H,0,-4.8551865731,-2.8227300743,0.1447526398
H,0,-3.7642750374,-2.5722017397,1.5233335051
H,0,-4.9398343766,-1.3146217662,1.0789729531
H,0,0.2906997399,-0.3582911094,-0.327359847
N,0,1.2803641477,-0.6183850742,-0.4279150846
C,0,1.9694658929,-0.1762066098,-1.6472664216
C,0,3.2446886622,-0.9917893523,-1.8265660999
H,0,1.2813023711,-0.3281939011,-2.4835921043
H,0,2.1619473046,0.9011043089,-1.5781764892
C,0,1.8621813917,-1.2249784923,0.594097683
N,0,3.1738550304,-1.4793212018,0.597088524
C,0,3.879029033,-2.1119888367,1.7135237989
C,0,4.0306558048,-1.0279766316,-0.5196616508
H,0,4.4059693995,-3.0012408855,1.3532680681
H,0,4.6119948667,-1.4114057515,2.1286973859
H,0,3.1922485531,-2.4082580031,2.502550681
H,0,4.4387791039,-0.0387109014,-0.2724831904
C,0,0.9858070405,-1.6218597915,1.7507605146
H,0,2.998463997,-2.0154947978,-2.1328966478
H,0,3.8643786047,-0.5487175253,-2.6117652929
H,0,4.8685877206,-1.7274748351,-0.590048748
H,0,1.0075984194,-2.706707013,1.895360331
H,0,1.3239257592,-1.1475566042,2.6770632735
H,0,-0.0435951878,-1.3169430562,1.5585681596

tsaxAB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.824032082

Zero-point correction= 0.452643 (Hartree/Particle)
Thermal correction to Energy= 0.476337
Thermal correction to Enthalpy= 0.477281
Thermal correction to Gibbs Free Energy= 0.399425
Sum of electronic and zero-point Energies= -962.371390
Sum of electronic and thermal Energies= -962.347695
Sum of electronic and thermal Enthalpies= -962.346751
Sum of electronic and thermal Free Energies= -962.424607

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.906	89.385	163.862

C,0,-1.4629132232,2.4728145391,0.8560201038
C,0,-0.1961960162,2.2595488381,1.6911625679

C,0,1.0580927611,2.7709771263,0.9701820124
C,0,1.1634130339,2.3122849699,-0.4931864917
C,0,-0.0499894486,2.1277344789,-1.2064038299
C,0,-1.2968166282,1.9763832407,-0.5617491825
O,0,2.3090097033,2.1730758071,-0.9915796256
O,0,-1.4350298739,0.1772618508,-0.4242454119
O,0,-2.3574642084,-0.4194265415,0.5572764899
C,0,-3.451433967,-1.0813106787,-0.1117877171
C,0,-4.2568224011,-0.0813998389,-0.9499058593
C,0,-2.921004792,-2.2276166493,-0.9832076809
C,0,-4.2884425508,-1.6178558557,1.0567265595
H,0,0.0188407183,1.9522085751,-2.2778479135
H,0,-2.18757031,2.0983259469,-1.1758112785
H,0,-1.7008904926,3.5466503885,0.8028019306
H,0,-2.3183097887,1.9755054957,1.3251252042
H,0,-0.3021610777,2.7422121568,2.6720726605
H,0,-0.0949430089,1.184798366,1.8818677933
H,0,1.0620436156,3.8718900889,0.964444933
H,0,1.9746045915,2.4649254293,1.489351663
H,0,-3.7421327384,-2.7606607291,-1.4764949011
H,0,-2.2521230795,-1.8310950249,-1.7518486499
H,0,-2.3634699809,-2.9471286934,-0.3719538264
H,0,-5.1237177365,-0.5692090399,-1.4110624211
H,0,-4.6182025538,0.7405846083,-0.3221768142
H,0,-3.6311773757,0.335167449,-1.7434189386
H,0,-5.1659723819,-2.157560235,0.6835982966
H,0,-3.6974688727,-2.3046871803,1.6725055582
H,0,-4.631600177,-0.7950406279,1.6926366944
H,0,-0.0046136263,-0.6327829355,-0.5639748955
N,0,0.9952083098,-0.9859450311,-0.6142258788
C,0,1.7174075868,-0.733768598,-1.8679166275
C,0,3.1171903567,-1.3327912292,-1.7951916389
H,0,1.1277645548,-1.173354566,-2.6785096053
H,0,1.7887766332,0.3505182529,-2.009200717
C,0,1.5725665389,-1.2703807158,0.5330639641
N,0,2.9097189865,-1.357042485,0.6479024158
C,0,3.589523248,-1.6040093125,1.9136207647
C,0,3.7534969029,-0.9024206096,-0.4756883902
H,0,4.4429086389,-2.2668472472,1.7383264112
H,0,3.9615837396,-0.6676076655,2.3496916202
H,0,2.9251316196,-2.0858628889,2.6294183161
H,0,3.8351269888,0.1918131669,-0.4377337949
C,0,0.6748487157,-1.5298257983,1.7143064994
H,0,3.0893692739,-2.4279075488,-1.8554055663

H,0,3.7178963792,-0.9646979619,-2.6323568935
H,0,4.7443616451,-1.3462693898,-0.3432677762
H,0,0.7723408682,-2.5718927906,2.0412410293
H,0,0.9367077738,-0.8844873624,2.5578728782
H,0,-0.3672405827,-1.3440677964,1.4424913024

2nd tsaxAB3 DBU model - 6-31G*

E(RB+HF-LYP) = -962.822771071

Zero-point correction= 0.452274 (Hartree/Particle)
Thermal correction to Energy= 0.476067
Thermal correction to Enthalpy= 0.477011
Thermal correction to Gibbs Free Energy= 0.398497
Sum of electronic and zero-point Energies= -962.370497
Sum of electronic and thermal Energies= -962.346704
Sum of electronic and thermal Enthalpies= -962.345760
Sum of electronic and thermal Free Energies= -962.424274

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.736	89.428	165.246

C,0,-1.8042348647,2.3699884006,1.138601134
C,0,-0.3839926168,2.4379513141,1.7093511269
C,0,0.5507990684,3.2514924264,0.8043689148
C,0,0.4890272201,2.8713725298,-0.6831441008
C,0,-0.7458124322,2.3516325274,-1.1833257506
C,0,-1.813609273,1.8554570056,-0.2974398267
O,0,1.4873549036,3.0894371541,-1.401406958
O,0,-1.3060027221,0.5219837402,-0.4286528848
O,0,-2.1942635608,-0.7277042016,0.6197156565
C,0,-2.9483633404,-1.5875473961,-0.1960477023
C,0,-4.0363173742,-0.8159476809,-0.9673811679
C,0,-2.0523376633,-2.3604273809,-1.1853832709
C,0,-3.6167735755,-2.5772277932,0.7869288228
H,0,-0.8403789777,2.2070855856,-2.2546094101
H,0,-2.8233447397,1.9036974418,-0.7227299212
H,0,-2.2609330733,3.3703521047,1.1448706768
H,0,-2.434729336,1.7104792295,1.7442940329
H,0,-0.4005229215,2.8625505033,2.7215963068
H,0,0.001030035,1.4155423869,1.8075201008
H,0,0.2891363771,4.3191759604,0.8673201371
H,0,1.596238391,3.1766841936,1.1261453107
H,0,-2.6325570002,-3.0573907212,-1.8033227543

H,0,-1.5406804754,-1.6552979189,-1.8480448076
H,0,-1.2945698523,-2.9397223257,-0.6428567102
H,0,-4.6932913718,-1.4928027836,-1.5284308409
H,0,-4.6509135997,-0.2372738442,-0.2688509295
H,0,-3.5738310209,-0.121409487,-1.675509213
H,0,-4.244342575,-3.3022758436,0.2527574654
H,0,-2.8560426122,-3.1284987923,1.3511168129
H,0,-4.242967386,-2.0328310535,1.5014032794
H,0,0.2276384867,-0.0767626797,-0.3332745609
N,0,1.2082877106,-0.4479843183,-0.3808162472
C,0,1.9967846538,-0.0564030846,-1.5543248889
C,0,3.1661462614,-1.0186914222,-1.721953934
H,0,1.32186257,-0.0878600016,-2.4136315774
H,0,2.3134529515,0.9873715355,-1.4437363322
C,0,1.6629116965,-1.1499823642,0.6331500347
N,0,2.949079077,-1.5489558181,0.6821669575
C,0,3.5427102834,-2.232628502,1.8258247284
C,0,3.8919283033,-1.1827402623,-0.3889414841
H,0,3.9311091758,-3.2121470861,1.5222387773
H,0,4.3749523469,-1.6372164189,2.2204709793
H,0,2.8149452148,-2.3738723441,2.6215683927
H,0,4.4109068336,-0.2558887111,-0.1084058539
C,0,0.6935367639,-1.4983046835,1.7296832044
H,0,2.8075780634,-1.9971019858,-2.063388684
H,0,3.8632195904,-0.6389010906,-2.4747523082
H,0,4.6428803822,-1.9775332802,-0.4487097412
H,0,0.740247809,-2.5680777814,1.957484341
H,0,0.9345548443,-0.945462205,2.6450345173
H,0,-0.3333432729,-1.2537269779,1.4199359952

tsaxAB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.900689997

Zero-point correction= 0.448927 (Hartree/Particle)
Thermal correction to Energy= 0.473034
Thermal correction to Enthalpy= 0.473978
Thermal correction to Gibbs Free Energy= 0.393922
Sum of electronic and zero-point Energies= -962.451763
Sum of electronic and thermal Energies= -962.427656
Sum of electronic and thermal Enthalpies= -962.426712
Sum of electronic and thermal Free Energies= -962.506767

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	296.833	90.274	168.492

C,0,-1.5374614185,2.5082830006,0.8697517688
C,0,-0.2634731615,2.3533851593,1.7070895065
C,0,0.9730082099,2.8912241497,0.97325309
C,0,1.0879171489,2.4248353405,-0.4852036433
C,0,-0.1145117683,2.1587984715,-1.1891193163
C,0,-1.3599310585,1.976121805,-0.5344218056
O,0,2.2394972333,2.3441140345,-0.9921550876
O,0,-1.4143885993,0.2060986549,-0.3662111584
O,0,-2.3685706112,-0.4225801869,0.5728102078
C,0,-3.4249255219,-1.1105093193,-0.1375786552
C,0,-4.2190431113,-0.1335699603,-1.0132933506
C,0,-2.8426305103,-2.2553508785,-0.9780393775
C,0,-4.296739567,-1.6553139526,1.0019889165
H,0,-0.0428319691,1.9680453627,-2.2571336651
H,0,-2.2512628711,2.0652793176,-1.1529875528
H,0,-1.8035390392,3.572595704,0.7829898175
H,0,-2.379989689,2.0038867912,1.3541559749
H,0,-0.3840090692,2.8558858749,2.675681584
H,0,-0.1269104684,1.287513335,1.9236777977
H,0,0.9472249596,3.9909510748,0.95049641
H,0,1.8994269866,2.6178387796,1.491462446
H,0,-3.6401845354,-2.809195953,-1.4857691541
H,0,-2.1619057254,-1.8588880776,-1.7358867428
H,0,-2.2906970059,-2.9556915592,-0.3413558078
H,0,-5.0667508375,-0.6432415477,-1.4847833974
H,0,-4.6060450721,0.6936448298,-0.4096203576
H,0,-3.5827037625,0.2758337481,-1.8016091713
H,0,-5.1420137467,-2.219669118,0.5938924345
H,0,-3.716924211,-2.3217692298,1.6487213955
H,0,-4.6884712499,-0.8360351771,1.6127125356
H,0,0.0421249211,-0.5513633567,-0.4879270544
N,0,1.0349312304,-0.9160069218,-0.561581113
C,0,1.7376739838,-0.6696403163,-1.8270443717
C,0,3.0655968786,-1.4179947367,-1.8355171641
H,0,1.080831708,-1.0030107392,-2.635252684
H,0,1.9022740486,0.4112190151,-1.921752702
C,0,1.6259256772,-1.2727272563,0.5572311264
N,0,2.9560036614,-1.4784623678,0.6225039481
C,0,3.6590361282,-1.7588677602,1.8711147737
C,0,3.8053211598,-1.1264135559,-0.5325992983
H,0,4.4486628449,-2.4911086914,1.6790197102
H,0,4.1197097511,-0.8478725944,2.2742171422

H,0,2.986061472,-2.1735118,2.6189192738
H,0,4.0692030571,-0.0625343056,-0.4726431123
C,0,0.7541615932,-1.4711237679,1.7682271053
H,0,2.9099277742,-2.4988533668,-1.9382875981
H,0,3.6716338314,-1.084637226,-2.6827007651
H,0,4.7215419358,-1.7188866071,-0.4570392855
H,0,0.7999152532,-2.5124453954,2.1045436307
H,0,1.0790348615,-0.8318403943,2.5939093135
H,0,-0.2817305511,-1.2287322208,1.5233022172

2nd tsaxAB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.899796469

Zero-point correction= 0.448861 (Hartree/Particle)
Thermal correction to Energy= 0.472906
Thermal correction to Enthalpy= 0.473851
Thermal correction to Gibbs Free Energy= 0.394685
Sum of electronic and zero-point Energies= -962.450936
Sum of electronic and thermal Energies= -962.426890
Sum of electronic and thermal Enthalpies= -962.425946
Sum of electronic and thermal Free Energies= -962.505111

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.753	90.250	166.617

C,0,-1.8219827801,2.3823585275,1.1462088355
C,0,-0.4156148268,2.4411258503,1.7518379648
C,0,0.5554356974,3.2309034465,0.8627129178
C,0,0.5151794587,2.8506501478,-0.621612318
C,0,-0.7105713871,2.3392113272,-1.1500931434
C,0,-1.8017717058,1.8545671761,-0.2849642409
O,0,1.5315802475,3.0614109454,-1.324670067
O,0,-1.2986139381,0.5102917624,-0.393956698
O,0,-2.2189012045,-0.7479856594,0.614420005
C,0,-2.9888493337,-1.5840769457,-0.2188377536
C,0,-4.0574918617,-0.784168955,-0.9886287205
C,0,-2.1013114923,-2.3649753096,-1.2103288916
C,0,-3.6822130683,-2.5727895219,0.7485617675
H,0,-0.7844200871,2.1942786156,-2.2227607118
H,0,-2.7990936572,1.9060790641,-0.7364103457
H,0,-2.2673869635,3.3872117146,1.1263834775
H,0,-2.4749814032,1.739527889,1.7454569875
H,0,-0.4535587394,2.8825543322,2.7556215971

H,0,-0.0479560805,1.4159291889,1.8761823727
H,0,0.3164101837,4.3040024772,0.9111439803
H,0,1.5914916942,3.1352604448,1.2065002073
H,0,-2.6943918386,-3.0478822972,-1.8307260026
H,0,-1.5776544551,-1.6667644039,-1.8703243217
H,0,-1.3560039244,-2.9584616106,-0.6677959596
H,0,-4.7159313508,-1.4464973481,-1.5637728681
H,0,-4.671665326,-0.2075511399,-0.2889878523
H,0,-3.5793812377,-0.0886016749,-1.6843716455
H,0,-4.3145406859,-3.2785315298,0.1954065035
H,0,-2.9359047259,-3.1429064119,1.3116873595
H,0,-4.3072617777,-2.0272093908,1.4620314967
H,0,0.2230765291,-0.1228763956,-0.3694814517
N,0,1.2043917438,-0.4910396697,-0.4232255109
C,0,1.973806336,-0.136033782,-1.6215586093
C,0,3.1701871636,-1.0710249585,-1.7551124294
H,0,1.2972771389,-0.2265693112,-2.4751168868
H,0,2.2674246682,0.9186540382,-1.5591708398
C,0,1.684762426,-1.1390647452,0.6157976327
N,0,2.9785688206,-1.5143441198,0.6668379083
C,0,3.5962498696,-2.138078906,1.8338663627
C,0,3.9063210791,-1.15403764,-0.4206971312
H,0,4.0620114257,-3.0872081152,1.5468070695
H,0,4.3718813432,-1.4792757002,2.2423053772
H,0,2.8633961928,-2.3308705297,2.6130693723
H,0,4.3877450513,-0.1964933515,-0.1799171636
C,0,0.7355242184,-1.4560918284,1.7382087182
H,0,2.8407046148,-2.0736376473,-2.0521315875
H,0,3.850476152,-0.7020248989,-2.52766326
H,0,4.6866295079,-1.9206922282,-0.4517060626
H,0,0.7650740752,-2.5243860436,1.9735224742
H,0,1.0076372518,-0.9009510248,2.6421618275
H,0,-0.2903071248,-1.1969998708,1.4482583879

Int axBB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.826959810

Zero-point correction= 0.454082 (Hartree/Particle)
Thermal correction to Energy= 0.477971
Thermal correction to Enthalpy= 0.478915
Thermal correction to Gibbs Free Energy= 0.400278
Sum of electronic and zero-point Energies= -962.372878
Sum of electronic and thermal Energies= -962.348989
Sum of electronic and thermal Enthalpies= -962.348044

Sum of electronic and thermal Free Energies= -962.426682

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.932	90.708	165.507

C,0,-1.2067163348,2.431667423,1.1759262679
C,0,0.1051717461,2.1348452451,1.9078141346
C,0,1.3194110069,2.4973336256,1.0432149439
C,0,1.2394586156,2.0116624067,-0.4153035152
C,0,-0.0252489134,1.7852805507,-0.9632974225
C,0,-1.268460059,1.7317257703,-0.1796618544
O,0,2.3452101904,1.9012684967,-1.0404310551
O,0,-1.4831496916,0.2494140858,0.0139533037
O,0,-2.7738958304,-0.0278955009,0.7281728434
C,0,-3.656581105,-0.7891131164,-0.1155230659
C,0,-3.9913425533,-0.0339738898,-1.4075630559
C,0,-3.0511061386,-2.1671593573,-0.4220168528
C,0,-4.901703815,-0.9345382964,0.7721123587
H,0,-0.0944969375,1.5819980488,-2.0296873881
H,0,-2.1520716112,2.0668195181,-0.7364209399
H,0,-1.2919897453,3.5122817285,0.9931213409
H,0,-2.0700657648,2.1350353364,1.7815988568
H,0,0.1375478415,2.6725726007,2.8653225607
H,0,0.1282128116,1.0647424501,2.1550176397
H,0,1.4361025919,3.5913934839,1.0095644743
H,0,2.2534218561,2.117337644,1.4789320108
H,0,-3.7672560933,-2.7970153004,-0.9625275333
H,0,-2.1546256655,-2.069849649,-1.0419725692
H,0,-2.7780309667,-2.6767148263,0.50880688
H,0,-4.7060709901,-0.6032641266,-2.0135584295
H,0,-4.4341951992,0.9409599187,-1.1785268304
H,0,-3.0879118387,0.1275186719,-2.002210467
H,0,-5.6740047055,-1.5127928129,0.2527102528
H,0,-4.6514323522,-1.4489269151,1.7057550999
H,0,-5.3115699641,0.0495516431,1.020434016
H,0,-0.0192906747,-0.9449555272,-0.5083194642
N,0,0.8422030746,-1.4244315088,-0.2173850928
C,0,0.8787909071,-1.7923298652,1.2000944001
C,0,2.1715984222,-1.2891401506,1.8329599357
H,0,-0.0039835847,-1.345666465,1.6621216356
H,0,0.7980872552,-2.8833248004,1.2893693614
C,0,1.9244192631,-1.1514639598,-0.9404394659
N,0,3.1548638815,-1.316549686,-0.4463474227

C,0,4.311117073,-0.7536180498,-1.1617608352
C,0,3.359712071,-1.6965528327,0.9660467986
H,0,4.251635778,0.3407346424,-1.1236574648
H,0,5.2219932531,-1.1118370367,-0.6796490079
H,0,4.3267785761,-1.0849197928,-2.2013812913
H,0,3.5340283478,-2.779609651,1.0179706449
C,0,1.7346210618,-0.6607636165,-2.3398749572
H,0,2.1389945663,-0.1988504911,1.9154472764
H,0,2.2922399906,-1.7036423242,2.8387365751
H,0,4.2681620751,-1.1979502715,1.3119431995
H,0,2.0185734999,0.4082170465,-2.3394219942
H,0,2.3571607716,-1.2276533942,-3.0384162392
H,0,0.6904233531,-0.7607889584,-2.6349022198

Int axBB3 DBU model – PCM Dichloroethane - 6-31G*

E(RB+HF-LYP) = -962.848186241

Zero-point correction= 0.452581 (Hartree/Particle)
Thermal correction to Energy= 0.476230
Thermal correction to Enthalpy= 0.477174
Thermal correction to Gibbs Free Energy= 0.393389
Sum of electronic and zero-point Energies= -962.395605
Sum of electronic and thermal Energies= -962.371956
Sum of electronic and thermal Enthalpies= -962.371012
Sum of electronic and thermal Free Energies= -962.454798

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.839	88.961	176.342

C,0,-1.5330261807,2.6225550746,0.568744156
C,0,-0.1526766138,2.666603433,1.2291589434
C,0,0.9272858089,3.0855628333,0.2246995255
C,0,0.8484698801,2.3742417054,-1.1378544077
C,0,-0.3626091488,1.7988954132,-1.5159586656
C,0,-1.5460025521,1.6873584873,-0.6408969193
O,0,1.9051708086,2.4008003745,-1.856207202
O,0,-1.5127491339,0.2607458612,-0.1926985085
O,0,-2.7243057822,-0.073752388,0.6148172858
C,0,-3.4614606428,-1.1315324358,-0.0376772711
C,0,-3.9237298657,-0.708312372,-1.436706199
C,0,-2.6150195335,-2.4105463017,-0.0971715466
C,0,-4.6604713847,-1.3170457198,0.902740239
H,0,-0.4251267028,1.3494605377,-2.5069640259

H,0,-2.4975085601,1.7857413989,-1.1802364355
H,0,-1.8095464768,3.6282386801,0.2195358085
H,0,-2.3031209993,2.3058694768,1.2812403497
H,0,-0.1625364807,3.343687272,2.0941513154
H,0,0.0805807439,1.6669782477,1.6193946221
H,0,0.8617936371,4.1696125131,0.0372542239
H,0,1.9329812853,2.9140580606,0.6306775704
H,0,-3.2004980279,-3.2450638394,-0.499757965
H,0,-1.7413022002,-2.2659446518,-0.7389872612
H,0,-2.2700753309,-2.6844207286,0.9063305309
H,0,-4.5312873634,-1.4976429319,-1.8943906911
H,0,-4.5281727728,0.2035491964,-1.3835774341
H,0,-3.0625109023,-0.5195169586,-2.0837005758
H,0,-5.314856888,-2.1111065212,0.5268881528
H,0,-4.3253642843,-1.5923147376,1.908493343
H,0,-5.2426950373,-0.3920848894,0.9727669559
H,0,0.1775945384,-0.5477245296,-0.0237979222
N,0,1.0191972965,-0.9981517209,0.3611709348
C,0,1.0135786091,-1.2986171156,1.7928498166
C,0,2.3952658723,-1.002985904,2.3651279825
H,0,0.2353715502,-0.6863450958,2.2542616198
H,0,0.7464134404,-2.3528075083,1.9443473627
C,0,2.0917726467,-1.1114259029,-0.4119399513
N,0,3.2591810643,-1.5233001179,0.0913126797
C,0,4.4408509437,-1.7439121497,-0.7525773867
C,0,3.4513692986,-1.7354361623,1.54432933
H,0,4.8777816177,-0.7952827937,-1.08307371
H,0,5.1805885306,-2.2843894358,-0.1599264428
H,0,4.1971986791,-2.3547911895,-1.6241432481
H,0,3.429953763,-2.8148014023,1.7435476613
C,0,1.9537714649,-0.7382335745,-1.85513663
H,0,2.5826560693,0.0766905137,2.3389554326
H,0,2.4582955634,-1.3295357674,3.4077880795
H,0,4.4506766736,-1.3678605227,1.7975559353
H,0,2.1880369212,0.3353705784,-1.9866931703
H,0,2.5999168651,-1.338039816,-2.4972139783
H,0,0.91697487,-0.8747869162,-2.1657901012

Int axBB3 DBU model – 6-31+G**

E(RB+HF-LYP) = -962.826959810

Zero-point correction=	0.454082 (Hartree/Particle)
Thermal correction to Energy=	0.477971
Thermal correction to Enthalpy=	0.478915

Thermal correction to Gibbs Free Energy= 0.400278
Sum of electronic and zero-point Energies= -962.372878
Sum of electronic and thermal Energies= -962.348989
Sum of electronic and thermal Enthalpies= -962.348044
Sum of electronic and thermal Free Energies= -962.426682

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.932	90.708	165.507

C,0,-1.465333962,2.5287081345,1.2127140984
C,0,-0.2531954839,2.2338754834,2.1013200111
C,0,1.0561269527,2.4671232819,1.3366413103
C,0,1.0935265512,1.8581256007,-0.0717309016
C,0,-0.1209466131,1.5568596676,-0.70298902
C,0,-1.4530625209,1.6665130378,-0.0517887737
O,0,2.2422038391,1.6628471966,-0.5913398712
O,0,-1.7961013778,0.2625087707,0.2784477647
O,0,-3.2014723363,0.2123964737,0.7658194772
C,0,-3.9408896104,-0.7556238036,-0.0088785677
C,0,-3.9992612691,-0.3495150231,-1.4875338072
C,0,-3.327892952,-2.1532973433,0.1616505359
C,0,-5.3338373954,-0.6905426399,0.6331133831
H,0,-0.1031446541,1.3383099832,-1.7698754925
H,0,-2.2328765263,2.0060700659,-0.7454679896
H,0,-1.448739574,3.5822856211,0.9000091604
H,0,-2.4020662317,2.3635704138,1.7549594663
H,0,-0.2831605,2.8548522176,3.0059630155
H,0,-0.3102471075,1.189601868,2.4357788055
H,0,1.2273527412,3.5468026275,1.2102133589
H,0,1.9230115026,2.0944439299,1.8960891513
H,0,-3.9358833823,-2.9059380915,-0.3528290424
H,0,-2.3180921272,-2.1823916389,-0.2555695752
H,0,-3.2741725078,-2.4159385705,1.223166194
H,0,-4.6027666053,-1.0653332523,-2.0568169527
H,0,-4.4483963205,0.6428142619,-1.5959803399
H,0,-2.9949340381,-0.3263022565,-1.9182661473
H,0,-6.0083840877,-1.3970844335,0.1379578186
H,0,-5.2809721538,-0.9465887158,1.6956997385
H,0,-5.754899792,0.3151912849,0.5398943507
H,0,0.4794206757,-0.4617039758,-0.820288744
N,0,1.2117664249,-1.1679685427,-0.6072036041
C,0,1.1486683168,-1.6913952308,0.7606199465
C,0,2.4018689988,-1.2802618628,1.52913807

H,0,0.2384077384,-1.289991843,1.2109642812
H,0,1.0585668346,-2.784468965,0.7179904972
C,0,2.3723500861,-0.9608262156,-1.2275183685
N,0,3.5302687182,-1.3583835555,-0.6836987715
C,0,4.8090566902,-1.1822360847,-1.3707047436
C,0,3.6362613099,-1.7142937366,0.7469036799
H,0,5.227762998,-0.1904701404,-1.1618175486
H,0,5.5026637265,-1.9469348184,-1.0114864728
H,0,4.6979733533,-1.3053157235,-2.4469201955
H,0,3.7984656464,-2.7978574755,0.823858118
C,0,2.3396673299,-0.4207444288,-2.6264740878
H,0,2.4103826857,-0.1942334083,1.651893565
H,0,2.4179426757,-1.741581586,2.5212294349
H,0,4.5284829088,-1.2153192246,1.1391247253
H,0,3.0104316557,0.4328693729,-2.7225094955
H,0,2.6161812896,-1.2077633771,-3.3393197367
H,0,1.3317636021,-0.0839620119,-2.8616428741

Int axBB3 DBU model – PCM Dichloroethane - 6-31+G**

E(RB+HF-LYP) = -962.931089719

Zero-point correction=	0.449743 (Hartree/Particle)
Thermal correction to Energy=	0.473420
Thermal correction to Enthalpy=	0.474365
Thermal correction to Gibbs Free Energy=	0.394307
Sum of electronic and zero-point Energies=	-962.481347
Sum of electronic and thermal Energies=	-962.457669
Sum of electronic and thermal Enthalpies=	-962.456725
Sum of electronic and thermal Free Energies=	-962.536783

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	297.076	89.538	168.496

C,0,-1.741169548,2.2290685591,1.250781529
C,0,-0.3280909787,2.2753478861,1.8392151158
C,0,0.6278562758,3.0631328082,0.9334341713
C,0,0.5140927528,2.7319056343,-0.5603410619
C,0,-0.6487852163,2.1329626651,-1.0295749561
C,0,-1.7441823064,1.6449526065,-0.161744119
O,0,1.5094179811,3.0769204893,-1.3049766911
O,0,-1.5209488781,0.1614895177,-0.1175954231
O,0,-2.6327238517,-0.5200652983,0.605185073
C,0,-3.3076604954,-1.4447690586,-0.2878162667

C,0,-3.9182111454,-0.7103435863,-1.4870967509
C,0,-2.3405522813,-2.5460223661,-0.7419452467
C,0,-4.4047862342,-2.022515475,0.6166346912
H,0,-0.7302887866,1.9397949571,-2.0988712748
H,0,-2.7358134957,1.7597685249,-0.6158672303
H,0,-2.1525842956,3.246795331,1.1902201181
H,0,-2.4151961785,1.6463577792,1.8880139124
H,0,-0.3484546573,2.711521664,2.8464562356
H,0,0.0399507872,1.2478820573,1.9533446816
H,0,0.4393057811,4.1429282234,1.0403873333
H,0,1.6717842472,2.9091306664,1.2343252533
H,0,-2.8694907253,-3.2965155533,-1.3392675507
H,0,-1.5380178131,-2.127967474,-1.3555575181
H,0,-1.8962205179,-3.0457672651,0.1251428725
H,0,-4.4657616162,-1.4159768238,-2.121497683
H,0,-4.6166118922,0.0633205504,-1.1521653746
H,0,-3.1377422516,-0.2413831461,-2.091765724
H,0,-4.995217383,-2.7575089257,0.0597254652
H,0,-3.968027274,-2.5198117639,1.4885909863
H,0,-5.0762996867,-1.2316219896,0.9649534276
H,0,0.2195666583,-0.5342456268,-0.0144913211
N,0,1.1301095981,-0.9562930468,0.2123338489
C,0,1.28103157,-1.5713895248,1.5337410231
C,0,2.7004161334,-1.3333251401,2.0375637266
H,0,0.5354125747,-1.1267969233,2.1967667141
H,0,1.0678632633,-2.6458212807,1.4614969094
C,0,2.1306860139,-0.7927466536,-0.643905482
N,0,3.369864175,-1.1931198143,-0.3480253829
C,0,4.4669183093,-1.0840167522,-1.3223814823
C,0,3.7032331163,-1.7693815689,0.9746973456
H,0,4.6891051693,-0.0380317687,-1.5538855917
H,0,5.3537691199,-1.5399710742,-0.8823715397
H,0,4.2326831608,-1.6200362319,-2.2457237614
H,0,3.7336318371,-2.8630979111,0.8826777026
C,0,1.8344464098,-0.125758832,-1.952239398
H,0,2.8404987028,-0.271131587,2.267926576
H,0,2.8781132166,-1.9007994432,2.9558633668
H,0,4.7075096784,-1.4259783056,1.2375593099
H,0,2.0523280374,0.9524100043,-1.8828258702
H,0,2.4143129054,-0.5621901869,-2.7662351989
H,0,0.7726587583,-0.218731329,-2.178125193

tsaxBB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.823755913

Zero-point correction= 0.452744 (Hartree/Particle)
Thermal correction to Energy= 0.476284
Thermal correction to Enthalpy= 0.477228
Thermal correction to Gibbs Free Energy= 0.399923
Sum of electronic and zero-point Energies= -962.371012
Sum of electronic and thermal Energies= -962.347472
Sum of electronic and thermal Enthalpies= -962.346528
Sum of electronic and thermal Free Energies= -962.423833

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	298.872	89.230	162.701

C,0,-1.2350469784,2.4225336598,0.9535541259
C,0,0.0343260457,2.1033952631,1.7492164827
C,0,1.2991704223,2.5681560694,1.0149309189
C,0,1.3469636233,2.1557922271,-0.4661334813
C,0,0.1092105197,2.0502135863,-1.1482259083
C,0,-1.134602872,1.9574935224,-0.4816774422
O,0,2.4756453271,1.9905262608,-0.9981388014
O,0,-1.4259160182,0.1839751023,-0.4019463337
O,0,-2.4543674129,-0.2967103373,0.5345546901
C,0,-3.5744664325,-0.8530618264,-0.1837910918
C,0,-4.2230684805,0.2008762198,-1.0890036361
C,0,-3.1248554164,-2.075261327,-0.9958842346
C,0,-4.5254055897,-1.2644108466,0.948200782
H,0,0.1413978847,1.9129269865,-2.2262480693
H,0,-2.023967518,2.173864425,-1.0715597498
H,0,-1.3999940165,3.5110252818,0.9345612144
H,0,-2.1118871927,1.9710866751,1.4287246137
H,0,-0.0199554757,2.5537066484,2.7494667528
H,0,0.0745816543,1.0172270864,1.8987521865
H,0,1.3634736285,3.6667371555,1.0462213416
H,0,2.2107495573,2.1986675594,1.5016788636
H,0,-3.9735674871,-2.5412174629,-1.5100670352
H,0,-2.3870628674,-1.775535983,-1.7452199874
H,0,-2.6679835907,-2.8237769602,-0.3380362468
H,0,-5.1160837199,-0.2043919176,-1.5794393255
H,0,-4.5202235426,1.0772987642,-0.5026776487
H,0,-3.519738208,0.5214278116,-1.8619472687
H,0,-5.430521491,-1.7277917638,0.5401003325
H,0,-4.0398073883,-1.9838764191,1.6163010724
H,0,-4.8193672767,-0.3908564918,1.5394582178

H,0,-0.1643856493,-0.8254250259,-0.2174972522
N,0,0.7237334473,-1.3472910854,0.0533098507
C,0,0.8218397645,-1.7721837944,1.4477603755
C,0,2.1363057511,-1.2824899987,2.0498377465
H,0,-0.0487864969,-1.3680175481,1.9690410997
H,0,0.7584526082,-2.8677052044,1.4959668364
C,0,1.7841034895,-1.1544911675,-0.7132422238
N,0,3.0307164782,-1.3693270107,-0.2699807244
C,0,4.1888401923,-0.9616583581,-1.0760456003
C,0,3.2978526654,-1.6895101957,1.1459964178
H,0,4.285513571,0.1299938066,-1.0550791255
H,0,5.081658821,-1.432580136,-0.6597088111
H,0,4.081597759,-1.2957040665,-2.1089514309
H,0,3.5047549932,-2.7649500428,1.2303490602
C,0,1.5618374654,-0.7173229488,-2.1300193533
H,0,2.1098181173,-0.1924326648,2.1439863677
H,0,2.2868059353,-1.7037640713,3.0488816607
H,0,4.206166308,-1.1551324043,1.4386346539
H,0,2.028561694,0.2652912465,-2.2753174694
H,0,1.9944762056,-1.4493166316,-2.8213576141
H,0,0.4932535204,-0.631200695,-2.3209208291

tsAxBB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.900565519

Zero-point correction= 0.449017 (Hartree/Particle)
Thermal correction to Energy= 0.472991
Thermal correction to Enthalpy= 0.473936
Thermal correction to Gibbs Free Energy= 0.395050
Sum of electronic and zero-point Energies= -962.451548
Sum of electronic and thermal Energies= -962.427574
Sum of electronic and thermal Enthalpies= -962.426630
Sum of electronic and thermal Free Energies= -962.505515

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.807	90.216	166.028

C,0,-1.2821683242,2.4586358971,1.0046404393
C,0,-0.0255535369,2.1515352691,1.8262298902
C,0,1.2533372487,2.6002155145,1.1049068617
C,0,1.3237373468,2.1719955113,-0.3689097871
C,0,0.0998825183,2.0645583954,-1.0742168644
C,0,-1.1586700919,1.9765505126,-0.423333971

O,0,2.4632811664,1.9896282859,-0.8807577027
O,0,-1.4186798123,0.2182236543,-0.3373623056
O,0,-2.5063657303,-0.2845626934,0.5236506515
C,0,-3.5821988637,-0.8412703966,-0.2672679799
C,0,-4.2030866121,0.2272576726,-1.1760925359
C,0,-3.0777182552,-2.0365655703,-1.0871729437
C,0,-4.5827883372,-1.2955151578,0.8044568939
H,0,0.1485483996,1.9159863111,-2.1494013046
H,0,-2.0357505632,2.1907499411,-1.0315991666
H,0,-1.4479625491,3.5458927729,0.9665294601
H,0,-2.1672064926,2.0132434242,1.4702481778
H,0,-0.0945117221,2.6236081242,2.8148497613
H,0,0.0114294528,1.0693487918,2.0004699912
H,0,1.3235270781,3.6981538535,1.1165694517
H,0,2.1537499064,2.2345155477,1.6123900945
H,0,-3.9010211156,-2.502847771,-1.6397524461
H,0,-2.3212507726,-1.7098752484,-1.8054038998
H,0,-2.6334870216,-2.7912475278,-0.4291620269
H,0,-5.0691313044,-0.1793268621,-1.7104400442
H,0,-4.5354641935,1.0865766562,-0.5847972889
H,0,-3.4751838731,0.5711984112,-1.9151313076
H,0,-5.4593368377,-1.7531858754,0.3336970373
H,0,-4.1250725583,-2.0316849689,1.4729418002
H,0,-4.9170902384,-0.4444213141,1.405755524
H,0,-0.1399398818,-0.7744922029,-0.1368332921
N,0,0.7510559734,-1.2993871062,0.1118918967
C,0,0.9096782107,-1.7024472831,1.5079533966
C,0,2.2599823538,-1.2210075828,2.0327129835
H,0,0.0757334359,-1.2750806512,2.0681707729
H,0,0.8324275942,-2.7956022616,1.5798267436
C,0,1.7795557853,-1.1812990971,-0.7120069417
N,0,3.0339359986,-1.4500860108,-0.3205791457
C,0,4.177182884,-1.2084878605,-1.2080970777
C,0,3.3698225619,-1.6922239895,1.0974978187
H,0,4.4338016067,-0.1429715211,-1.2138577482
H,0,5.0244771596,-1.7928209071,-0.8433171787
H,0,3.9583032781,-1.5310596753,-2.2254095104
H,0,3.5733488805,-2.7630670467,1.2305463598
C,0,1.5136570346,-0.7638713741,-2.1265876072
H,0,2.2608288624,-0.1281911352,2.0829419519
H,0,2.4443524541,-1.6056942988,3.040248207
H,0,4.29547561,-1.1493476981,1.3101989031
H,0,2.0255132823,0.1852784632,-2.3198833167
H,0,1.8676652097,-1.5317446761,-2.8220356339

H,0,0.4444865814,-0.6202555765,-2.2700699268

tsaxAB3PCM DBU model – PCM dichloroethane – 6-31G*

E(RB+HF-LYP) = -962.924991813

Zero-point correction= 0.450769 (Hartree/Particle)
Thermal correction to Energy= 0.474956
Thermal correction to Enthalpy= 0.475900
Thermal correction to Gibbs Free Energy= 0.395556
Sum of electronic and zero-point Energies= -962.392509
Sum of electronic and thermal Energies= -962.368322
Sum of electronic and thermal Enthalpies= -962.367378
Sum of electronic and thermal Free Energies= -962.447722

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.039	89.885	169.098

C,0,-1.9307790793,2.0847520427,1.2372189756
C,0,-0.5483270793,2.1784290427,1.8904859756
C,0,0.3081419207,3.2649990427,1.2301289756
C,0,0.3336469207,3.1861300427,-0.3031050244
C,0,-0.7935180793,2.6019130427,-0.9515200244
C,0,-1.8240460793,1.9611520427,-0.2608350244
O,0,1.3049889207,3.6957160427,-0.9111290244
O,0,-1.3907280793,0.0605780427,-0.4345600244
O,0,-2.0705680793,-0.8800619573,0.4544779756
C,0,-2.9522500793,-1.7403359573,-0.3009830244
C,0,-4.0224780793,-0.9110069573,-1.0205580244
C,0,-2.1410610793,-2.5773539573,-1.2988970244
C,0,-3.5820070793,-2.6261849573,0.7808509756
H,0,-0.8042170793,2.6285630427,-2.0406880244
H,0,-2.7647340793,1.8033000427,-0.7819870244
H,0,-2.5153780793,2.9917110427,1.4646289756
H,0,-2.4916630793,1.2317730427,1.6320109756
H,0,-0.6440580793,2.3652200427,2.9681559756
H,0,-0.0504360793,1.2079370427,1.7772909756
H,0,-0.0820960793,4.2610080427,1.4954899756
H,0,1.3444309207,3.2373100427,1.5881809756
H,0,-2.7947380793,-3.2297429573,-1.8894320244
H,0,-1.5979590793,-1.9145269573,-1.9777030244
H,0,-1.4144230793,-3.2070479573,-0.7720650244
H,0,-4.7257340793,-1.5623769573,-1.5527820244
H,0,-4.5875610793,-0.3092129573,-0.2996920244

H,0,-3.5527920793,-0.2392179573,-1.7433490244
H,0,-4.2773510793,-3.3435199573,0.3309279756
H,0,-2.8102510793,-3.1875249573,1.3191889756
H,0,4.1336230793,-2.0168619573,1.5050729756
H,0,0.1609189207,-0.2744569573,-0.3481490244
N,0,1.2154259207,-0.4625789573,-0.4163110244
C,0,1.9205329207,0.1756090427,-1.5305310244
C,0,3.1670589207,-0.6313899573,-1.8760960244
H,0,1.2212039207,0.2179450427,-2.3704890244
H,0,2.1665559207,1.2104720427,-1.2637940244
C,0,1.8072489207,-1.2164269573,0.4866759756
N,0,3.1290859207,-1.4453549573,0.4610029756
C,0,3.8401389207,-2.2238829573,1.4733259756
C,0,3.9786989207,-0.8899849573,-0.6101460244
H,0,4.1844669207,-3.1757939573,1.0514539756
H,0,4.7134019207,-1.6549009573,1.8102069756
H,0,3.2089089207,-2.4241569573,2.3367079756
H,0,4.4494779207,0.0329140427,-0.2447480244
C,0,0.9427739207,-1.8192599573,1.5621749756
H,0,2.8793999207,-1.5872599573,-2.3304050244
H,0,3.7838329207,-0.0898659573,-2.6001580244
H,0,4.7760929207,-1.6153349573,-0.8031950244
H,0,1.0880729207,-2.9031639573,1.6143229756
H,0,1.1960099207,-1.3977679573,2.5417589756
H,0,-0.1095320793,-1.6126849573,1.3509389756

2nd tsaxAB3PCM DBU model – PCM dichloroethane – 6-31G*

E(RB+HF-LYP) = -962.843032970

Zero-point correction= 0.451265 (Hartree/Particle)
Thermal correction to Energy= 0.475487
Thermal correction to Enthalpy= 0.476431
Thermal correction to Gibbs Free Energy= 0.395373
Sum of electronic and zero-point Energies= -962.391768
Sum of electronic and thermal Energies= -962.367546
Sum of electronic and thermal Enthalpies= -962.366602
Sum of electronic and thermal Free Energies= -962.447660

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.373	89.913	170.601

C,0,-2.287932946,1.5537454503,1.5906728803
C,0,-0.8974947579,2.0912444435,1.9465919829

C,0,-0.50643307,3.2851330347,1.0648385358
C,0,-0.7731215932,3.1075300184,-0.4350697994
C,0,-1.7944834285,2.192213975,-0.8318389411
C,0,-2.4066979846,1.2271658215,0.1058826463
O,0,-0.1539008576,3.8342335051,-1.2459352112
O,0,-1.4705831786,0.2745803894,-0.3621627465
O,0,-1.6927366278,-1.4018379147,0.5478164015
C,0,-2.1648355868,-2.3618536822,-0.3579673103
C,0,-3.5500500419,-1.9712981275,-0.9135096779
C,0,-1.179866986,-2.5767242595,-1.5266737334
C,0,-2.2928062424,-3.6728421648,0.4549449948
H,0,-2.0570603292,2.142280787,-1.8848031198
H,0,-3.4297805753,0.9240151179,-0.1510580791
H,0,-3.0579011607,2.2990125823,1.8397243563
H,0,-2.5087829849,0.6443767366,2.1603420942
H,0,-0.8613431993,2.378899615,3.0051540558
H,0,-0.1639678312,1.2871774089,1.8186168069
H,0,-1.0786257124,4.1748411859,1.3735903598
H,0,0.5505480288,3.5491895804,1.1922137754
H,0,-1.5337396059,-3.3471095637,-2.2242043614
H,0,-1.0542449255,-1.6404329195,-2.0797175736
H,0,-0.198727535,-2.8871340622,-1.1472341441
H,0,-3.972490244,-2.75944173,-1.5502859904
H,0,-4.2455164235,-1.7850656379,-0.0868110167
H,0,-3.4696650284,-1.0554927165,-1.5077151987
H,0,-2.6780294824,-4.4916157751,-0.1668768472
H,0,-1.3167360532,-3.9725851359,0.8531703156
H,0,-2.9758643016,-3.5277879408,1.2994532739
H,0,0.2453714166,-0.0550444125,-0.1400182137
N,0,1.2716765013,-0.0556100629,-0.2760975734
C,0,1.7836662241,0.758279171,-1.3821809419
C,0,3.1131872857,0.1815756683,-1.8541639638
H,0,1.0287259886,0.7419736334,-2.1719054144
H,0,1.888742714,1.79981205,-1.0561021909
C,0,2.0299013564,-0.7727179928,0.5356691549
N,0,3.361779523,-0.7777395891,0.4153094701
C,0,4.2524776107,-1.4932445719,1.3291241458
C,0,4.0391223812,-0.0241420872,-0.6592534024
H,0,4.6849874462,-2.3704371011,0.8336066747
H,0,5.06492432,-0.8215770505,1.6252776005
H,0,3.726197616,-1.810280605,2.2272388978
H,0,4.3819770172,0.9362008376,-0.2512631787
C,0,1.3347895408,-1.5775440245,1.5976049076
H,0,2.9445202543,-0.7766333042,-2.3599242077

H,0,3.5878328893,0.8589768756,-2.5706722332
H,0,4.9248828556,-0.5979481496,-0.9505999897
H,0,1.709936885,-2.6054899258,1.6103009485
H,0,1.5146290519,-1.1398647197,2.5869178032
H,0,0.2562414817,-1.5942999683,1.3933251

tsaxAB3BBPCM DBU model – PCM dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.924991813

Zero-point correction= 0.447370 (Hartree/Particle)
Thermal correction to Energy= 0.470821
Thermal correction to Enthalpy= 0.471765
Thermal correction to Gibbs Free Energy= 0.393708
Sum of electronic and zero-point Energies= -962.477620
Sum of electronic and thermal Energies= -962.454169
Sum of electronic and thermal Enthalpies= -962.453225
Sum of electronic and thermal Free Energies= -962.531282

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.445	88.485	164.285

C,0,-2.1966040305,1.5893610427,1.442786
C,0,-0.8434780305,2.1576750427,1.882118
C,0,-0.5162270305,3.4573480427,1.136337
C,0,-0.7337170305,3.3796410427,-0.376712
C,0,-1.6432620305,2.4074520427,-0.876904
C,0,-2.2861170305,1.4746890427,-0.056139
O,0,-0.1525540305,4.2306130427,-1.106479
O,0,-1.3062850305,-0.2156089573,-0.352986
O,0,-1.7483190305,-1.3358619573,0.474307
C,0,-2.3947290305,-2.3563419573,-0.328097
C,0,-3.6233140305,-1.7849429573,-1.046118
C,0,-1.3983090305,-2.9507889573,-1.332431
C,0,-2.8099560305,-3.4000189573,0.716789
H,0,-1.8323410305,2.4064580427,-1.949529
H,0,-3.1827450305,0.9961080427,-0.436604
H,0,-3.0094090305,2.2543600427,1.778448
H,0,-2.3807670305,0.6089460427,1.892704
H,0,-0.8327220305,2.3284770427,2.965865
H,0,-0.0683740305,1.4124920427,1.667997
H,0,-1.1563090305,4.2746990427,1.5043
H,0,0.5179839695,3.7740500427,1.31548
H,0,-1.8713140305,-3.7443199573,-1.921593

H,0,-1.0436390305,-2.1738229573,-2.014507
H,0,-0.5356420305,-3.3783749573,-0.810099
H,0,-4.1420730305,-2.5743369573,-1.601394
H,0,-4.3249600305,-1.3545299573,-0.323713
H,0,-3.3226170305,-1.0060409573,-1.751321
H,0,-3.3090430305,-4.2439999573,0.229015
H,0,-1.9355690305,-3.7819639573,1.253944
H,0,-3.5011920305,-2.9641579573,1.445484
H,0,0.2626219695,-0.2297709573,-0.286772
N,0,1.3357839695,-0.2068109573,-0.368401
C,0,1.8939169695,0.5543400427,-1.487806
C,0,3.2250679695,-0.0576949573,-1.910321
H,0,1.1607549695,0.5321300427,-2.298192
H,0,2.0224349695,1.6025840427,-1.189418
C,0,2.0837639695,-0.8517109573,0.505897
N,0,3.4233579695,-0.8536359573,0.426947
C,0,4.2928579695,-1.4940569573,1.415052
C,0,4.1307059695,-0.1957179573,-0.690994
H,0,4.7369209695,-2.4069909573,1.000778
H,0,5.0983289695,-0.8008619573,1.676866
H,0,3.7490379695,-1.7420049573,2.323654
H,0,4.4898089695,0.7849440427,-0.350688
C,0,1.3805819695,-1.5917569573,1.610894
H,0,3.0548979695,-1.0422459573,-2.361602
H,0,3.7151069695,0.5728080427,-2.658494
H,0,5.0073449695,-0.8076639573,-0.927468
H,0,1.7242399695,-2.6290619573,1.664294
H,0,1.5812669695,-1.1185179573,2.578243
H,0,0.3041489695,-1.5842529573,1.429658

2nd tsaxAB3BBPCM DBU model – PCM dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.926859787

Zero-point correction= 0.447998 (Hartree/Particle)
Thermal correction to Energy= 0.471364
Thermal correction to Enthalpy= 0.472309
Thermal correction to Gibbs Free Energy= 0.394614
Sum of electronic and zero-point Energies= -962.478862
Sum of electronic and thermal Energies= -962.455495
Sum of electronic and thermal Enthalpies= -962.454551
Sum of electronic and thermal Free Energies= -962.532246

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	295.786	88.451	163.522

C,0,-1.914808,-0.851066,-1.8313609756
C,0,-1.205791,-2.102165,-1.3018209756
C,0,-2.172461,-3.009988,-0.5301019756
C,0,-3.096183,-2.284679,0.4518760244
C,0,-3.315865,-0.902658,0.2871720244
C,0,-2.58724,-0.072403,-0.7011449756
O,0,-3.697958,-2.990243,1.3230020244
O,0,-1.662145,0.42035,0.2753390244
O,0,-0.600596,1.63338,-0.4242759756
C,0,-0.848899,2.899332,0.1920830244
C,0,-2.287545,3.36108,-0.0873509756
C,0,-0.587522,2.837489,1.7066760244
C,0, 0.150949,3.862337,-0.4810789756
H,0,-4.007582,-0.406146,0.9639330244
H,0,-3.181701,0.760111,-1.1011079756
H,0,-2.689812,-1.132957,-2.5588509756
H,0,-1.209793,-0.189681,-2.3475939756
H,0,-0.744456,-2.659106,-2.1273609756
H,0,-0.394431,-1.787702,-0.6360699756
H,0,-2.828513,-3.544901,-1.2345009756
H,0,-1.630878,-3.785189,0.0255640244
H,0,-0.772366,3.810525,2.1756040244
H,0,-1.243473,2.096222,2.1709130244
H,0,0.453498,2.559718,1.9078810244
H,0,-2.455918,4.367707,0.3121240244
H,0,-2.478303,3.380899,-1.1655169756
H,0,-3.003606,2.680856,0.3813800244
H,0,0.029644,4.874989,-0.0788309756
H,0,1.182922,3.545052,-0.2974929756
H,0,-0.017034,3.897345,-1.5623019756
H,0,0.691683,0.662319,0.0673200244
N,0,1.497985,0.050138,0.3387330244
C,0,1.475155,-0.582713,1.6591750244
C,0,2.905706,-0.782539,2.1478170244
H,0,0.902869,0.063017,2.3282020244
H,0,0.943615,-1.540081,1.5945050244
C,0,2.488356,-0.09934,-0.5245429756
N,0,3.558963,-0.849448,-0.2428869756
C,0,4.658397,-1.078931,-1.1832359756
C,0,3.717225,-1.501478,1.0752030244
H,0,5.54574,-0.514264,-0.8754109756
H,0,4.902598,-2.145555,-1.1831599756

H,0,4.384306,-0.790912,-2.1955689756
H,0,3.413401,-2.552703,0.9829820244
C,0,2.362661,0.603024,-1.8488169756
H,0,3.362028,0.189292,2.3706790244
H,0,2.913956,-1.374768,3.0676490244
H,0,4.783746,-1.482954,1.3206680244
H,0,3.216745,1.26418,-2.0232199756
H,0,2.319915,-0.121902,-2.6681209756
H,0,1.445346,1.192051,-1.8610229756

tsaxBB3PCM DBU model – PCM dichloroethane – 6-31G*

E(RB+HF-LYP) = -962.841832029

Zero-point correction= 0.450623 (Hartree/Particle)
Thermal correction to Energy= 0.474920
Thermal correction to Enthalpy= 0.475864
Thermal correction to Gibbs Free Energy= 0.394191
Sum of electronic and zero-point Energies= -962.391209
Sum of electronic and thermal Energies= -962.366912
Sum of electronic and thermal Enthalpies= -962.365968
Sum of electronic and thermal Free Energies= -962.447641

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.017	89.877	171.895

C,0,-1.6516109695,2.1805239695,1.2963830122
C,0,-0.2338109695,2.1692499695,1.8764770122
C,0,0.6742780305,3.1750629695,1.1588770122
C,0,0.6111550305,3.0848449695,-0.3727289878
C,0,-0.5961239695,2.6002789695,-0.9527149878
C,0,-1.6359039695,2.0415499695,-0.2045559878
O,0,1.5896850305,3.5031189695,-1.0368499878
O,0,-1.3793449695,0.1254259695,-0.3939109878
O,0,-2.1909519695,-0.7347260305,0.4689250122
C,0,-3.1406659695,-1.4850490305,-0.3168949878
C,0,-4.0805059695,-0.5419440305,-1.0781659878
C,0,-2.4010609695,-2.4211340305,-1.2822839878
C,0,-3.9079419695,-2.2838190305,0.7441160122
H,0,-0.6640439695,2.6240249695,-2.0399099878
H,0,-2.6148189695,1.9674069695,-0.6708489878
H,0,-2.1504499695,3.1319999695,1.5450930122
H,0,-2.2584399695,1.3778609695,1.7274730122
H,0,-0.2583059695,2.3733499695,2.9549640122

H,0,0.1793470305,1.1609049695,1.7520920122
H,0,0.3852200305,4.2023529695,1.4340540122
H,0,1.7220370305,3.0609239695,1.4626000122
H,0,-3.1071189695,-3.0132470305,-1.8762409878
H,0,-1.7766699695,-1.8349080305,-1.9617719878
H,0,-1.7556159695,-3.1113740305,-0.7264019878
H,0,-4.8423879695,-1.1089990305,-1.6259929878
H,0,-4.5885539695,0.1339579695,-0.3809749878
H,0,-3.5123369695,0.0586769695,-1.7933239878
H,0,-4.6612049695,-2.9237760305,0.2714640122
H,0,-3.2237699695,-2.9199860305,1.3163070122
H,0,-4.4157859695,-1.6087910305,1.4416530122
H,0,0.0161490305,-0.5344420305,-0.1170509878
N,0,0.9402210305,-1.0330200305,0.1159800122
C,0,0.9896890305,-1.8334800305,1.3395170122
C,0,2.3946520305,-1.7861990305,1.9305250122
H,0,0.2407680305,-1.4309420305,2.0255770122
H,0,0.6996850305,-2.8666260305,1.1061460122
C,0,1.9873040305,-0.8067720305,-0.6521119878
N,0,3.1996000305,-1.3015600305,-0.3599819878
C,0,4.3788480305,-1.1210800305,-1.2044049878
C,0,3.4143360305,-2.1239010305,0.8461670122
H,0,5.1708890305,-0.6302650305,-0.6280779878
H,0,4.7457890305,-2.0973660305,-1.5427509878
H,0,4.1537420305,-0.5097760305,-2.0753739878
H,0,3.3583710305,-3.1849270305,0.5666350122
C,0,1.7654800305,0.0381419695,-1.8777039878
H,0,2.5981410305,-0.7851860305,2.3289610122
H,0,2.4892620305,-2.4995690305,2.7552360122
H,0,4.4320070305,-1.9275720305,1.1987580122
H,0,2.2699970305,1.0065909695,-1.7873949878
H,0,2.1270810305,-0.4709280305,-2.7760919878
H,0,0.6984610305,0.2344919695,-1.9850819878

2nd tsaxBB3PCM DBU model – PCM dichloroethane – 6-31G*

E(RB+HF-LYP) = -962.844439077

Zero-point correction= 0.451581 (Hartree/Particle)
Thermal correction to Energy= 0.475623
Thermal correction to Enthalpy= 0.476567
Thermal correction to Gibbs Free Energy= 0.396212
Sum of electronic and zero-point Energies= -962.392858
Sum of electronic and thermal Energies= -962.368816
Sum of electronic and thermal Enthalpies= -962.367872

Sum of electronic and thermal Free Energies= -962.448227

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.458	89.686	169.122

C,0,2.039487441,-0.6931479636,1.8521617771
C,0,1.201896507,-1.94504621,1.5750614153
C,0,2.0140720171,-2.9998926408,0.814451181
C,0,2.8388319764,-2.4623709214,-0.3678612317
C,0,3.1408974777,-1.0870942321,-0.3970565066
C,0,2.6049627494,-0.1009531126,0.561847614
O,0,3.276045842,-3.3043924532,-1.2010202205
O,0,1.5713593505,0.4109171655,-0.3092109076
O,0,0.7392966785,1.6946194494,0.4019375419
C,0,0.9753842086,2.8901839747,-0.3489318163
C,0,2.4647922293,3.2614427388,-0.3116927732
C,0,0.4930721351,2.7387836269,-1.800062276
C,0,0.1452721878,3.9587890169,0.3873563563
H,0,3.7598061847,-0.7208193207,-1.2138944859
H,0,3.2999243876,0.7190261508,0.791402272
H,0,2.8835636929,-0.9442840386,2.511468584
H,0,1.4440213776,0.0723908265,2.3638090018
H,0,0.8157773665,-2.3631568791,2.5146460656
H,0,0.3274935486,-1.6557211532,0.9798144996
H,0,2.724124737,-3.4883882929,1.5010723293
H,0,1.3681471784,-3.8022434553,0.4348551483
H,0,0.6530384248,3.6650693856,-2.3644044907
H,0,1.0403342109,1.9312652143,-2.2941849905
H,0,-0.5779744417,2.505554005,-1.8316463622
H,0,2.6387436638,4.2246419277,-0.8058036767
H,0,2.8124999159,3.3375852231,0.7244431707
H,0,3.0594058994,2.4994861157,-0.8231847302
H,0,0.2738855061,4.937680659,-0.0898196152
H,0,-0.9217185565,3.7093751171,0.3672835204
H,0,0.4624210954,4.0387554605,1.4325177949
H,0,-0.7632824565,0.8425335605,0.1980727706
N,0,-1.7256896676,0.4448422454,0.2488932003
C,0,-2.5973518805,0.9758340544,1.2987598422
C,0,-3.6030507496,-0.0956311077,1.7054293112
H,0,-1.9592505497,1.2732236474,2.1352339673
H,0,-3.1116480636,1.8735229071,0.9302896706
C,0,-2.1039501423,-0.4810327472,-0.6181889434
N,0,-3.3363738999,-0.9966763264,-0.5889307651

C,0,-3.8255651534,-1.9655281613,-1.5721371786
C,0,-4.3076040341,-0.6298019354,0.4628426987
H,0,-3.8249942007,-2.9777642664,-1.1507731363
H,0,-4.8519127703,-1.6966768214,-1.8398529338
H,0,-3.2220857143,-1.9501530817,-2.4778101095
H,0,-5.0054101187,0.1108329189,0.0500997149
C,0,-1.1017125102,-0.9338766173,-1.6427076094
H,0,-3.0851109416,-0.9127679973,2.2212141552
H,0,-4.3451797273,0.3187613346,2.3946058029
H,0,-4.8816167419,-1.5309042851,0.7029514071
H,0,-1.0806983158,-2.0253488929,-1.7092227153
H,0,-1.3649799138,-0.5393386889,-2.6314682775
H,0,-0.1031014286,-0.5823985798,-1.3707338722

tsaxBB3BBPCM DBU model – PCM dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.924560565

Zero-point correction= 0.447056 (Hartree/Particle)
Thermal correction to Energy= 0.470654
Thermal correction to Enthalpy= 0.471598
Thermal correction to Gibbs Free Energy= 0.392933
Sum of electronic and zero-point Energies= -962.477505
Sum of electronic and thermal Energies= -962.453907
Sum of electronic and thermal Enthalpies= -962.452962
Sum of electronic and thermal Free Energies= -962.531628

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.340	88.625	165.566

C,0,-2.027500909,1.7054756659,1.4847028789
C,0,-0.6488206864,2.2985065783,1.793032643
C,0,-0.3818427998,3.5518240276,0.9500662673
C,0,-0.7047860325,3.3834810127,-0.5361724983
C,0,-1.6360732851,2.3771375075,-0.9123245209
C,0,-2.2212818342,1.4977451443,0.0051384232
O,0,-0.1865124806,4.1951422046,-1.3528732521
O,0,-1.2866608152,-0.2225008271,-0.2523028722
O,0,-1.8389542068,-1.3127853949,0.5491916152
C,0,-2.4729973008,-2.3070659701,-0.2931037474
C,0,-3.6383803626,-1.6922614502,-1.0785319048
C,0,-1.4444071223,-2.9369362005,-1.2424655556
C,0,-2.9819583862,-3.3383840444,0.7220386509
H,0,-1.8964439469,2.3090029809,-1.9677399302

H,0,-3.1438626408,1.0024446401,-0.2795799379
H,0,-2.8161685441,2.3921909703,1.83421031
H,0,-2.1796192378,0.7563755829,2.0079017359
H,0,-0.5619627192,2.5329916917,2.861292711
H,0,0.1136451141,1.543144251,1.5682168506
H,0,-0.9991760896,4.3884449975,1.3133705626
H,0,0.6605745654,3.8801940701,1.036751625
H,0,-1.9079609156,-3.7294719643,-1.8404369604
H,0,-1.042064719,-2.179914418,-1.9203856702
H,0,-0.6159065954,-3.3729119081,-0.6739721685
H,0,-4.1411768716,-2.4584128121,-1.679431091
H,0,-4.3741378255,-1.2537884761,-0.395734308
H,0,-3.2728420583,-0.9109605571,-1.7498237412
H,0,-3.485507608,-4.1611618691,0.2036087602
H,0,-2.1508745503,-3.7526116419,1.3021164627
H,0,-3.6944545644,-2.8793752015,1.4151549157
H,0,0.215772592,-0.4706884754,0.0490585001
N,0,1.2457988229,-0.709124622,0.2648961635
C,0,1.5625272841,-1.3282087102,1.5523378751
C,0,2.9711592278,-0.9298445652,1.9809060589
H,0,0.8097134044,-1.0000609076,2.2730075746
H,0,1.4774329421,-2.4191801164,1.461515111
C,0,2.1633053881,-0.419532224,-0.6373878664
N,0,3.4656843984,-0.6684196722,-0.4325944634
C,0,4.5081500527,-0.4150007962,-1.4282952994
C,0,3.9497071102,-1.2231515448,0.8480763862
H,0,5.1228911568,0.4412335807,-1.1275606001
H,0,5.1495999238,-1.2991414669,-1.5005243706
H,0,4.0829561901,-0.2205690889,-2.4101560054
H,0,4.1040627398,-2.3039922915,0.7272219199
C,0,1.6945866483,0.2040044831,-1.923753874
H,0,2.9974971692,0.1381143016,2.2273961676
H,0,3.2710160029,-1.4855825069,2.8745453285
H,0,4.9243883802,-0.7685989429,1.0528185685
H,0,2.2058367025,1.1532220073,-2.1084579267
H,0,1.8935208523,-0.4619679971,-2.7699383681
H,0,0.6215666686,0.3882602839,-1.8682653544

2nd tsaxBB3BBPCM DBU model – PCM dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.927256281

Zero-point correction=	0.447886 (Hartree/Particle)
Thermal correction to Energy=	0.471236
Thermal correction to Enthalpy=	0.472181

Thermal correction to Gibbs Free Energy= 0.394609
Sum of electronic and zero-point Energies= -962.479371
Sum of electronic and thermal Energies= -962.456020
Sum of electronic and thermal Enthalpies= -962.455076
Sum of electronic and thermal Free Energies= -962.532648

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.705	88.382	163.264

C,0,2.0039412257,-0.7283985773,1.8757071373
C,0,1.2446342329,-1.9976574284,1.475662681
C,0,2.1419735833,-2.9710732759,0.6996219235
C,0,3.0158085989,-2.3292418357,-0.3808079178
C,0,3.2701175724,-0.9430334693,-0.3188462293
C,0,2.6216580622,-0.0391173033,0.6601515966
O,0,3.5525708436,-3.0992540231,-1.2379111521
O,0,1.6542506974,0.4020976017,-0.2957269375
O,0,0.6323576524,1.6830018092,0.3840019137
C,0,0.861131191,2.9008287008,-0.3243487875
C,0,2.3164268827,3.3620597378,-0.1448344899
C,0,0.5260685083,2.7475214233,-1.8184961968
C,0,-0.0938716542,3.9206380399,0.3314969904
H,0,3.9285878904,-0.5048632737,-1.0651640981
H,0,3.2534508477,0.804519738,0.9686836107
H,0,2.8154250348,-0.9761766691,2.5753184492
H,0,1.3397129218,-0.0202848533,2.3838409005
H,0,0.8350441401,-2.4929616057,2.3650777707
H,0,0.3900236886,-1.7129626915,0.8520904349
H,0,2.8321303208,-3.4776804145,1.3921414987
H,0,1.5515701205,-3.7659113252,0.2279914988
H,0,0.6848535614,3.6908548811,-2.3535515442
H,0,1.1609866423,1.9801988877,-2.2695093397
H,0,-0.5219178034,2.456278984,-1.9526919901
H,0,2.4763447301,4.3381346254,-0.6172243994
H,0,2.558095898,3.4499092316,0.9196885729
H,0,3.0027464078,2.6430657944,-0.6000366363
H,0,0.0229665005,4.9052416982,-0.1366538401
H,0,-1.1376421957,3.610461838,0.2143394798
H,0,0.1228005546,4.0168130801,1.4001944091
H,0,-0.8299632593,0.8571980326,0.2362685533
N,0,-1.7806879564,0.412188964,0.2847405193
C,0,-2.6606959276,0.8332881578,1.3780176602
C,0,-3.6144770399,-0.3040124904,1.7277284444

H,0,-2.0274212728,1.104479132,2.2269681993
H,0,-3.2196381923,1.7283271447,1.07540394
C,0,-2.1329150998,-0.4756229227,-0.6312367565
N,0,-3.3387980677,-1.0546566365,-0.617525758
C,0,-3.7935194798,-1.9940411518,-1.6460681516
C,0,-4.3130163285,-0.7909756914,0.4627599186
H,0,-3.7589403155,-3.0227697291,-1.2696473403
H,0,-4.8275272673,-1.7492364975,-1.9061045941
H,0,-3.1895105621,-1.9196327633,-2.5477022413
H,0,-5.0437457757,-0.0554923808,0.1024010017
C,0,-1.1275517688,-0.8158163403,-1.6950656553
H,0,-3.0563335142,-1.1291649417,2.1866384809
H,0,-4.3627649329,0.0347918863,2.4500107091
H,0,-4.8473151,-1.7273510078,0.6540064415
H,0,-1.0150514793,-1.8989724929,-1.7922129312
H,0,-1.4505224036,-0.4208968715,-2.6650167985
H,0,-0.1577519175,-0.3874802703,-1.4376151236

Int eqAB3BB DBU model – 6-31G*

E(RB+HF-LYP) = -962.825708289

Zero-point correction= 0.453871 (Hartree/Particle)
Thermal correction to Energy= 0.477904
Thermal correction to Enthalpy= 0.478848
Thermal correction to Gibbs Free Energy= 0.398726
Sum of electronic and zero-point Energies= -962.371837
Sum of electronic and thermal Energies= -962.347804
Sum of electronic and thermal Enthalpies= -962.346860
Sum of electronic and thermal Free Energies= -962.426982

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.889	90.570	168.631

C,0,-1.4220643096,2.1441709402,1.3335880124
C,0,-0.3697461018,3.2555331106,1.3158561508
C,0,1.0139196314,2.6498840978,1.061729202
C,0,1.0538782675,1.7543175527,-0.1873530132
C,0,-0.1599133543,1.2781884036,-0.693376995
C,0,-1.4788241786,1.4018755997,-0.0126218122
O,0,2.2027225366,1.4945544546,-0.6752129633
O,0,-1.8848877839,0.0077383161,0.1982968029
O,0,-3.2699985267,0.0082574878,0.727184125
C,0,-4.0740312333,-0.8754888825,-0.0761751283

C,0,-4.1541209905,-0.3804012237,-1.5259442725
C,0,-3.5217153897,-2.3062289788,-0.0043301092
C,0,-5.442153295,-0.7829102366,0.6129417072
H,0,-0.1774084392,0.9010923619,-1.7157914412
H,0,-2.2508026982,1.8463286992,-0.6586856925
H,0,-2.4151950132,2.5286331875,1.589433647
H,0,-1.1594862298,1.4118913654,2.1088381372
H,0,-0.6038677845,3.9784997024,0.521889557
H,0,-0.3844585871,3.8116156821,2.2628149047
H,0,1.7798623799,3.4220831407,0.9209502228
H,0,1.3283262088,2.0680499566,1.9435736374
H,0,-4.1714654844,-3.0023253036,-0.5479023368
H,0,-2.5215499658,-2.3519592351,-0.4435655759
H,0,-3.456626364,-2.6342256329,1.0387833944
H,0,-4.8058754797,-1.0296584068,-2.122435561
H,0,-4.5564175023,0.6377720323,-1.5605304284
H,0,-3.1601859302,-0.376428602,-1.9812006747
H,0,-6.1673619445,-1.4263194566,0.1026172603
H,0,-5.3690106544,-1.1015145263,1.6578867058
H,0,-5.8153058987,0.2462784048,0.5915167255
H,0,0.5268091766,-0.6724698633,-0.5555494509
N,0,1.3373999775,-1.2802563058,-0.3120382324
C,0,1.4186891716,-1.5647250305,1.1243988359
C,0,2.6693073591,-0.9181033144,1.7147442457
H,0,0.5012228751,-1.1747429,1.5714077819
H,0,1.4349477318,-2.652396359,1.2729808066
C,0,2.4293828594,-1.0114258665,-1.0315986973
N,0,3.6580898131,-1.2240051032,-0.5372500102
C,0,4.8550447839,-0.944653254,-1.3263154631
C,0,3.887172325,-1.364425467,0.914230463
H,0,5.6815261555,-1.5375611393,-0.924869541
H,0,4.713157707,-1.2267118972,-2.3695045187
H,0,5.1140443108,0.120090318,-1.2720710227
H,0,4.1490028133,-2.4098274154,1.1286572364
C,0,2.2493444192,-0.7094723664,-2.4918126853
H,0,2.5819661921,0.1690314945,1.6439972479
H,0,2.7959812356,-1.1973915844,2.7655524389
H,0,4.7540394246,-0.7463167944,1.170231354
H,0,2.8068528776,0.1840668059,-2.7696978884
H,0,2.5760968338,-1.5663656055,-3.0958394465
H,0,1.1950439245,-0.5306011384,-2.6983761441

Int eqAB3BB DBU model – PCM Dichloroethane - 6-31G*

E(RB+HF-LYP) = -962.845008985

Zero-point correction= 0.452764 (Hartree/Particle)
Thermal correction to Energy= 0.475396
Thermal correction to Enthalpy= 0.476341
Thermal correction to Gibbs Free Energy= 0.400257
Sum of electronic and zero-point Energies= -962.392245
Sum of electronic and thermal Energies= -962.369613
Sum of electronic and thermal Enthalpies= -962.368668
Sum of electronic and thermal Free Energies= -962.444752

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.316	86.774	160.132

C,0,-1.1266346035,2.3617806557,0.5063772934
C,0,-0.2373528575,3.5513699218,0.1334251454
C,0,1.0608111749,3.0467938706,-0.5032604839
C,0,0.8145482975,2.1006947994,-1.6914215663
C,0,-0.4350370743,1.494755378,-1.7828331593
C,0,-1.4567372888,1.4842572394,-0.7156809108
O,0,1.7684967562,1.9629064634,-2.5310031659
O,0,-1.5095278907,0.0477555534,-0.3072805097
O,0,-2.5575274055,-0.1450852688,0.7401928836
C,0,-3.4885550971,-1.1580655069,0.299962966
C,0,-4.2109982466,-0.7224388442,-0.9801195114
C,0,-2.7654195834,-2.4972544415,0.1043551297
C,0,-4.4635083441,-1.2328771457,1.4834462793
H,0,-0.6500331769,0.9043715998,-2.6738825635
H,0,-2.4751133578,1.690595723,-1.075750786
H,0,-2.050895245,2.6886937887,0.9960229043
H,0,-0.591503629,1.7425447761,1.2385731551
H,0,-0.7644263683,4.2016765747,-0.578687863
H,0,-0.0308802256,4.1602783924,1.0246358464
H,0,1.6802674087,3.8760185696,-0.8692109956
H,0,1.6692249532,2.5255642819,0.254691938
H,0,-3.480750576,-3.2898682044,-0.1432169298
H,0,-2.03760936,-2.4272617938,-0.7091284825
H,0,-2.2379179729,-2.7832772011,1.0213400816
H,0,-4.9629296434,-1.4661654427,-1.2685951001
H,0,-4.7164954167,0.2372476353,-0.8273775234
H,0,-3.5004876588,-0.614515773,-1.804406744
H,0,-5.2353264891,-1.9850543296,1.287034597
H,0,-3.9364328021,-1.5097158861,2.40260782
H,0,-4.953907495,-0.2665982025,1.6415238492

H,0,0.0785962637,-0.669208753,0.2144305533
N,0,0.9816959418,-0.967423538,0.6185590125
C,0,1.0902038976,-0.9619892084,2.078027359
C,0,2.4946116258,-0.5193604959,2.4724986762
H,0,0.3243220264,-0.2848177919,2.4642615493
H,0,0.8751025398,-1.9669604608,2.4648190468
C,0,2.0026307617,-1.1904609413,-0.1984211258
N,0,3.2235737597,-1.4443409188,0.283453564
C,0,4.3821422106,-1.7161284786,-0.5727931847
C,0,3.5208633756,-1.3690734557,1.7313160162
H,0,5.0761421688,-2.3485966333,-0.0139284674
H,0,4.0932802091,-2.2486487223,-1.4779557353
H,0,4.8932780273,-0.786098086,-0.8481514963
H,0,3.555095245,-2.3907144549,2.1317111955
C,0,1.7426805863,-1.1261028659,-1.6733044592
H,0,2.6337774158,0.5385802458,2.2209751362
H,0,2.6434917357,-0.6295166311,3.5511190241
H,0,4.5205552535,-0.9356029002,1.8356435069
H,0,2.0751732138,-0.154069548,-2.0759904772
H,0,2.2423895907,-1.9377102811,-2.2066503325
H,0,0.6701007651,-1.1888361625,-1.8552651897

Int eqAB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.902046132

Zero-point correction= 0.450332 (Hartree/Particle)
Thermal correction to Energy= 0.474633
Thermal correction to Enthalpy= 0.475577
Thermal correction to Gibbs Free Energy= 0.394600
Sum of electronic and zero-point Energies= -962.451714
Sum of electronic and thermal Energies= -962.427413
Sum of electronic and thermal Enthalpies= -962.426469
Sum of electronic and thermal Free Energies= -962.507446

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	297.837	91.368	170.430

C,0,-1.4449507487,2.0771116129,1.389955846
C,0,-0.4367169242,3.229536107,1.3613849562
C,0,0.965826933,2.6893676137,1.0608041852
C,0,1.0110694686,1.7833994073,-0.1787000739
C,0,-0.1876417851,1.2287664729,-0.6441453513
C,0,-1.5115085087,1.3652214134,0.0308028188

O,0,2.1553725047,1.5773598887,-0.7078896404
O,0,-1.9599235484,-0.0225775104,0.2047498737
O,0,-3.3559259616,0.005710642,0.7020431072
C,0,-4.1689693603,-0.8541659025,-0.1262520043
C,0,-4.2093339047,-0.3420985396,-1.5721390126
C,0,-3.6531839611,-2.2986082196,-0.0578099821
C,0,-5.5474461071,-0.7344770919,0.5377323009
H,0,-0.2059154977,0.8490328879,-1.6650917098
H,0,-2.2678621743,1.8428647725,-0.6106793685
H,0,-2.4432321696,2.4196581764,1.6801843553
H,0,-1.1315060243,1.3401744473,2.1415666649
H,0,-0.7233002039,3.954737937,0.5870889262
H,0,-0.4475329938,3.7696818804,2.3169954519
H,0,1.6857072529,3.4969582503,0.8851284256
H,0,1.3416474843,2.1294369507,1.9319622483
H,0,-4.3130801103,-2.9692824864,-0.6196354934
H,0,-2.6480187336,-2.3671798948,-0.4811357272
H,0,-3.6154790802,-2.6382038949,0.9822699709
H,0,-4.8676966813,-0.9704741797,-2.1823669499
H,0,-4.5852579554,0.6854670512,-1.6049475131
H,0,-3.2094055136,-0.3611907635,-2.0128786222
H,0,-6.2737335714,-1.3572203648,0.0048984174
H,0,-5.5037349658,-1.0653704498,1.5798806405
H,0,-5.8979244555,0.3020682535,0.5176857086
H,0,0.614775531,-0.6757611784,-0.4652131056
N,0,1.4409165146,-1.2685106908,-0.2326914593
C,0,1.5856245298,-1.5439864736,1.1995084975
C,0,2.844906568,-0.865125309,1.7326792102
H,0,0.6819605129,-1.1760098532,1.6895843917
H,0,1.6336070753,-2.6302042466,1.3499422326
C,0,2.5021315725,-1.0493763274,-1.0088438769
N,0,3.7486684508,-1.2285588325,-0.5505494771
C,0,4.9211550555,-1.0393413843,-1.4035014608
C,0,4.0400984955,-1.3059238754,0.8961075845
H,0,5.7355003512,-1.6556737939,-1.0136492233
H,0,4.7190195734,-1.353916292,-2.426144436
H,0,5.2345615377,0.0115853942,-1.4041823973
H,0,4.3408439249,-2.3347788806,1.1358896746
C,0,2.2668509307,-0.7703162944,-2.463746335
H,0,2.7303859326,0.2193621126,1.6549665345
H,0,3.0154086507,-1.1270711707,2.7813197751
H,0,4.8982971892,-0.653910967,1.0888986718
H,0,2.8100514801,0.1224033028,-2.7737414711
H,0,2.5754939703,-1.6332720735,-3.0667877492

H,0,1.2056674265,-0.5982676833,-2.6333723074

Int eqAB3BB DBU model – PCM Dichloroethane - 6-31+G**

E(RB+HF-LYP) = -962.929006771

Zero-point correction= 0.449391 (Hartree/Particle)
Thermal correction to Energy= 0.473296
Thermal correction to Enthalpy= 0.474240
Thermal correction to Gibbs Free Energy= 0.393564
Sum of electronic and zero-point Energies= -962.479616
Sum of electronic and thermal Energies= -962.455711
Sum of electronic and thermal Enthalpies= -962.454767
Sum of electronic and thermal Free Energies= -962.535442

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.997	89.680	169.795

C,0,-1.4364469239,1.6134040963,1.5762306563
C,0,-1.0758284227,3.0820052328,1.8163868289
C,0,0.0866411024,3.4973419075,0.9064580835
C,0,-0.1654175588,3.1736269043,-0.5723319167
C,0,-1.1077999791,2.2004590688,-0.8795620378
C,0,-1.8119511968,1.3478994911,0.1091375941
O,0,0.4894399283,3.8649957811,-1.4389757858
O,0,-1.4152810269,-0.0441937434,-0.2679792077
O,0,-2.1947360602,-1.0245342729,0.5370788722
C,0,-2.9412123608,-1.9000087536,-0.3509905791
C,0,-3.9494759942,-1.1026236151,-1.186650682
C,0,-1.981075679,-2.6952843887,-1.2444430505
C,0,-3.6586937364,-2.8250878809,0.6412722646
H,0,-1.3610779856,2.0468248115,-1.9288968617
H,0,-2.9025905875,1.3480820545,-0.0193192284
H,0,-2.2487173401,1.2907057501,2.2364124307
H,0,-0.5653070433,0.9930804737,1.8241934162
H,0,-1.9472590425,3.71823675,1.6076096337
H,0,-0.8185864625,3.2362720114,2.8729232906
H,0,0.2795676423,4.5748559436,0.9778118077
H,0,1.0136898488,2.9972537591,1.2285161698
H,0,-2.538311011,-3.4109768286,-1.8585186887
H,0,-1.4317507758,-2.0272982588,-1.9130039556
H,0,-1.262967723,-3.2529456031,-0.6340202346
H,0,-4.5452020588,-1.781980718,-1.8057226509
H,0,-4.6299337743,-0.5412220456,-0.5386069675

H,0,-3.4343875657,-0.4008821698,-1.8477104962
H,0,-4.2661063957,-3.5529100128,0.0932778938
H,0,-2.9370440115,-3.371022588,1.2570589686
H,0,-4.3177368096,-2.2508891129,1.2998646208
H,0,0.2826547845,-0.6156918063,0.0019176404
N,0,1.2429279436,-0.9309787926,0.2167117833
C,0,1.4412849905,-1.719709888,1.4368607015
C,0,2.853101417,-1.4852815857,1.9618802216
H,0,0.6832260283,-1.4091103383,2.1596347124
H,0,1.2778197603,-2.7821716782,1.2143090513
C,0,2.2226355541,-0.5787857101,-0.6052038884
N,0,3.4856338921,-0.9429671001,-0.3714843532
C,0,4.6001465386,-0.6320198143,-1.2707511094
C,0,3.8570325641,-1.7103653423,0.8368825577
H,0,5.1552963942,-1.5531138593,-1.4745951331
H,0,4.2493296788,-0.2250759688,-2.2158842398
H,0,5.2740535166,0.089267571,-0.7963121574
H,0,3.9229356727,-2.7731842962,0.5683021012
C,0,1.8604828895,0.2419331764,-1.8086507714
H,0,2.9423397638,-0.461287884,2.3434523895
H,0,3.0697492173,-2.1715340164,2.7858782078
H,0,4.8555251748,-1.3789748777,1.137728827
H,0,2.4471295697,1.1638773304,-1.8405040089
H,0,2.0499086728,-0.3209354511,-2.728499553
H,0,0.8078980552,0.5252127974,-1.7640292623

tseqAB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.898243086

Zero-point correction= 0.448904 (Hartree/Particle)
Thermal correction to Energy= 0.473024
Thermal correction to Enthalpy= 0.473968
Thermal correction to Gibbs Free Energy= 0.394255
Sum of electronic and zero-point Energies= -962.449339
Sum of electronic and thermal Energies= -962.425219
Sum of electronic and thermal Enthalpies= -962.424275
Sum of electronic and thermal Free Energies= -962.503988

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.827	90.264	167.770

C,0,-1.4758490062,2.389675029,1.0221446007
C,0,-0.2839536887,3.256657393,1.450907499

C,0,1.0378370924,2.5698633039,1.0942808824
C,0,1.1294721529,2.2040712554,-0.3949058314
C,0,-0.0944891334,2.0745652612,-1.093275224
C,0,-1.3338910205,1.8858503151,-0.4146503237
O,0,2.2760119313,2.042656935,-0.8987415671
O,0,-1.4263695276,0.145025733,-0.3315244681
O,0,-2.4312617572,-0.4583157369,0.572771268
C,0,-3.4824483749,-1.1084431341,-0.1787641895
C,0,-4.2263853921,-0.1019159717,-1.0653080201
C,0,-2.9046123923,-2.2589888553,-1.0143032725
C,0,-4.4015017889,-1.6431953426,0.9283660307
H,0,-0.055794441,1.9321558324,-2.1699587546
H,0,-2.2272891188,2.0239341005,-1.0201367719
H,0,-2.4094140588,2.9572776059,1.1170495257
H,0,-1.5802704122,1.5292697732,1.6931667172
H,0,-0.3293863857,4.2243158712,0.9359674444
H,0,-0.339213487,3.4643308235,2.5277973086
H,0,1.9042637762,3.1984984852,1.3284019308
H,0,1.1470523998,1.6520045244,1.6927968413
H,0,-3.7022309297,-2.7957928839,-1.5397615265
H,0,-2.2016839393,-1.8722206616,-1.7567108467
H,0,-2.3763846624,-2.9701888578,-0.3700546986
H,0,-5.0719457585,-0.5855643371,-1.5671880628
H,0,-4.6114077734,0.7271131775,-0.4629719831
H,0,-3.5589295508,0.3018458102,-1.8307169509
H,0,-5.2502496663,-2.1774714905,0.4884541778
H,0,-3.8587437988,-2.3338031803,1.5815416915
H,0,-4.7874716687,-0.8212157395,1.5390326748
H,0,-0.0491757598,-0.6902997058,-0.0785233973
N,0,0.8673119862,-1.1619613999,0.177965068
C,0,1.0715234746,-1.4808205525,1.5901500931
C,0,2.4859514247,-1.0920246443,2.0116161199
H,0,0.3123522145,-0.9397503842,2.1592972419
H,0,0.898819799,-2.5536432772,1.7482618674
C,0,1.8515192078,-1.1220744308,-0.7026061433
N,0,3.1128865134,-1.4362481432,-0.3660228282
C,0,4.2284520495,-1.2791120263,-1.3026459757
C,0,3.4949491815,-1.6911973013,1.0366984752
H,0,5.0153110938,-1.9848030198,-1.0253818753
H,0,3.9201182453,-1.5001421634,-2.3227457612
H,0,4.6210045969,-0.2565156166,-1.2627260905
H,0,3.5943503272,-2.7752040975,1.1835084183
C,0,1.5227830944,-0.7377518204,-2.1136946504
H,0,2.5830214898,-0.0022534026,2.0109993731

H,0,2.6976813823,-1.4497858144,3.0236493873
H,0,4.4809065831,-1.2442318399,1.193762172
H,0,2.0194560506,0.2117926606,-2.3431134742
H,0,1.8423036666,-1.5166148535,-2.8125414142
H,0,0.4483738322,-0.5914568559,-2.2088531276

2nd tseqAB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.839963975

Zero-point correction= 0.451435 (Hartree/Particle)
Thermal correction to Energy= 0.475547
Thermal correction to Enthalpy= 0.476491
Thermal correction to Gibbs Free Energy= 0.395510
Sum of electronic and zero-point Energies= -962.388529
Sum of electronic and thermal Energies= -962.364417
Sum of electronic and thermal Enthalpies= -962.363473
Sum of electronic and thermal Free Energies= -962.444454

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	298.410	89.687	170.439

C,0,1.8041705643,-0.7206185053,1.7980343713
C,0,2.1634678475,-2.2023518419,1.9539588278
C,0,1.9723700102,-2.9445778442,0.6263654629
C,0,2.8314174841,-2.3360677244,-0.4938889717
C,0,3.132867207,-0.9637235994,-0.3859895525
C,0,2.5024839857,-0.0507430325,0.5903757344
O,0,3.2698708985,-3.098717361,-1.3980905648
O,0,1.5535925656,0.5089894681,-0.3433123403
O,0,0.6476494729,1.7412864529,0.3773459034
C,0,0.8740061571,2.9579204725,-0.339665201
C,0,2.3485413931,3.372353504,-0.2283114002
C,0,0.4588582347,2.8180291154,-1.8127588892
C,0,-0.0203918882,3.9874837018,0.3766766941
H,0,3.7876594526,-0.5243494896,-1.1358833232
H,0,3.167009952,0.7593895118,0.9211199084
H,0,2.0398744147,-0.1709488969,2.7177825409
H,0,0.7217809108,-0.6281526075,1.6497366731
H,0,3.2118630217,-2.2999435605,2.2685303972
H,0,1.5534929082,-2.6539423858,2.7487486929
H,0,2.2452254766,-4.00368079,0.7103908811
H,0,0.9101424628,-2.9170561397,0.3350925713
H,0,0.606614825,3.7605904794,-2.3531256312

H,0,1.0547187909,2.0405027572,-2.2984045473
H,0,-0.6005241894,2.5456966218,-1.8927180692
H,0,2.5199253,4.3430962551,-0.7084228145
H,0,2.6422540376,3.4513005921,0.8242939576
H,0,2.9875712939,2.628686657,-0.7122476461
H,0,0.1009486057,4.9786372136,-0.0764697971
H,0,-1.0777216718,3.7085757198,0.3025485839
H,0,0.2461681091,4.0567395766,1.4366880081
H,0,-0.8281133105,0.8627856619,0.1676722027
N,0,-1.7740489855,0.4259899229,0.2258368017
C,0,-2.6888127026,0.9775572028,1.2276136229
C,0,-3.6543680969,-0.1123949332,1.6798776252
H,0,-2.0805884688,1.3507953947,2.0559094712
H,0,-3.2345193435,1.82819734,0.7978791629
C,0,-2.0952738933,-0.5634417744,-0.5928205532
N,0,-3.3036325492,-1.1325178229,-0.5526541355
C,0,-3.7348634838,-2.1732600112,-1.4879970254
C,0,-4.3101880061,-0.7491004526,0.4590487347
H,0,-3.7282229266,-3.1554219542,-1.0007842103
H,0,-4.7562124727,-1.9475448794,-1.8100801344
H,0,-3.0976318608,-2.2027654677,-2.3696872522
H,0,-5.0314525772,-0.065702579,-0.0084325675
C,0,-1.0543876977,-1.0244039515,-1.5739103554
H,0,-3.1115988173,-0.8739453193,2.2521911089
H,0,-4.4275104521,0.3079773775,2.3302445098
H,0,-4.8489695821,-1.6595524695,0.7417919034
H,0,-0.9780039462,-2.1154316837,-1.5773501944
H,0,-1.3192000237,-0.7014312027,-2.5879147519
H,0,-0.0794953635,-0.6058368694,-1.3085770324

Int eqBB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.825022182

Zero-point correction= 0.453871 (Hartree/Particle)
Thermal correction to Energy= 0.477936
Thermal correction to Enthalpy= 0.478881
Thermal correction to Gibbs Free Energy= 0.399909
Sum of electronic and zero-point Energies= -962.371152
Sum of electronic and thermal Energies= -962.347086
Sum of electronic and thermal Enthalpies= -962.346142
Sum of electronic and thermal Free Energies= -962.425113

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	299.910	90.832	166.209

C,0,-1.2059963681,2.168275155,1.151531667
C,0,-0.0886490341,3.2080666982,1.2797434339
C,0,1.2380712449,2.609460379,0.8049555827
C,0,1.1492504175,2.0320028822,-0.6186624721
C,0,-0.1267757636,1.7643219825,-1.1231390086
C,0,-1.3275881902,1.62149463,-0.2860211491
O,0,2.2422744929,1.8645294313,-1.2467907265
O,0,-1.5021277071,0.1198337998,-0.2462620245
O,0,-2.6464801201,-0.2942783614,0.6397852561
C,0,-3.6331619295,-0.9995327803,-0.1377707601
C,0,-4.2284632022,-0.0971975953,-1.2253786733
C,0,-3.0266239721,-2.2723456865,-0.744798579
C,0,-4.6887917216,-1.3499894514,0.921243676
H,0,-0.2197122154,1.5069156505,-2.1766778941
H,0,-2.2462175835,1.9808461681,-0.7660100456
H,0,-2.1676503849,2.5801845547,1.4780643126
H,0,-0.9926501615,1.3293724447,1.8252594642
H,0,-0.3257589394,4.0859220298,0.6648345742
H,0,-0.0174048347,3.5574393213,2.3193775155
H,0,2.0428251417,3.3545236768,0.7968362897
H,0,1.5645869488,1.8215242068,1.5065673172
H,0,-3.7920329048,-2.8586028017,-1.266361042
H,0,-2.2428483318,-2.0174627698,-1.4638947675
H,0,-2.5896391917,-2.8991713862,0.0409248004
H,0,-5.0249508937,-0.6199054818,-1.76799245
H,0,-4.6522907719,0.8091592091,-0.7802964004
H,0,-3.4584072434,0.1963384211,-1.9439583912
H,0,-5.5146643185,-1.9058088561,0.463516465
H,0,-4.2519136598,-1.9672017666,1.713260002
H,0,-5.0926967943,-0.4398473582,1.3761713377
H,0,0.0666832944,-0.8307458598,-0.5142851295
N,0,1.0471864305,-1.1534635881,-0.5617063192
C,0,1.7142567137,-1.009140237,-1.8635508557
C,0,3.1468770285,-1.5189641009,-1.7618995169
H,0,1.1298582448,-1.5723383001,-2.5975963387
H,0,1.7272801623,0.061276339,-2.1117963763
C,0,1.676065161,-1.2125467793,0.5974256085
N,0,3.0148814555,-1.218324158,0.66986791
C,0,3.7333512728,-1.1997503304,1.9392659307
C,0,3.7974754791,-0.8778634742,-0.5384429396
H,0,4.6704516994,-1.7514857771,1.8215641568
H,0,3.96974123,-0.1718923234,2.2439003719

H,0,3.1529961931,-1.6791513839,2.7271597196
H,0,3.7999615798,0.215172304,-0.6496881526
C,0,0.8284161043,-1.3041599637,1.8379965077
H,0,3.1821951075,-2.6124796137,-1.6783381093
H,0,3.6987563749,-1.2318409136,-2.6619709243
H,0,4.8154435497,-1.2461271699,-0.383658118
H,0,0.9726358612,-2.2730508773,2.3296482054
H,0,1.0914502227,-0.5171999681,2.5507031493
H,0,-0.2261153515,-1.1953144221,1.5787545684

Int eqBB3 DBU model – 6-31+G**

E(RB+HF-LYP) = -962.901398516

Zero-point correction= 0.450583 (Hartree/Particle)
Thermal correction to Energy= 0.474948
Thermal correction to Enthalpy= 0.475893
Thermal correction to Gibbs Free Energy= 0.395875
Sum of electronic and zero-point Energies= -962.450816
Sum of electronic and thermal Energies= -962.426450
Sum of electronic and thermal Enthalpies= -962.425506
Sum of electronic and thermal Free Energies= -962.505523

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.035	91.679	168.410

C,0,-1.2987294015,2.233793169,1.1614978179
C,0,-0.1652038071,3.2516167367,1.3306588212
C,0,1.1724267224,2.6291409912,0.9175928995
C,0,1.1384211135,2.0385656928,-0.5010153975
C,0,-0.1175048671,1.775398528,-1.0577744227
C,0,-1.349465635,1.6429113238,-0.2630001739
O,0,2.2581319237,1.8529794064,-1.0829085751
O,0,-1.5035907962,0.132694635,-0.1778829554
O,0,-2.7058039093,-0.2686142188,0.6316685629
C,0,-3.6431636513,-0.9968234407,-0.1923717179
C,0,-4.161668138,-0.1267086921,-1.3441000214
C,0,-3.0015188916,-2.2885123988,-0.7185039539
C,0,-4.7693119097,-1.3151593077,0.8022479814
H,0,-0.1714943636,1.5146491864,-2.112674842
H,0,-2.2499271367,1.9675523065,-0.7964398071
H,0,-2.265511107,2.6823898481,1.4147573102
H,0,-1.152637015,1.4107503646,1.8713667041
H,0,-0.3582104215,4.1322078298,0.7049600832

H,0,-0.1306469361,3.6019803775,2.3713152042
H,0,1.9857357956,3.3637615418,0.9347539246
H,0,1.4565154669,1.842890836,1.6367048385
H,0,-3.7357774805,-2.8883967956,-1.2673657958
H,0,-2.17531588,-2.0583089459,-1.3965912098
H,0,-2.6176568608,-2.8895229054,0.1127290304
H,0,-4.9210722587,-0.6686176342,-1.9187304998
H,0,-4.612956976,0.7922782318,-0.9572768989
H,0,-3.3472770894,0.1429653436,-2.0212449434
H,0,-5.5627620398,-1.879194539,0.3006128031
H,0,-4.3914228258,-1.9144296051,1.6364446151
H,0,-5.199703346,-0.3934155519,1.2050050396
H,0,0.073510279,-0.854263394,-0.4335591553
N,0,1.0492750792,-1.1762384339,-0.5227489135
C,0,1.6486086736,-1.0593259036,-1.8588398447
C,0,3.070723802,-1.6053275565,-1.8311950741
H,0,1.0134339939,-1.612577769,-2.5563780877
H,0,1.6622951284,0.0058720549,-2.1189494194
C,0,1.7431715214,-1.2087798181,0.6018516232
N,0,3.0825451417,-1.2410773936,0.6009071369
C,0,3.8702692644,-1.1802498187,1.8298781221
C,0,3.8135069167,-0.9730052726,-0.6573379863
H,0,4.7897769142,-1.7531244292,1.6854262576
H,0,4.1369750838,-0.1439477876,2.0716976802
H,0,3.3278324844,-1.6155913216,2.667571297
H,0,3.8743389057,0.1151765356,-0.7904818397
C,0,0.9647939029,-1.2397590732,1.8889798319
H,0,3.0760124789,-2.698241587,-1.7368911577
H,0,3.5781477719,-1.346084331,-2.7646748312
H,0,4.816237571,-1.394427057,-0.5477327636
H,0,1.0976294035,-2.2018863215,2.3951308524
H,0,1.2952433174,-0.4470188567,2.5644832754
H,0,-0.0960858431,-1.0953443703,1.6804974842

Int eqBB3 DBU model – PCM Dichloroethane - 6-31G*

E(RB+HF-LYP) = -962.844738623

Zero-point correction= 0.453435 (Hartree/Particle)
Thermal correction to Energy= 0.477708
Thermal correction to Enthalpy= 0.478652
Thermal correction to Gibbs Free Energy= 0.398080
Sum of electronic and zero-point Energies= -962.391304
Sum of electronic and thermal Energies= -962.367030
Sum of electronic and thermal Enthalpies= -962.366086

Sum of electronic and thermal Free Energies= -962.446658

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.766	90.837	169.578

C,0,-1.1642170122,2.1940779024,1.1098230122
C,0,-0.0977960122,3.2932129024,1.1339470122
C,0,1.2212999878,2.7518269024,0.5748870122
C,0,1.0633089878,2.1388049024,-0.8259339878
C,0,-0.2186210122,1.7629849024,-1.2193859878
C,0,-1.3683950122,1.6078339024,-0.3027829878
O,0,2.1172259878,2.0493059024,-1.5444049878
O,0,-1.5278410122,0.1222549024,-0.2145859878
O,0,-2.6726910122,-0.2332510976,0.6738410122
C,0,-3.6250290122,-1.0296260976,-0.0658919878
C,0,-4.2103750122,-0.2356610976,-1.2393259878
C,0,-2.9731630122,-2.3334410976,-0.5451239878
C,0,-4.6976140122,-1.3133600976,0.9946620122
H,0,-0.3598850122,1.4196939024,-2.2447209878
H,0,-2.3189190122,1.9535079024,-0.7321259878
H,0,-2.1183820122,2.5607069024,1.5056660122
H,0,-0.8471960122,1.3812709024,1.7747560122
H,0,-0.4272660122,4.1467519024,0.5254170122
H,0,0.0317099878,3.6670489024,2.1592520122
H,0,1.9839269878,3.5383259024,0.5030960122
H,0,1.6343119878,1.9943499024,1.2620470122
H,0,-3.7157720122,-2.9839730976,-1.0210519878
H,0,-2.1850000122,-2.1257180976,-1.2746279878
H,0,-2.5332270122,-2.8736930976,0.3007090122
H,0,-4.9728700122,-0.8258800976,-1.7607129878
H,0,-4.6753900122,0.6896149024,-0.8822589878
H,0,-3.4257290122,0.0220279024,-1.9561219878
H,0,-5.4990260122,-1.9240050976,0.5645990122
H,0,-4.2685530122,-1.8540790976,1.8449060122
H,0,-5.1338570122,-0.3782480976,1.3615880122
H,0,0.0868799878,-0.8339340976,-0.3965069878
N,0,1.0673949878,-1.1378490976,-0.4544529878
C,0,1.6938379878,-1.0802780976,-1.7830669878
C,0,3.1166339878,-1.6202750976,-1.6973539878
H,0,1.0766989878,-1.6765940976,-2.4631889878
H,0,1.7018059878,-0.0332580976,-2.1092509878
C,0,1.7243329878,-1.2056390976,0.6917910122
N,0,3.0593559878,-1.2259370976,0.7264070122

C,0,3.8286659878,-1.3062230976,1.9670290122
C,0,3.8133849878,-0.9519350976,-0.5148399878
H,0,4.6981909878,-1.9483990976,1.8007320122
H,0,4.1793639878,-0.3125810976,2.2725720122
H,0,3.2337369878,-1.7377820976,2.7709470122
H,0,3.8474499878,0.1347429024,-0.6721779878
C,0,0.9074829878,-1.2773340976,1.9531080122
H,0,3.1228099878,-2.7093870976,-1.5682389878
H,0,3.6545519878,-1.3873270976,-2.6218289878
H,0,4.8289729878,-1.3308760976,-0.3756349878
H,0,1.0211399878,-2.2602600976,2.4249990122
H,0,1.2244109878,-0.5173380976,2.6735120122
H,0,-0.1481250122,-1.1244930976,1.7219250122

Int eqBB3 DBU model – PCM Dichloroethane - 6-31+G**

E(RB+HF-LYP) = -962.926817039

Zero-point correction= 0.449737 (Hartree/Particle)
Thermal correction to Energy= 0.473501
Thermal correction to Enthalpy= 0.474446
Thermal correction to Gibbs Free Energy= 0.394925
Sum of electronic and zero-point Energies= -962.477080
Sum of electronic and thermal Energies= -962.453316
Sum of electronic and thermal Enthalpies= -962.452371
Sum of electronic and thermal Free Energies= -962.531892

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	297.127	89.656	167.366

C,0,-1.3397017083,2.1094979925,1.2619632696
C,0,-0.4133704163,3.325105907,1.3588546156
C,0,0.9517119602,2.9996899247,0.7421696994
C,0,0.8426872009,2.4749083463,-0.6929303309
C,0,-0.3758630653,1.9414892129,-1.0997983006
C,0,-1.4987969016,1.6061559023,-0.1864521289
O,0,1.8874893316,2.5871979256,-1.4382083283
O,0,-1.5087649183,0.1096303062,-0.2001388042
O,0,-2.6115343631,-0.4142150651,0.6499317873
C,0,-3.4934774289,-1.2445538634,-0.1507829066
C,0,-4.1470705423,-0.4267231193,-1.2705653409
C,0,-2.7288839272,-2.4498009475,-0.7127544431
C,0,-4.5361154288,-1.6926819814,0.8820924347
H,0,-0.489315584,1.6501908196,-2.1440391511

H,0,-2.4801407513,1.884659166,-0.5924964719
H,0,-2.3222857109,2.3283847929,1.6941014337
H,0,-0.9144646077,1.2935970383,1.8593199451
H,0,-0.8571911939,4.1780855418,0.82746759
H,0,-0.3049786039,3.6274879518,2.4092398245
H,0,1.6023650834,3.8824612624,0.7196256191
H,0,1.4732242016,2.2503152072,1.3593315722
H,0,-3.4149813789,-3.123739164,-1.2373161835
H,0,-1.9623311289,-2.1267559718,-1.4223823435
H,0,-2.24783091,-3.0101447811,0.0958262219
H,0,-4.8539648611,-1.049600522,-1.8296130525
H,0,-4.693056191,0.4267730185,-0.8560923368
H,0,-3.3925011272,-0.0551099971,-1.9687394915
H,0,-5.2786579066,-2.3385930293,0.4018653623
H,0,-4.0627894995,-2.2545246767,1.6936089757
H,0,-5.0546182334,-0.8291794737,1.3103102019
H,0,0.1802146782,-0.6962535351,-0.4209129204
N,0,1.1658404576,-0.9737168813,-0.5005136878
C,0,1.7991971123,-0.7337277022,-1.8045485678
C,0,3.2010131213,-1.3322398034,-1.8114214648
H,0,1.171978839,-1.2083722954,-2.5664134436
H,0,1.7973782916,0.347662709,-1.9812219752
C,0,1.8087710982,-1.2568874373,0.6204278945
N,0,3.1418160351,-1.3506543612,0.6522160338
C,0,3.8975310532,-1.6542681166,1.8694755469
C,0,3.9336180921,-0.9496037665,-0.5296651317
H,0,4.7127827924,-2.3368642951,1.6155009357
H,0,4.3241503959,-0.7384527313,2.2958116253
H,0,3.2682433506,-2.1361340349,2.6151871708
H,0,4.1068338142,0.133658578,-0.4856062947
C,0,0.9797865785,-1.4845639139,1.8547410581
H,0,3.1492149553,-2.4248827412,-1.888603441
H,0,3.7593208134,-0.962198161,-2.676570604
H,0,4.9016716335,-1.4532519836,-0.4649328992
H,0,1.0517938085,-2.5296135888,2.174917618
H,0,1.3188302433,-0.8517452114,2.6795425462
H,0,-0.0662318529,-1.2589463314,1.6438548843

Int gaucheB3 DBU model - 6-31G*

E(RB+HF-LYP) = -962.825878133

Zero-point correction=	0.454975 (Hartree/Particle)
Thermal correction to Energy=	0.478533
Thermal correction to Enthalpy=	0.479477

Thermal correction to Gibbs Free Energy= 0.402756
Sum of electronic and zero-point Energies= -962.370904
Sum of electronic and thermal Energies= -962.347345
Sum of electronic and thermal Enthalpies= -962.346401
Sum of electronic and thermal Free Energies= -962.423122

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	300.284	90.134	161.473

C,0,-0.8308554138,2.9623179239,0.7709786372
C,0,0.5873233122,2.7510073155,1.3125038486
C,0,1.6145347965,2.6735709827,0.1747708287
C,0,1.1893951663,1.8069470107,-1.0241561936
C,0,-0.1610139715,1.5358035357,-1.1963143136
C,0,-1.2184208877,1.8747887618,-0.2343303174
O,0,2.1261772563,1.4384161614,-1.8172293224
O,0,-1.6217409521,0.7233163925,0.69679726
O,0,-2.0272956845,-0.4021613873,-0.1465516074
C,0,-3.3655913643,-0.8239469221,0.2193025174
C,0,-3.3970995057,-1.2725447676,1.6854945622
C,0,-4.366764088,0.3065261693,-0.0400033424
C,0,-3.611254407,-2.0047339769,-0.7278286098
H,0,-0.4666786436,1.0320544943,-2.109768905
H,0,-2.1640634465,2.1293817769,-0.7285181645
H,0,-0.8888780816,3.9253299032,0.2462597901
H,0,-1.5603151907,2.9989384606,1.5906440576
H,0,0.8477472507,3.5548332397,2.0151620101
H,0,0.5982825791,1.818529534,1.8928257526
H,0,1.8161176227,3.6836535903,-0.2136151153
H,0,2.5829970001,2.3043745161,0.5400040427
H,0,-5.3863464928,-0.0284033899,0.1826433475
H,0,-4.1395991986,1.1688257544,0.5915424324
H,0,-4.3267595379,0.6211803668,-1.0878835655
H,0,-4.3959705864,-1.632110926,1.9575502077
H,0,-2.6840211017,-2.0878856708,1.8550024714
H,0,-3.1363747258,-0.4392527148,2.3427078379
H,0,-4.6114887539,-2.4180512106,-0.5606227418
H,0,-3.5398315101,-1.6836885634,-1.7720715351
H,0,-2.8803237457,-2.8032532529,-0.5574928471
H,0,-0.3761439825,-1.3403087759,-0.1560558193
N,0,0.5707120215,-1.5816230944,0.1556965367
C,0,0.7767088342,-1.5031411749,1.6045821209
C,0,2.1474191065,-0.907084641,1.9053803495

H,0,-0.023591271,-0.8742402041,2.0013541344
H,0,0.6808318881,-2.5069640113,2.0387233712
C,0,1.5382942895,-1.474131926,-0.7494176261
N,0,2.8263846236,-1.4975236355,-0.3964995545
C,0,3.8658682225,-1.1065408899,-1.3663952091
C,0,3.2044985073,-1.569591355,1.026202851
H,0,3.7338426047,-0.0431505268,-1.6072440774
H,0,4.8406634975,-1.2961398096,-0.9144137221
H,0,3.7930413376,-1.7077387807,-2.2753330172
H,0,3.3475922308,-2.6223117463,1.3062863905
C,0,1.1622777217,-1.3322260652,-2.1871145748
H,0,2.1334221002,0.1672615045,1.7002446648
H,0,2.3989311079,-1.0493647199,2.9610858659
H,0,4.1653068422,-1.0633023917,1.1398799697
H,0,1.4689338193,-0.3091081734,-2.4878082555
H,0,1.6787061092,-2.0781900776,-2.7995538233
H,0,0.0852468946,-1.4455603043,-2.3119774472

Int gaucheB3 DBU model - 6-31+G**

E(RB+HF-LYP) = -962.901682774

Zero-point correction= 0.451487 (Hartree/Particle)
Thermal correction to Energy= 0.475532
Thermal correction to Enthalpy= 0.476477
Thermal correction to Gibbs Free Energy= 0.397937
Sum of electronic and zero-point Energies= -962.450196
Sum of electronic and thermal Energies= -962.426150
Sum of electronic and thermal Enthalpies= -962.425206
Sum of electronic and thermal Free Energies= -962.503746

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.401	91.174	165.300

C,0,-0.8971873686,2.9994145981,0.7821362374
C,0,0.4988611654,2.8163147239,1.389789456
C,0,1.5765273862,2.7283237189,0.3000217396
C,0,1.2201760718,1.8200430581,-0.8888164041
C,0,-0.1217251658,1.5527245198,-1.1365614804
C,0,-1.2265110938,1.8967929534,-0.2276545199
O,0,2.2010853558,1.409647742,-1.608465838
O,0,-1.6555821253,0.749094562,0.7022984583
O,0,-2.0299160328,-0.3963428619,-0.1279405639
C,0,-3.3863020063,-0.8124959742,0.1927482045

C,0,-3.4756799056,-1.2295601477,1.6661134298
C,0,-4.3784438576,0.3095127958,-0.1312390786
C,0,-3.5932359827,-2.0145204706,-0.7371743286
H,0,-0.3765886158,1.0193230686,-2.0480689702
H,0,-2.1512435386,2.132326241,-0.7670109034
H,0,-0.9444919803,3.9545097734,0.242894662
H,0,-1.6625805782,3.0346333041,1.5674840241
H,0,0.7182424303,3.6402813122,2.0820844718
H,0,0.499251433,1.8972000028,1.9907689788
H,0,1.770560781,3.7277862915,-0.1168253065
H,0,2.5355828364,2.3939576896,0.7165165765
H,0,-5.4033507076,-0.0273602125,0.0586372944
H,0,-4.182594079,1.1856475129,0.4910906925
H,0,-4.2992885715,0.6016826081,-1.1827496832
H,0,-4.4839648279,-1.5876597099,1.9005644057
H,0,-2.768058213,-2.0374567419,1.8823334766
H,0,-3.2480029372,-0.3821354036,2.3168551759
H,0,-4.5961645043,-2.4281391446,-0.5918197481
H,0,-3.4918621301,-1.716317921,-1.7851599775
H,0,-2.8659037992,-2.8053833863,-0.5254413171
H,0,-0.3545914912,-1.3215092534,-0.1364675334
N,0,0.5941901347,-1.5863292061,0.1467658764
C,0,0.8607855888,-1.5311084398,1.5862883823
C,0,2.2065767971,-0.8567207394,1.8291085849
H,0,0.0436799414,-0.9665428494,2.0405493799
H,0,0.8507780862,-2.5488177396,1.9977741254
C,0,1.5409909415,-1.5140815793,-0.7844701181
N,0,2.8359963438,-1.5501954458,-0.4667559979
C,0,3.8658619931,-1.2744425368,-1.4820690787
C,0,3.2721894637,-1.4941375382,0.9431008482
H,0,3.8550187284,-0.2026276004,-1.7148952315
H,0,4.8320194197,-1.5787061102,-1.0766336108
H,0,3.6829540832,-1.8537395063,-2.3874963679
H,0,3.5154781478,-2.5106949095,1.2799358542
C,0,1.1216423645,-1.4023271059,-2.2154680613
H,0,2.1278131519,0.2069116712,1.5901048094
H,0,2.4966425671,-0.9518544089,2.8796804856
H,0,4.190257419,-0.9030044242,0.9757313964
H,0,1.4521919567,-0.4127527023,-2.5660743083
H,0,1.5774712981,-2.1920277292,-2.8197140698
H,0,0.0375824141,-1.4734437117,-2.2969772602

Int gaucheB3 DBU model – PCM Dichloroethane - 6-31G*

E(RB+HF-LYP) = -962.845136389

Zero-point correction= 0.454455 (Hartree/Particle)
Thermal correction to Energy= 0.478157
Thermal correction to Enthalpy= 0.479101
Thermal correction to Gibbs Free Energy= 0.401697
Sum of electronic and zero-point Energies= -962.390681
Sum of electronic and thermal Energies= -962.366980
Sum of electronic and thermal Enthalpies= -962.366035
Sum of electronic and thermal Free Energies= -962.443439

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	300.048	90.218	162.910

C,0,-0.8072824052,2.9422553416,0.796111605
C,0,0.6420295601,2.7169602498,1.2387144427
C,0,1.5986994685,2.7220733176,0.0394281517
C,0,1.1043285987,1.9358373721,-1.186513934
C,0,-0.2403033836,1.6167550951,-1.2708201744
C,0,-1.2500882715,1.8889903805,-0.2248225926
O,0,1.9900993871,1.6688409629,-2.0849446715
O,0,-1.5795659996,0.7104147959,0.6610297289
O,0,-2.0036358227,-0.395698243,-0.1987848595
C,0,-3.3324912464,-0.8406319815,0.1930569064
C,0,-3.3244459461,-1.3198190607,1.6489291732
C,0,-4.3514613317,0.2830355703,-0.019547992
C,0,-3.5847073835,-2.0040616522,-0.7732250834
H,0,-0.5868366512,1.1113831621,-2.1703646096
H,0,-2.2197373917,2.1684696527,-0.6583160296
H,0,-0.9035187904,3.9262219318,0.3168679135
H,0,-1.4860318594,2.9382574042,1.6589689992
H,0,0.938100913,3.4789914914,1.9728010027
H,0,0.6978773549,1.7491516519,1.7527561151
H,0,1.7849535027,3.7590931475,-0.2843548904
H,0,2.5819216348,2.3221186828,0.3227332743
H,0,-5.3602878679,-0.0713845633,0.2203115103
H,0,-4.1232299501,1.1352219306,0.6259231813
H,0,-4.3418863472,0.6190156653,-1.0617318821
H,0,-4.314282398,-1.6953679051,1.9318320273
H,0,-2.6015115682,-2.1322944256,1.7863568196
H,0,-3.0602928726,-0.4989708946,2.3207550275
H,0,-4.5778874365,-2.4283811464,-0.5920475315
H,0,-3.5391918467,-1.6620804003,-1.8124654253
H,0,-2.8438060369,-2.7991975322,-0.6339051525

H,0,-0.3809736728,-1.3573721603,-0.0415421185
N,0,0.5718354138,-1.5786708352,0.2640231302
C,0,0.7924178351,-1.6093095945,1.7134637478
C,0,2.1722304176,-1.0498495995,2.0453244632
H,0,0.0023744562,-1.0077447035,2.1695327126
H,0,0.6917493927,-2.6418003656,2.0713803646
C,0,1.5313442676,-1.4403440723,-0.6431251952
N,0,2.8199764506,-1.4569585553,-0.3007203725
C,0,3.8541390188,-1.1529816603,-1.3018587908
C,0,3.2178277824,-1.6474093609,1.1076073976
H,0,3.6620926631,-0.1620521354,-1.7281798815
H,0,4.8233466778,-1.1592328035,-0.8023631343
H,0,3.8728710993,-1.9070629516,-2.0949397306
H,0,3.3517384459,-2.7204457489,1.2997656172
C,0,1.143736792,-1.2857353723,-2.0795961474
H,0,2.1688166092,0.0394873172,1.9344721797
H,0,2.432032169,-1.2825703908,3.0827279768
H,0,4.1841755835,-1.158391732,1.2510627107
H,0,1.4450706571,-0.2790760544,-2.4188129399
H,0,1.6443060983,-2.0461098014,-2.6889782869
H,0,0.0643412266,-1.3915205523,-2.1905225731

Int gaucheB3 DBU model – PCM Dichloroethane - 6-31+G**

E(RB+HF-LYP) = -962.926189324

Zero-point correction= 0.450342 (Hartree/Particle)
Thermal correction to Energy= 0.474668
Thermal correction to Enthalpy= 0.475612
Thermal correction to Gibbs Free Energy= 0.395179
Sum of electronic and zero-point Energies= -962.475847
Sum of electronic and thermal Energies= -962.451521
Sum of electronic and thermal Enthalpies= -962.450577
Sum of electronic and thermal Free Energies= -962.531010

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	297.859	91.300	169.286

C,0,-1.4383120854,2.7529750854,1.0564830305
C,0,0.0031489146,2.7307310854,1.5782460305
C,0,0.9992769146,3.0868500854,0.4666970305
C,0,0.7296519146,2.4036080854,-0.8794729695
C,0,-0.5148260854,1.8473510854,-1.1145229695
C,0,-1.6189440854,1.7926890854,-0.1237109695

O,0,1.7033769146,2.4267550854,-1.7366469695
O,0,-1.7680120854,0.4659400854,0.5787750305
O,0,-1.8948590854,-0.5815579146,-0.4355469695
C,0,-3.1335160854,-1.3279339146,-0.2342269695
C,0,-3.1327230854,-1.9928639146,1.1468050305
C,0,-4.3436620854,-0.4063399146,-0.4127499695
C,0,-3.0652900854,-2.3734039146,-1.3540079695
H,0,-0.6961830854,1.3960080854,-2.0882319695
H,0,-2.5946620854,1.9514810854,-0.6005749695
H,0,-1.6937810854,3.7615940854,0.7046170305
H,0,-2.1490560854,2.5025640854,1.8539570305
H,0,0.1106029146,3.4219310854,2.4245580305
H,0,0.2225409146,1.7260640854,1.9610530305
H,0,0.9898879146,4.1738230854,0.2887560305
H,0,2.0257009146,2.8416990854,0.7685870305
H,0,-5.2693840854,-0.9850049146,-0.3254669695
H,0,-4.3525270854,0.3722660854,0.3540790305
H,0,-4.3251900854,0.0685220854,-1.3986329695
H,0,-4.0351550854,-2.6006309146,1.2724790305
H,0,-2.2627260854,-2.6481009146,1.2613710305
H,0,-3.1114100854,-1.2393889146,1.9380810305
H,0,-3.9570190854,-3.0073519146,-1.3192339695
H,0,-3.0230000854,-1.8906519146,-2.3351789695
H,0,-2.1863950854,-3.0163379146,-1.2403179695
H,0,-0.1141680854,-1.1421539146,-0.1322169695
N,0,0.8279739146,-1.3481829146,0.2163610305
C,0,0.9638979146,-1.5822419146,1.6578240305
C,0,2.3068779146,-1.0434069146,2.1380010305
H,0,0.1295439146,-1.0760359146,2.1489170305
H,0,0.8794269146,-2.6574699146,1.8607830305
C,0,1.8465739146,-1.1451299146,-0.6100709695
N,0,3.1110139146,-1.2307949146,-0.1889309695
C,0,4.2340079146,-1.0963209146,-1.1263399695
C,0,3.4207269146,-1.5417439146,1.2223340305
H,0,4.1400399146,-0.1853319146,-1.7211869695
H,0,5.1541379146,-1.0311459146,-0.5458689695
H,0,4.3050149146,-1.9628519146,-1.7925159695
H,0,3.5643599146,-2.6254799146,1.3292790305
C,0,1.5446719146,-0.7940399146,-2.0324449695
H,0,2.2923439146,0.0520310854,2.1356250305
H,0,2.5013389146,-1.3743759146,3.1624540305
H,0,4.3659569146,-1.0509299146,1.4680170305
H,0,1.6952249146,0.2901410854,-2.1712119695
H,0,2.1858749146,-1.3467539146,-2.7226059695

H,0.5023369146,-1.0190579146,-2.2570829695

tbuoocyclohexanoneB3 - 6-31G*

E(RB+HF-LYP) = -617.499588925

Zero-point correction=	0.271937 (Hartree/Particle)
Thermal correction to Energy=	0.286175
Thermal correction to Enthalpy=	0.287119
Thermal correction to Gibbs Free Energy=	0.230167
Sum of electronic and zero-point Energies=	-617.227652
Sum of electronic and thermal Energies=	-617.213414
Sum of electronic and thermal Enthalpies=	-617.212470
Sum of electronic and thermal Free Energies=	-617.269422

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.577	53.931	119.865

C,0,-0.2082626084,1.5757296991,1.4395737677
C,0,1.2443463653,1.3699834312,1.8874995072
C,0,2.2322231147,2.1438568235,0.9911788145
C,0,2.0099955034,1.866073017,-0.4895291744
C,0,0.5571098109,1.9327871165,-0.9581940138
C,0,-0.4048800636,1.1751473886,-0.0292816389
O,0,2.9215595296,1.6420022912,-1.2609805007
O,0,-0.0816237829,-0.2008999151,-0.2507348727
O,0,-1.0584445429,-0.9868308029,0.5090255164
C,0,-1.4657809575,-2.1127049523,-0.3061584993
C,0,-2.173382945,-1.6289823369,-1.5768026125
C,0,-0.2531198183,-2.9932097222,-0.6294119132
C,0,-2.4406801424,-2.8355259134,0.6319113739
H,0,0.2515079185,2.9891123968,-0.9623841121
H,0,-1.4448413831,1.3460105387,-0.338005399
H,0,-0.4989721138,2.6304171476,1.5514706131
H,0,-0.8880969924,0.9870113858,2.0626954063
H,0,1.3679261529,1.68496584,2.930116725
H,0,1.4793639128,0.3005607201,1.8465676078
H,0,2.0836849363,3.2249772353,1.1439418805
H,0,3.2752669385,1.9188766222,1.2322557013
H,0,-0.5674105165,-3.8914741127,-1.172753793
H,0,0.4670732054,-2.4509373743,-1.2476414788
H,0,0.2480034752,-3.3033063792,0.2934776163
H,0,-2.538993587,-2.4816052872,-2.1598243459
H,0,-3.0296853477,-0.995214379,-1.3212972002

H,0,-1.4873850476,-1.0545924746,-2.2050386172
H,0,-2.8291718932,-3.7343400653,0.1417817717
H,0,-1.937084217,-3.1348225288,1.5564965538
H,0,-3.2856337314,-2.1884813826,0.8891563198
H,0,0.4971091045,1.5597422032,-1.9842100599

tbuoocyclohexanoneB3BB - 6-31+G**

E(RB+HF-LYP) = -617.545699234

Zero-point correction= 0.269910 (Hartree/Particle)
Thermal correction to Energy= 0.284254
Thermal correction to Enthalpy= 0.285198
Thermal correction to Gibbs Free Energy= 0.227904
Sum of electronic and zero-point Energies= -617.275789
Sum of electronic and thermal Energies= -617.261446
Sum of electronic and thermal Enthalpies= -617.260501
Sum of electronic and thermal Free Energies= -617.317795

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	178.372	54.380	120.585

C,0,-0.183259816,1.5627637924,1.4588934479
C,0,1.274542316,1.3508455338,1.8869814489
C,0,2.2543083871,2.1350640829,0.9904651262
C,0,2.0120019256,1.8932943201,-0.4909086363
C,0,0.5564261304,1.9411318851,-0.9456897961
C,0,-0.4022910763,1.1840064507,-0.0123581808
O,0,2.9208343431,1.7178601991,-1.2834493726
O,0,-0.1082389816,-0.1968822179,-0.2593256987
O,0,-1.0961811041,-0.978594171,0.493144476
C,0,-1.4771604985,-2.1281451846,-0.3098981683
C,0,-2.1676070272,-1.6739625189,-1.6009256695
C,0,-0.2489985817,-3.000268104,-0.5952362615
C,0,-2.4608490154,-2.8445968308,0.6239196662
H,0,0.2485483737,2.9963760415,-0.947247042
H,0,-1.4428595297,1.3742370842,-0.306901344
H,0,-0.4700879223,2.6164503988,1.5857004298
H,0,-0.8569081248,0.9696887394,2.0838692952
H,0,1.4094502202,1.6548372506,2.9308916035
H,0,1.510960701,0.2824631574,1.8335921018
H,0,2.114226065,3.214180477,1.1614825754
H,0,3.299165957,1.9016707817,1.2125120361
H,0,-0.5475914751,-3.9103241844,-1.1263952694

H,0,0.4755837826,-2.4636649153,-1.2122774737
H,0,0.2390498,-3.2889305849,0.3407611383
H,0,-2.5153911334,-2.5427488275,-2.1696713839
H,0,-3.0333855757,-1.04384271,-1.3726900516
H,0,-1.4769910146,-1.1082358449,-2.2310891822
H,0,-2.8299172936,-3.7538744645,0.1392853792
H,0,-1.9712720831,-3.125870451,1.5609033793
H,0,-3.3173300655,-2.2039242151,0.8550484498
H,0,0.4907587946,1.5716412247,-1.9721877411

tbuoocyclohexanoneB3 – PCM Dichloroethane - 6-31G*

E(RB+HF-LYP) = -617.507326327

Zero-point correction= 0.271406 (Hartree/Particle)
Thermal correction to Energy= 0.285591
Thermal correction to Enthalpy= 0.286536
Thermal correction to Gibbs Free Energy= 0.229988
Sum of electronic and zero-point Energies= -617.235921
Sum of electronic and thermal Energies= -617.221735
Sum of electronic and thermal Enthalpies= -617.220791
Sum of electronic and thermal Free Energies= -617.277338

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.211	53.947	119.014

C,0,-0.239571168,1.5901028417,1.399131551
C,0,1.2052583881,1.4600889618,1.8970473775
C,0,2.1903522428,2.2263612325,0.9898803048
C,0,2.0190033888,1.8686273337,-0.475996206
C,0,0.584985224,1.8639284651,-0.9894679564
C,0,-0.3810100391,1.1186629849,-0.0537066734
O,0,2.9649575136,1.6344514327,-1.2113560377
O,0,-0.0072379256,-0.2583554863,-0.2071409459
O,0,-0.9764272294,-1.053330703,0.5495393715
C,0,-1.4742180058,-2.1148996739,-0.3062355902
C,0,-2.2117102976,-1.5351306357,-1.5177246933
C,0,-0.3200982002,-3.0306106781,-0.7291420668
C,0,-2.4419912121,-2.8427792312,0.6349526332
H,0,0.2481628079,2.9096777081,-1.0475477474
H,0,-1.4143232771,1.2477254384,-0.4019991922
H,0,-0.5705364949,2.6371440595,1.4536938029
H,0,-0.9162732735,1.0055547425,2.0304402591
H,0,1.2886726771,1.8347254,2.9236985571

H,0,1.4835419273,0.4000016412,1.9188982128
H,0,1.9931654937,3.3068740061,1.0803044017
H,0,3.2334398956,2.0556249362,1.2748041027
H,0,-0.6994033781,-3.8799430476,-1.3084013709
H,0,0.3995637846,-2.4865712248,-1.3471218076
H,0,0.2016685967,-3.4177512808,0.1526602032
H,0,-2.6440511715,-2.3415345578,-2.1205535487
H,0,-3.0239466372,-0.8749911489,-1.1941416111
H,0,-1.5271886422,-0.9651716986,-2.15218678
H,0,-2.8904034998,-3.6961613816,0.115567889
H,0,-1.9162087348,-3.2140374821,1.5207530597
H,0,-3.2459632025,-2.1741755454,0.9602802291
H,0,0.5637423361,1.4447778839,-1.9999198457

tbuoocyclohexanoneB3BB – PCM Dichloroethane - 6-31+G**

E(RB+HF-LYP) = -617.507326327

Zero-point correction= 0.271406 (Hartree/Particle)
Thermal correction to Energy= 0.285591
Thermal correction to Enthalpy= 0.286536
Thermal correction to Gibbs Free Energy= 0.229988
Sum of electronic and zero-point Energies= -617.235921
Sum of electronic and thermal Energies= -617.221735
Sum of electronic and thermal Enthalpies= -617.220791
Sum of electronic and thermal Free Energies= -617.277338

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.211	53.947	119.014

C,0,-0.239571168,1.5901028417,1.399131551
C,0,1.2052583881,1.4600889618,1.8970473775
C,0,2.1903522428,2.2263612325,0.9898803048
C,0,2.0190033888,1.8686273337,-0.475996206
C,0,0.584985224,1.8639284651,-0.9894679564
C,0,-0.3810100391,1.1186629849,-0.0537066734
O,0,2.9649575136,1.6344514327,-1.2113560377
O,0,-0.0072379256,-0.2583554863,-0.2071409459
O,0,-0.9764272294,-1.053330703,0.5495393715
C,0,-1.4742180058,-2.1148996739,-0.3062355902
C,0,-2.2117102976,-1.5351306357,-1.5177246933
C,0,-0.3200982002,-3.0306106781,-0.7291420668
C,0,-2.4419912121,-2.8427792312,0.6349526332
H,0,0.2481628079,2.9096777081,-1.0475477474

H,0,-1.4143232771,1.2477254384,-0.4019991922
H,0,-0.5705364949,2.6371440595,1.4536938029
H,0,-0.9162732735,1.0055547425,2.0304402591
H,0,1.2886726771,1.8347254,2.9236985571
H,0,1.4835419273,0.4000016412,1.9188982128
H,0,1.9931654937,3.3068740061,1.0803044017
H,0,3.2334398956,2.0556249362,1.2748041027
H,0,-0.6994033781,-3.8799430476,-1.3084013709
H,0,0.3995637846,-2.4865712248,-1.3471218076
H,0,0.2016685967,-3.4177512808,0.1526602032
H,0,-2.6440511715,-2.3415345578,-2.1205535487
H,0,-3.0239466372,-0.8749911489,-1.1941416111
H,0,-1.5271886422,-0.9651716986,-2.15218678
H,0,-2.8904034998,-3.6961613816,0.115567889
H,0,-1.9162087348,-3.2140374821,1.5207530597
H,0,-3.2459632025,-2.1741755454,0.9602802291
H,0,0.5637423361,1.4447778839,-1.9999198457

tseqBB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.822351428

Zero-point correction= 0.452736 (Hartree/Particle)
Thermal correction to Energy= 0.476433
Thermal correction to Enthalpy= 0.477377
Thermal correction to Gibbs Free Energy= 0.399388
Sum of electronic and zero-point Energies= -962.369615
Sum of electronic and thermal Energies= -962.345919
Sum of electronic and thermal Enthalpies= -962.344975
Sum of electronic and thermal Free Energies= -962.422964

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.966	89.369	164.142

C,0,-1.0931994859,2.6175580956,0.5763299367
C,0,0.1495416323,3.2516783959,1.2157954765
C,0,1.3526998311,2.3106900573,1.1120731463
C,0,1.6339257367,1.8817153249,-0.3368523392
C,0,0.5504161022,1.9567290998,-1.2446136626
C,0,-0.7976352932,2.0440653178,-0.8085490202
O,0,2.7955629837,1.492770691,-0.6272204474
O,0,-1.290000885,0.339546881,-0.7471821452
O,0,-2.4230535817,-0.0324726631,0.1159883567
C,0,-3.550308931,-0.4584983955,-0.6800206473

C,0,-4.0244248365,0.6765554018,-1.5948748066
C,0,-3.1775823075,-1.7048511137,-1.4930867487
C,0,-4.6082972935,-0.786116102,0.3816761163
H,0,0.7549556574,1.7561713783,-2.2941345798
H,0,-1.5252760722,2.3248055451,-1.5672505642
H,0,-1.8948996868,3.362922775,0.4967755902
H,0,-1.4904153712,1.8217732092,1.2162670297
H,0,0.3900997843,4.1867425302,0.6940106276
H,0,-0.0577230856,3.5147897032,2.2620946431
H,0,2.2688954376,2.7708404509,1.5005475571
H,0,1.174808564,1.412097482,1.7257462339
H,0,-4.0310565029,-2.0602015884,-2.0821360328
H,0,-2.3556909828,-1.4712538552,-2.1750727447
H,0,-2.8589986519,-2.5151476329,-0.8268826516
H,0,-4.9288080055,0.3825864672,-2.1404889451
H,0,-4.2526345451,1.5716290877,-1.0060455239
H,0,-3.2478447932,0.9266552127,-2.3222784228
H,0,-5.5316977856,-1.1353322229,-0.0935838387
H,0,-4.2496948204,-1.5717565529,1.055672384
H,0,-4.8405836804,0.1011425774,0.9799660856
H,0,-0.0309321385,-0.7322626511,-0.5639772122
N,0,0.8730425882,-1.256328243,-0.3996191203
C,0,1.8270057769,-1.2756243984,-1.5157511441
C,0,3.0624395052,-2.0817965882,-1.1321520388
H,0,1.3119687711,-1.7070901731,-2.3797647076
H,0,2.1149215038,-0.2407780266,-1.7321714449
C,0,1.1960668257,-1.4740131747,0.8581986151
N,0,2.4547093982,-1.7709954409,1.2237284817
C,0,2.8597861135,-1.9322657159,2.6151654321
C,0,3.5427094416,-1.6077821492,0.2374656323
H,0,3.6290650568,-2.7084107203,2.6729981687
H,0,3.2771385039,-0.9990426483,3.0155626491
H,0,2.0194002746,-2.23885562,3.2365130575
H,0,3.8172415377,-0.5458690814,0.1936501355
C,0,0.0886532956,-1.4095099521,1.8770004418
H,0,2.8432252508,-3.1563003099,-1.0991588562
H,0,3.8504539706,-1.9220924005,-1.8743242024
H,0,4.3950862622,-2.1963324198,0.5888410537
H,0,-0.0514832752,-2.3896594651,2.3476042775
H,0,0.3230080618,-0.6869852777,2.6647810392
H,0,-0.8476379599,-1.1134838771,1.3979612142

2nd tseqBB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.818858563

Zero-point correction= 0.452404 (Hartree/Particle)
Thermal correction to Energy= 0.476295
Thermal correction to Enthalpy= 0.477239
Thermal correction to Gibbs Free Energy= 0.398459
Sum of electronic and zero-point Energies= -962.366455
Sum of electronic and thermal Energies= -962.342564
Sum of electronic and thermal Enthalpies= -962.341620
Sum of electronic and thermal Free Energies= -962.420399

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	298.879	89.806	165.806

C,0,-1.7784212684,2.4891694415,0.8793995587
C,0,-0.5461741999,3.3014396919,1.3044072713
C,0,0.7590857554,2.5795378235,0.9472114063
C,0,0.8629425568,2.2826220247,-0.5525154573
C,0,-0.3703982321,2.1127656683,-1.2556528332
C,0,-1.6216033992,1.855341119,-0.5137854685
O,0,1.9922522157,2.1986288249,-1.0868802981
O,0,-1.2109693024,0.4891640888,-0.4738367932
O,0,-2.2318442746,-0.69227017,0.6178503676
C,0,-3.1427490038,-1.4513428374,-0.1266151337
C,0,-4.2280076608,-0.5581546466,-0.7619349048
C,0,-2.4370804859,-2.2733016816,-1.2263225302
C,0,-3.8021607759,-2.4114314148,0.8929407427
H,0,-0.344514838,1.9622977935,-2.32975375
H,0,-2.5295559165,1.9678982515,-1.1169012691
H,0,-2.6650737804,3.1353516902,0.8889292143
H,0,-1.9767304731,1.6657023872,1.5737251557
H,0,-0.5555286212,4.2717514822,0.79000828
H,0,-0.5859120698,3.5179184925,2.3799605154
H,0,1.641826316,3.1663343152,1.2260806903
H,0,0.8182003996,1.63122012,1.5020723998
H,0,-3.1409476885,-2.902726463,-1.7859594905
H,0,-1.9453923738,-1.5966684454,-1.9337548319
H,0,-1.675351184,-2.9267691318,-0.7827904282
H,0,-5.0151569837,-1.1509997956,-1.2454441441
H,0,-4.6900264231,0.0697485919,0.0080408035
H,0,-3.783752706,0.0972827176,-1.5183162854
H,0,-4.5528951198,-3.0519201537,0.4116928505
H,0,-3.0434586336,-3.0538099854,1.3543590757
H,0,-4.2903771433,-1.8369177107,1.6872353027

H,0,0.0864823488,-0.6862118626,-0.5954932567
N,0,1.0712207556,-0.993220304,-0.5839861043
C,0,1.8229780562,-0.7951537142,-1.8291028773
C,0,3.2607102375,-1.268366762,-1.6472885771
H,0,1.3103566215,-1.3587659884,-2.6149160705
H,0,1.8005449152,0.2734761056,-2.0705280552
C,0,1.6016375377,-1.1514593137,0.6143226306
N,0,2.9326720425,-1.15152492,0.7835252335
C,0,3.5708040253,-1.3031662974,2.086271798
C,0,3.7956208299,-0.709430694,-0.330764882
H,0,4.4574516542,-1.9359430726,1.9786663684
H,0,3.883700991,-0.3296731841,2.4849889854
H,0,2.8957186723,-1.7757110979,2.7976356012
H,0,3.7986281442,0.3879105667,-0.3581276094
C,0,0.6563315976,-1.3529774708,1.7658190086
H,0,3.3182855133,-2.3634789687,-1.6339188508
H,0,3.8745550663,-0.9103218545,-2.4791904274
H,0,4.8081910176,-1.0674411165,-0.1260304962
H,0,0.7813248347,-2.3611183562,2.1795754256
H,0,0.8601605821,-0.6334741698,2.5651019922
H,0,-0.3846052413,-1.2324521579,1.4308736775

tseqBB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.899268353

Zero-point correction= 0.449324 (Hartree/Particle)
Thermal correction to Energy= 0.473332
Thermal correction to Enthalpy= 0.474276
Thermal correction to Gibbs Free Energy= 0.395293
Sum of electronic and zero-point Energies= -962.449944
Sum of electronic and thermal Energies= -962.425937
Sum of electronic and thermal Enthalpies= -962.424992
Sum of electronic and thermal Free Energies= -962.503975

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	297.020	90.209	166.234

C,0,-1.1158607751,2.6421485486,0.6220762618
C,0,0.1201551086,3.3089971598,1.2416202586
C,0,1.3372185963,2.3828645982,1.1543942281
C,0,1.6143059564,1.9056678152,-0.2783784046
C,0,0.532037638,1.9492060323,-1.1897435164
C,0,-0.8203296433,2.0463054165,-0.7536092854

O,0,2.7795009898,1.5053677357,-0.5555128255
O,0,-1.2855285904,0.3509017478,-0.660532695
O,0,-2.4807809168,-0.0202058828,0.123295798
C,0,-3.5573358923,-0.459291923,-0.7397723916
C,0,-3.9760663944,0.6589619489,-1.7017372144
C,0,-3.1400426476,-1.7204696603,-1.5079245588
C,0,-4.6804292194,-0.7703939273,0.2590233314
H,0,0.7357108754,1.7325423484,-2.2355348595
H,0,-1.5445261443,2.3152082535,-1.5194754991
H,0,-1.9331112202,3.3683134388,0.5359003768
H,0,-1.4889606835,1.8496813629,1.2806056118
H,0,0.3450213554,4.2378275369,0.7027995108
H,0,-0.0864183195,3.5865457386,2.2837669503
H,0,2.2495460523,2.871046711,1.5149915205
H,0,1.1817403975,1.5025622931,1.7980122099
H,0,-3.9663427431,-2.0885230676,-2.1263219794
H,0,-2.2908696252,-1.5014886285,-2.1603687425
H,0,-2.8514895708,-2.5153018091,-0.8113983944
H,0,-4.8475211378,0.3506202789,-2.2900531192
H,0,-4.2385573291,1.5647827771,-1.1458689994
H,0,-3.1621817114,0.8946797355,-2.3918965437
H,0,-5.5688313954,-1.1290111939,-0.2715187208
H,0,-4.3657808091,-1.5437729977,0.9670336928
H,0,-4.9524132936,0.126399053,0.8242153288
H,0,-0.0468616877,-0.7459007233,-0.4926207316
N,0,0.8568878283,-1.2753312745,-0.3622687093
C,0,1.7580908057,-1.3191939998,-1.5196280964
C,0,2.9908235623,-2.1530982074,-1.1907792817
H,0,1.1962940233,-1.7412391264,-2.3580126574
H,0,2.0504202587,-0.2907018184,-1.7572155847
C,0,1.2384530817,-1.4782011972,0.8824871104
N,0,2.5065863636,-1.7976563436,1.19226316
C,0,2.977901764,-1.918453932,2.569292375
C,0,3.5518338514,-1.6926557439,0.1521138158
H,0,3.7484480566,-2.6930239794,2.6114259693
H,0,3.4129591421,-0.9737637483,2.9193180678
H,0,2.1698707478,-2.207452603,3.2391773686
H,0,3.8777425432,-0.6464093619,0.0891120576
C,0,0.1848490556,-1.3680880042,1.9520018188
H,0,2.7444019736,-3.2209750468,-1.1461490679
H,0,3.7461417638,-2.0153814727,-1.9697248318
H,0,4.3907483636,-2.3189131047,0.4674579299
H,0,0.0254605988,-2.3413264254,2.4287236495
H,0,0.482961718,-0.6548055551,2.725068837

H,0,-0.7570824905,-1.0356438902,1.5119685717

2nd tseqBB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.896635434

Zero-point correction=	0.448498 (Hartree/Particle)
Thermal correction to Energy=	0.472774
Thermal correction to Enthalpy=	0.473718
Thermal correction to Gibbs Free Energy=	0.392929
Sum of electronic and zero-point Energies=	-962.448138
Sum of electronic and thermal Energies=	-962.423861
Sum of electronic and thermal Enthalpies=	-962.422917
Sum of electronic and thermal Free Energies=	-962.503707

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.670	90.442	170.036

C,0,-1.8094453258,2.4324443434,0.9926855973
C,0,-0.7133727884,3.4761568336,1.2500887743
C,0,0.6499761371,2.9890164645,0.7442354721
C,0,0.6241634699,2.6478000117,-0.7490698287
C,0,-0.6297869248,2.2400802374,-1.2952166656
C,0,-1.7515452382,1.8339078608,-0.4274580862
O,0,1.6795975156,2.754339233,-1.4187553394
O,0,-1.2829276892,0.4670045248,-0.4536221276
O,0,-2.2054680773,-0.6954172661,0.6282451163
C,0,-3.0033412663,-1.5679861885,-0.1412383936
C,0,-4.0672329145,-0.7972765934,-0.9459372878
C,0,-2.1440403915,-2.4270982525,-1.0911125615
C,0,-3.7008706072,-2.4777329971,0.8973097262
H,0,-0.7024918199,2.0769888339,-2.3652339442
H,0,-2.728350061,1.8744802635,-0.9202864974
H,0,-2.7962957051,2.8805391987,1.157205142
H,0,-1.7273754576,1.5998102231,1.69930523
H,0,-0.9639713503,4.4104202866,0.7308942599
H,0,-0.6659540572,3.7156619655,2.3203122758
H,0,1.4352706575,3.7379072058,0.892221483
H,0,0.9579441105,2.0929150073,1.3053460031
H,0,-2.7578115841,-3.1414802953,-1.6531892296
H,0,-1.6228263871,-1.7835575444,-1.8062940993
H,0,-1.3973012981,-2.9925808863,-0.5215290914
H,0,-4.7470553985,-1.4822350157,-1.4670151727
H,0,-4.6592284131,-0.1640865558,-0.276798971

H,0,-3.5875276452,-0.1586644698,-1.6933499276
H,0,-4.3580972565,-3.2013332984,0.3992115676
H,0,-2.9581023768,-3.0294873047,1.4828587482
H,0,-4.3016822253,-1.8746212627,1.5848386689
H,0,0.2187028207,-0.2167692317,-0.3785818361
N,0,1.1901874753,-0.6104243889,-0.3959812974
C,0,1.953542157,-0.4290757029,-1.6351936127
C,0,3.1348604607,-1.3920440725,-1.6491075413
H,0,1.2697557244,-0.6240033101,-2.4651560249
H,0,2.2640186631,0.6207073938,-1.7074618135
C,0,1.680562493,-1.0950922259,0.7238503674
N,0,2.9718142311,-1.4688260523,0.8167559236
C,0,3.595999678,-1.9294364005,2.053776677
C,0,3.8890402421,-1.2965463174,-0.3251278907
H,0,3.9810933698,-2.9475794567,1.9262326067
H,0,4.4332132623,-1.2706037213,2.3117920574
H,0,2.889129223,-1.9232569196,2.8795139432
H,0,4.3954221703,-0.3263820265,-0.232721655
C,0,0.7424293567,-1.223936029,1.892345394
H,0,2.7873523106,-2.4212190842,-1.7980208852
H,0,3.8102038465,-1.1467937882,-2.473528377
H,0,4.6510238832,-2.0789673865,-0.2527553497
H,0,0.7784948419,-2.2361830545,2.3057550853
H,0,1.0183537844,-0.5211331702,2.685987635
H,0,-0.2851647961,-1.0202372704,1.5691037501

2nd tseqAB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.817227828

Zero-point correction= 0.451567 (Hartree/Particle)
Thermal correction to Energy= 0.475682
Thermal correction to Enthalpy= 0.476626
Thermal correction to Gibbs Free Energy= 0.396366
Sum of electronic and zero-point Energies= -962.365661
Sum of electronic and thermal Energies= -962.341546
Sum of electronic and thermal Enthalpies= -962.340602
Sum of electronic and thermal Free Energies= -962.420862

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.495	89.834	168.922

C,0,-1.8952414633,2.1669400939,1.1998947083

C,0,-0.8106549999,3.1771710791,1.5983296256
C,0,0.551392101,2.7939056888,1.0102083156
C,0,0.5094444451,2.6972555335,-0.5225907402
C,0,-0.7451990484,2.3489948311,-1.1010635851
C,0,-1.8265021753,1.7644465246,-0.2881039186
O,0,1.5515080986,2.9368227083,-1.1736243883
O,0,-1.3108685129,0.4296713668,-0.4987897508
O,0,-2.066289533,-0.8690764561,0.5161293092
C,0,-2.8866279322,-1.7006592434,-0.2676903618
C,0,-4.0567133253,-0.9158007951,-0.88855809
C,0,-2.0782263304,-2.4087689185,-1.3725506139
C,0,-3.4344527696,-2.7451339373,0.7320149567
H,0,-0.8319757044,2.3376224221,-2.1828364596
H,0,-2.8137638715,1.8247843057,-0.7588742873
H,0,-2.8860254776,2.585943558,1.4151708735
H,0,-1.8167434985,1.2472551114,1.7895261953
H,0,-1.0825556356,4.1720133072,1.2211420961
H,0,-0.7560084484,3.2617747815,2.6920995922
H,0,1.3306651552,3.5196354732,1.2685277822
H,0,0.8751088647,1.8244303228,1.4226344705
H,0,-2.6987881451,-3.1084459917,-1.9464011322
H,0,-1.6653160291,-1.6677099134,-2.064289371
H,0,-1.2463710217,-2.9718696412,-0.9315425063
H,0,-4.7525922376,-1.5784759035,-1.418637708
H,0,-4.6111232351,-0.3866156242,-0.105617772
H,0,-3.6779459693,-0.176966152,-1.601661616
H,0,-4.0948901309,-3.4628525806,0.2288652438
H,0,-2.6099925127,-3.2988700846,1.1949519574
H,0,-4.0005088733,-2.2473690409,1.5262242121
H,0,0.0586294556,-0.3540328851,-0.0702635879
N,0,0.9549155608,-0.8251340275,0.2047634285
C,0,0.991214518,-1.4342129652,1.5321649779
C,0,2.3988986134,-1.3224527051,2.106003263
H,0,0.2461407908,-0.9228207578,2.1440388376
H,0,0.6733748,-2.4810785461,1.4514694294
C,0,1.9964514616,-0.6955225235,-0.5907124744
N,0,3.217795314,-1.1243456072,-0.2190594181
C,0,4.3757414988,-1.049314055,-1.1081030739
C,0,3.4142389143,-1.8063473854,1.0713240804
H,0,4.50805763,-1.9772533146,-1.6797743329
H,0,4.280126928,-0.2120054499,-1.7979081163
H,0,5.2705106817,-0.8860594633,-0.5015867152
H,0,3.3358869425,-2.8930239393,0.9252985119
C,0,1.7799801628,-0.048738598,-1.9269479328

H,0,2.612579345,-0.2794869806,2.3661620053
H,0,2.4924631294,-1.9200504632,3.0179559135
H,0,4.434208495,-1.5934793238,1.4049918691
H,0,2.1363694754,0.9916672754,-1.911024793
H,0,2.2749065836,-0.6107717628,-2.7230266817
H,0,0.7093339441,0.0005520061,-2.1269781647

tseqAB3 DBU model – PCM Dichloroethane – 6-31G*

E(RB+HF-LYP) = -962.838772209

Zero-point correction= 0.450679 (Hartree/Particle)
Thermal correction to Energy= 0.475045
Thermal correction to Enthalpy= 0.475989
Thermal correction to Gibbs Free Energy= 0.394101
Sum of electronic and zero-point Energies= -962.388093
Sum of electronic and thermal Energies= -962.363727
Sum of electronic and thermal Enthalpies= -962.362783
Sum of electronic and thermal Free Energies= -962.444671

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.095	89.958	172.348

C,0,-1.7839749634,2.1510149268,1.1817669634
C,0,-0.7188189634,3.1315279268,1.6949509634
C,0,0.6472910366,2.8467889268,1.0615289634
C,0,0.5839340366,2.8854589268,-0.4709660366
C,0,-0.6481889634,2.4939849268,-1.0623510366
C,0,-1.6966559634,1.9278439268,-0.3205380366
O,0,1.5990060366,3.2511979268,-1.1135130366
O,0,-1.3795449634,0.0592049268,-0.4681560366
O,0,-2.1195529634,-0.8070540732,0.4530669634
C,0,-3.0761099634,-1.6131440732,-0.2673380366
C,0,-4.0842419634,-0.7275470732,-1.0095630366
C,0,-2.3454149634,-2.5496810732,-1.2387950366
C,0,-3.7636219634,-2.4067060732,0.8508799634
H,0,-0.7080029634,2.5158519268,-2.1499990366
H,0,-2.6548159634,1.8289109268,-0.8228270366
H,0,-2.7854609634,2.5284599268,1.4292469634
H,0,-1.6989569634,1.1831439268,1.6880889634
H,0,-1.0155489634,4.1577369268,1.4381439634
H,0,-0.6603539634,3.0853919268,2.7905629634
H,0,1.4063010366,3.5680239268,1.3873159634
H,0,1.0025970366,1.8514229268,1.3717239634

H,0,-3.0549969634,-3.1784610732,-1.7893670366
H,0,-1.7681079634,-1.9608700732,-1.9566440366
H,0,-1.6562869634,-3.2049080732,-0.6931400366
H,0,-4.8561839634,-1.3386960732,-1.4919130366
H,0,-4.5747279634,-0.0406360732,-0.3107350366
H,0,-3.5761419634,-0.1388380732,-1.7778060366
H,0,-4.5085289634,-3.0927220732,0.4325619634
H,0,-3.0293689634,-2.9951160732,1.4120069634
H,0,-4.2692529634,-1.7301830732,1.5485469634
H,0,0.0577630366,-0.5230850732,-0.1252630366
N,0,0.9918270366,-0.9535840732,0.1682389634
C,0,1.0527160366,-1.6253820732,1.4660879634
C,0,2.4597530366,-1.5088380732,2.0419319634
H,0,0.3050320366,-1.1602690732,2.1128389634
H,0,0.7677790366,-2.6783780732,1.3403359634
C,0,2.0340060366,-0.7853840732,-0.6219760366
N,0,3.2547910366,-1.2263580732,-0.2845570366
C,0,4.4322110366,-1.0991000732,-1.1413130366
C,0,3.4791620366,-1.9363170732,0.9892969634
H,0,4.8004100366,-2.0934360732,-1.4208520366
H,0,4.2051880366,-0.5396270732,-2.0458980366
H,0,5.2238020366,-0.5732090732,-0.5962840366
H,0,3.4295130366,-3.0185100732,0.8063989634
C,0,1.7957850366,-0.0642120732,-1.9207200366
H,0,2.6557710366,-0.4732640732,2.3442729634
H,0,2.5641320366,-2.1407060732,2.9295409634
H,0,4.4962200366,-1.7023010732,1.3194749634
H,0,2.2561070366,0.9302159268,-1.9018480366
H,0,2.1906820366,-0.6327010732,-2.7675070366
H,0,0.7228640366,0.0777169268,-2.0552350366

2nd tseqAB3BB – 6-31+G**

E(RB+HF-LYP) = -962.895307237

Zero-point correction=	0.448226 (Hartree/Particle)
Thermal correction to Energy=	0.472643
Thermal correction to Enthalpy=	0.473587
Thermal correction to Gibbs Free Energy=	0.392450
Sum of electronic and zero-point Energies=	-962.447082
Sum of electronic and thermal Energies=	-962.422664
Sum of electronic and thermal Enthalpies=	-962.421720
Sum of electronic and thermal Free Energies=	-962.502858

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	296.588	90.580	170.768

C,0,-1.8254779288,2.1220426276,1.2840550558
C,0,-0.7584424513,3.1672421656,1.6379261983
C,0,0.5939944115,2.8177587155,1.0050604859
C,0,0.5037886119,2.6876329924,-0.5197746636
C,0,-0.7642174627,2.3206449993,-1.0593579359
C,0,-1.823758633,1.7418851345,-0.2109488136
O,0,1.5225222066,2.9254428052,-1.2128505606
O,0,-1.3198399745,0.4102197074,-0.4649448413
O,0,-2.1267876269,-0.9219743841,0.5062436494
C,0,-2.9420721607,-1.717704708,-0.3243563102
C,0,-4.0857653233,-0.8951053658,-0.9478876864
C,0,-2.1178839351,-2.4023965514,-1.4336975628
C,0,-3.5324057825,-2.7892211478,0.6223754878
H,0,-0.8881872389,2.3115593704,-2.1370260855
H,0,-2.8262820468,1.8172058879,-0.6445647641
H,0,-2.8184147203,2.493397602,1.562842493
H,0,-1.6726227028,1.1998865544,1.8552375658
H,0,-1.0711657884,4.1527507998,1.2692328009
H,0,-0.6650481386,3.2557648858,2.7281753765
H,0,1.3563359265,3.5740554566,1.2204996041
H,0,0.9664648347,1.8676790004,1.4186858536
H,0,-2.7400298862,-3.0683041298,-2.0437575816
H,0,-1.6759156175,-1.6469481907,-2.0903382952
H,0,-1.3093514642,-2.996471026,-0.9921266881
H,0,-4.7711618942,-1.5325466086,-1.5195059992
H,0,-4.6568343724,-0.3890768414,-0.1623735791
H,0,-3.6794621593,-0.1372404629,-1.623983991
H,0,-4.192007174,-3.4708698647,0.0709815304
H,0,-2.7304819785,-3.3769909875,1.0809983974
H,0,-4.1098418433,-2.3127384416,1.420491088
H,0,0.0649261232,-0.3574939599,-0.054915081
N,0,0.9731031126,-0.8044958911,0.2277180523
C,0,1.040520794,-1.3481269918,1.583257268
C,0,2.4566641653,-1.199443309,2.1285000771
H,0,0.3044879239,-0.8130949972,2.1860885165
H,0,0.7293755911,-2.3994698671,1.5603753932
C,0,2.0019445142,-0.7061064691,-0.5896345588
N,0,3.2314417583,-1.1128292429,-0.2186567051
C,0,4.3864634529,-1.0743690529,-1.1145950196
C,0,3.4574224697,-1.726175084,1.1017793893
H,0,4.6199283689,-2.0754758737,-1.4986132519

H,0,4.208935209,-0.402678217,-1.9508765977
H,0,5.2529429432,-0.7022914932,-0.5607858522
H,0,3.3862558207,-2.8190109661,1.0097277328
C,0,1.760582301,-0.1259789465,-1.952536941
H,0,2.6681637671,-0.1449044305,2.3372832626
H,0,2.5665344245,-1.7528265125,3.0655949716
H,0,4.4813546873,-1.4882493817,1.4040970295
H,0,2.1860473818,0.8829175299,-2.0214745698
H,0,2.1802322978,-0.7683969812,-2.7307100724
H,0,0.6877085287,-0.0238409966,-2.1112614383

tseqAB3BB DBU model – PCM Dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.921368923

Zero-point correction= 0.447221 (Hartree/Particle)
Thermal correction to Energy= 0.470874
Thermal correction to Enthalpy= 0.471819
Thermal correction to Gibbs Free Energy= 0.392549
Sum of electronic and zero-point Energies= -962.474148
Sum of electronic and thermal Energies= -962.450494
Sum of electronic and thermal Enthalpies= -962.449550
Sum of electronic and thermal Free Energies= -962.528820

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.478	88.645	166.837

C,0,-1.9634489146,1.9762200061,1.2606550183
C,0,-1.0430899146,3.1450370061,1.6465300183
C,0,0.2676170854,3.1128600061,0.8499200183
C,0,0.0121730854,3.1037220061,-0.6577559817
C,0,-1.1591369146,2.4379180061,-1.1063609817
C,0,-1.9990329146,1.7230890061,-0.2372889817
O,0,0.8347810854,3.6828860061,-1.4217259817
O,0,-1.3461939146,-0.0860459939,-0.3819049817
O,0,-1.9667909146,-1.0578009939,0.5214930183
C,0,-2.7634099146,-2.0168249939,-0.2150059817
C,0,-3.9033549146,-1.3148289939,-0.9635759817
C,0,-1.8767439146,-2.8131469939,-1.1819539817
C,0,-3.3150459146,-2.9237149939,0.8923630183
H,0,-1.3433509146,2.4076600061,-2.1793739817
H,0,-2.9606989146,1.4109570061,-0.6312859817
H,0,-2.9844629146,2.1746320061,1.6113680183
H,0,-1.6510609146,1.0544180061,1.7634500183

H,0,-1.5529089146,4.0954210061,1.4392740183
H,0,-0.8405909146,3.1239770061,2.7248600183
H,0,0.9039270854,3.9733890061,1.0848480183
H,0,0.8422040854,2.2100960061,1.1068990183
H,0,-2.4634259146,-3.5789389939,-1.7016949817
H,0,-1.4368789146,-2.1461599939,-1.9277829817
H,0,-1.0668399146,-3.3092529939,-0.6362309817
H,0,-4.5405699146,-2.0501129939,-1.4677269817
H,0,-4.5235349146,-0.7417769939,-0.2660279817
H,0,-3.5011209146,-0.6328079939,-1.7170329817
H,0,-3.9410269146,-3.7104349939,0.4580100183
H,0,-2.4979399146,-3.3984199939,1.4454410183
H,0,-3.9231689146,-2.3475589939,1.5973030183
H,0,0.1493050854,-0.4284749939,-0.0081459817
N,0,1.1327180854,-0.7386539939,0.2857890183
C,0,1.3292960854,-1.1892499939,1.6641230183
C,0,2.7625100854,-0.9008449939,2.0991470183
H,0,0.6013400854,-0.6691129939,2.2911040183
H,0,1.1105210854,-2.2630419939,1.7292830183
C,0,2.1057980854,-0.6901759939,-0.6039449817
N,0,3.3624830854,-1.0459069939,-0.2998329817
C,0,4.4605340854,-1.0639239939,-1.2672879817
C,0,3.7308920854,-1.4691709939,1.0665650183
H,0,4.9548530854,-2.0403249939,-1.2281779817
H,0,4.1018270854,-0.9006249939,-2.2805789817
H,0,5.1939290854,-0.2884359939,-1.0192149817
H,0,3.7488050854,-2.5669059939,1.1018410183
C,0,1.7512480854,-0.2190789939,-1.9878919817
H,0,2.9137720854,0.1809750061,2.1941070183
H,0,2.9640400854,-1.3523469939,3.0752860183
H,0,4.7489260854,-1.1134369939,1.2547730183
H,0,2.3545750854,0.6471310061,-2.2741299817
H,0,1.9183670854,-1.0145389939,-2.7213009817
H,0,0.6995770854,0.0663570061,-2.0131479817

2nd tseqAB3BB DBU model – PCM Dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.923161942

Zero-point correction=	0.448142 (Hartree/Particle)
Thermal correction to Energy=	0.471463
Thermal correction to Enthalpy=	0.472407
Thermal correction to Gibbs Free Energy=	0.395039
Sum of electronic and zero-point Energies=	-962.475019
Sum of electronic and thermal Energies=	-962.451699

Sum of electronic and thermal Enthalpies= -962.450755
Sum of electronic and thermal Free Energies= -962.528123

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.847	88.356	162.833

C,0,1.9750592429,-0.7414562077,1.8710084104
C,0,2.0074427781,-2.2766127118,1.9158186915
C,0,1.6804438312,-2.8870475805,0.5457839951
C,0,2.6695579863,-2.414212843,-0.5212823355
C,0,3.1755783345,-1.1063248201,-0.3843365515
C,0,2.6229361571,-0.1466702975,0.6004873228
O,0,3.022202259,-3.2267956445,-1.4324093106
O,0,1.6541028846,0.3663808991,-0.3340145108
O,0,0.723196085,1.6590112391,0.3576921014
C,0,0.9954068469,2.8741550089,-0.3464491858
C,0,2.4731426168,3.2653094644,-0.193139282
C,0,0.6216182456,2.7482144207,-1.8331208477
C,0,0.1013804388,3.9256765466,0.3417379166
H,0,3.8892778162,-0.739175497,-1.1183809299
H,0,3.3272132661,0.6550820833,0.854446085
H,0,2.4728446191,-0.3337276744,2.7593066564
H,0,0.9399148521,-0.3854970926,1.9055181829
H,0,3.008049361,-2.6157196753,2.2156528603
H,0,1.3096587832,-2.6442311731,2.6796913037
H,0,1.7142188193,-3.9819480336,0.5755899953
H,0,0.661386653,-2.6049490235,0.2433774589
H,0,0.8072486246,3.6896377937,-2.3627045506
H,0,1.2140196257,1.9604261212,-2.3059188941
H,0,-0.4402373919,2.5015789955,-1.9461309466
H,0,2.6663323633,4.2389044641,-0.6578775883
H,0,2.7418511453,3.3291096122,0.8665481416
H,0,3.1160467046,2.522049479,-0.6721295612
H,0,0.2499037139,4.9086139639,-0.1204531657
H,0,-0.9574848689,3.6628823013,0.2467672514
H,0,0.3472563162,4.0022555913,1.4056638903
H,0,-0.7909597359,0.8871414622,0.2244899388
N,0,-1.7507361726,0.4737749744,0.2945458831
C,0,-2.6089693513,0.9618108119,1.3775588676
C,0,-3.6114359236,-0.1225664009,1.7577165626
H,0,-1.9636818429,1.2281062625,2.2189383736
H,0,-3.1291600337,1.8720801636,1.0510615819
C,0,-2.1412667308,-0.4221086509,-0.5994189582

N,0,-3.3680188099,-0.9530957134,-0.5645844388
C,0,-3.8742642239,-1.8891477478,-1.5719827358
C,0,-4.3294848735,-0.613734383,0.505871858
H,0,-3.9318054876,-2.901738758,-1.1568923914
H,0,-4.8789746344,-1.5719794177,-1.8672937549
H,0,-3.2454574528,-1.8988771681,-2.4589907907
H,0,-5.0248418578,0.1447910379,0.1224039531
C,0,-1.1564228847,-0.8203690266,-1.6621501577
H,0,-3.0938858448,-0.9583070011,2.2423254469
H,0,-4.3452491023,0.2697625417,2.4679801894
H,0,-4.9076550544,-1.5178365547,0.721943045
H,0,-1.0951612123,-1.9079481195,-1.7529504983
H,0,-1.4638953376,-0.4172226535,-2.6336293259
H,0,-0.1658326999,-0.4362843053,-1.4128497296

tseqBB3 DBU model – PCM Dichloroethane – 6-31G*

E(RB+HF-LYP) = -962.840339467

Zero-point correction= 0.451312 (Hartree/Particle)
Thermal correction to Energy= 0.475419
Thermal correction to Enthalpy= 0.476364
Thermal correction to Gibbs Free Energy= 0.396232
Sum of electronic and zero-point Energies= -962.389027
Sum of electronic and thermal Energies= -962.364920
Sum of electronic and thermal Enthalpies= -962.363976
Sum of electronic and thermal Free Energies= -962.444108

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.330	89.747	168.652

C,0,-2.201252939,1.9927560183,1.0417629329
C,0,-1.290776939,3.0558640183,1.6751729329
C,0,0.155578061,2.9045840183,1.1913719329
C,0,0.251519061,2.9738450183,-0.3377940671
C,0,-0.860000939,2.4659560183,-1.0627710671
C,0,-1.916697939,1.7834300183,-0.4371730671
O,0,1.285370061,3.4597530183,-0.8621630671
O,0,-1.371731939,-0.0335259817,-0.5272710671
O,0,-1.964214939,-0.9671109817,0.4290399329
C,0,-2.830029939,-1.9079299817,-0.2461490671
C,0,-3.979747939,-1.1722509817,-0.9446480671
C,0,-2.018292939,-2.7404429817,-1.2465330671
C,0,-3.355258939,-2.7783709817,0.9019659329

H,0,-0.804687939,2.4956110183,-2.1504550671
H,0,-2.794725939,1.5831460183,-1.0452700671
H,0,-3.253074939,2.2862750183,1.1630369329
H,0,-2.099394939,1.0315060183,1.5578449329
H,0,-1.649001939,4.0561010183,1.3951119329
H,0,-1.346601939,2.9964510183,2.7702509329
H,0,0.809476061,3.6796030183,1.6085499329
H,0,0.559202061,1.9349750183,1.5223629329
H,0,-2.656985939,-3.4659839817,-1.7635110671
H,0,-1.560360939,-2.0815229817,-1.9889840671
H,0,-1.221497939,-3.2899079817,-0.7318160671
H,0,-4.674924939,-1.8857569817,-1.4025450671
H,0,-4.536263939,-0.5619119817,-0.2245940671
H,0,-3.589705939,-0.5172419817,-1.7280700671
H,0,-4.036983939,-3.5452599817,0.5177799329
H,0,-2.529152939,-3.2804769817,1.4174459329
H,0,-3.897499939,-2.1676119817,1.6318389329
H,0,0.237688061,-0.2543779817,-0.3939090671
N,0,1.290430061,-0.4072919817,-0.4333380671
C,0,1.990199061,0.1664650183,-1.5868440671
C,0,3.277089061,-0.6113319817,-1.8387350671
H,0,1.307142061,0.1039410183,-2.4390020671
H,0,2.180358061,1.2299400183,-1.3985770671
C,0,1.896288061,-1.0474179817,0.5459719329
N,0,3.226499061,-1.2176169817,0.5605759329
C,0,3.951715061,-1.8630359817,1.6534629329
C,0,4.072809061,-0.7214699817,-0.5418180671
H,0,4.357604061,-2.8272959817,1.3248869329
H,0,4.784087061,-1.2189709817,1.9572689329
H,0,3.309780061,-2.0221879817,2.5174029329
H,0,4.495531061,0.2500820183,-0.2520340671
C,0,1.039347061,-1.5862769817,1.6600479329
H,0,3.041112061,-1.6151209817,-2.2123160671
H,0,3.884828061,-0.1072619817,-2.5967020671
H,0,4.904223061,-1.4249099817,-0.6563500671
H,0,1.246544061,-2.6476349817,1.8299799329
H,0,1.241243061,-1.0496579817,2.5944109329
H,0,-0.016759939,-1.4693369817,1.4047069329

2nd tseqBB3 DBU model – PCM Dichloroethane – 6-31G*

E(RB+HF-LYP) = -962.839393931

Zero-point correction=	0.451344 (Hartree/Particle)
Thermal correction to Energy=	0.475543

Thermal correction to Enthalpy= 0.476487
Thermal correction to Gibbs Free Energy= 0.396066
Sum of electronic and zero-point Energies= -962.388050
Sum of electronic and thermal Energies= -962.363851
Sum of electronic and thermal Enthalpies= -962.362907
Sum of electronic and thermal Free Energies= -962.443328

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.408	89.980	169.259

C,0,-2.3183927364,1.508897509,1.5507654899
C,0,-1.5950335369,2.8345919201,1.8286398022
C,0,-0.3505748721,2.9976885015,0.9456738617
C,0,-0.7067335341,2.948992127,-0.5444472822
C,0,-1.8131178658,2.1271373488,-0.9073748864
C,0,-2.4150968512,1.1716687903,0.049309272
O,0,-0.0507918878,3.6382737886,-1.3608020478
O,0,-1.4700723296,0.2082089529,-0.3958409381
O,0,-1.6415964787,-1.4148453529,0.5517816994
C,0,-2.1059858798,-2.4131600558,-0.3191787492
C,0,-3.5049429624,-2.0659059382,-0.8673612662
C,0,-1.1293534194,-2.6444518581,-1.4904440512
C,0,-2.1966370262,-3.6958492648,0.5408526571
H,0,-2.1127928255,2.0892530159,-1.9510552783
H,0,-3.4271676989,0.8508520437,-0.2242920753
H,0,-3.3275833272,1.5452404425,1.9804054048
H,0,-1.8041263069,0.6707775488,2.0327269701
H,0,-2.2769667028,3.6713909425,1.6238778137
H,0,-1.3267026292,2.9037927287,2.8911004753
H,0,0.158243726,3.9506377166,1.1325241341
H,0,0.3748692768,2.2018584104,1.171537696
H,0,-1.4705067313,-3.4492537425,-2.1544732763
H,0,-1.0353659099,-1.7265529323,-2.0794268468
H,0,-0.1361938283,-2.9137894532,-1.1111872928
H,0,-3.9188358264,-2.8811369351,-1.4747620696
H,0,-4.1937988846,-1.8687126664,-0.0377901138
H,0,-3.4500112497,-1.1671221285,-1.4895767307
H,0,-2.5753018826,-4.5420632581,-0.0471188817
H,0,-1.209380191,-3.9637699961,0.9339540919
H,0,-2.8702943341,-3.5345446259,1.3898526302
H,0,0.253853118,-0.0798312067,-0.1583695435
N,0,1.2810284586,-0.078580344,-0.2890048885
C,0,1.7896330125,0.6334962259,-1.4649514517

C,0,3.1432291773,0.0516391919,-1.8556607762
H,0,1.0502880122,0.511615144,-2.2605450233
H,0,1.8545749735,1.705744568,-1.2463133021
C,0,2.0446572533,-0.6871838497,0.6022601074
N,0,3.3779141039,-0.6659953999,0.5030819028
C,0,4.2700360701,-1.2601656349,1.4991745262
C,0,4.0533846325,-0.0065261536,-0.6328829063
H,0,4.7028375751,-2.1940721148,1.1212951121
H,0,5.0816757393,-0.5549583512,1.7041897987
H,0,3.7456575092,-1.4570663827,2.4323220841
H,0,4.3640446143,0.999206692,-0.3195789913
C,0,1.3538118027,-1.4004707044,1.7305655225
H,0,3.0116151628,-0.9570134118,-2.265166299
H,0,3.6117796175,0.6676573944,-2.6293040775
H,0,4.9585306832,-0.5822426323,-0.8520268347
H,0,1.7685593334,-2.4040188302,1.8649855537
H,0,1.4882329871,-0.8503376844,2.6697329786
H,0,0.284054047,-1.4849981285,1.5031938664

tseqBB3BB DBU model – PCM Dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.922154717

Zero-point correction= 0.447644 (Hartree/Particle)
Thermal correction to Energy= 0.472059
Thermal correction to Enthalpy= 0.473004
Thermal correction to Gibbs Free Energy= 0.391163
Sum of electronic and zero-point Energies= -962.474510
Sum of electronic and thermal Energies= -962.450095
Sum of electronic and thermal Enthalpies= -962.449151
Sum of electronic and thermal Free Energies= -962.530991

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.222	90.495	172.247

C,0,-1.9585729512,1.9451010183,1.298284939
C,0,-1.0313609512,3.0786140183,1.763329939
C,0,0.3025490488,3.0545730183,1.006544939
C,0,0.0992790488,3.1051580183,-0.508045061
C,0,-1.0789699512,2.5023440183,-1.021103061
C,0,-1.9667359512,1.7741200183,-0.211242061
O,0,0.9731120488,3.6751950183,-1.221676061
O,0,-1.3720669512,-0.0427709817,-0.446951061
O,0,-1.9429959512,-1.0375729817,0.461752939

C,0,-2.8175579512,-1.9527849817,-0.244219061
C,0,-3.9890519512,-1.1969589817,-0.882864061
C,0,-2.0240299512,-2.7356029817,-1.298692061
C,0,-3.3119659512,-2.8821089817,0.871864939
H,0,-1.2314699512,2.5284320183,-2.099142061
H,0,-2.9287779512,1.5213790183,-0.645191061
H,0,-2.9834379512,2.1364500183,1.641274939
H,0,-1.6647109512,0.9940440183,1.755325939
H,0,-1.5174809512,4.0467890183,1.583141939
H,0,-0.8628469512,3.0061200183,2.845295939
H,0,0.9450380488,3.8947520183,1.293091939
H,0,0.8557340488,2.1341020183,1.247930939
H,0,-2.6692079512,-3.4610499817,-1.806645061
H,0,-1.6116529512,-2.0521609817,-2.045393061
H,0,-1.1966689512,-3.2792729817,-0.829763061
H,0,-4.6826649512,-1.8991659817,-1.358944061
H,0,-4.5387419512,-0.6298399817,-0.124208061
H,0,-3.6250499512,-0.5024129817,-1.644252061
H,0,-3.9871999512,-3.6391919817,0.459239939
H,0,-2.4716249512,-3.3953759817,1.350594939
H,0,-3.8536109512,-2.3149639817,1.635729939
H,0,0.2056720488,-0.3154989817,-0.371822061
N,0,1.2620130488,-0.4663149817,-0.431380061
C,0,1.9282500488,0.0073950183,-1.647863061
C,0,3.1951900488,-0.8071169817,-1.885796061
H,0,1.2185730488,-0.0997399817,-2.472644061
H,0,2.1541730488,1.0760040183,-1.546981061
C,0,1.9066100488,-1.0216129817,0.577334939
N,0,3.2373960488,-1.1876889817,0.560201939
C,0,3.9985390488,-1.7486639817,1.677874939
C,0,4.0441410488,-0.8124829817,-0.619284061
H,0,4.3212590488,-2.7708979817,1.448147939
H,0,4.8858460488,-1.1297679817,1.843076939
H,0,3.4137600488,-1.7554739817,2.594947939
H,0,4.4937550488,0.1731110183,-0.438496061
C,0,1.0938050488,-1.4681089817,1.761933939
H,0,2.9313250488,-1.8356439817,-2.159653061
H,0,3.7734590488,-0.3795549817,-2.710356061
H,0,4.8579340488,-1.5400419817,-0.702546061
H,0,1.3100390488,-2.5118369817,2.008167939
H,0,1.3267260488,-0.8581339817,2.641600939
H,0,0.0308900488,-1.3731179817,1.533348939

2nd tseqBB3BB DBU model – PCM Dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.922272222

Zero-point correction=	0.448187 (Hartree/Particle)
Thermal correction to Energy=	0.472561
Thermal correction to Enthalpy=	0.473505
Thermal correction to Gibbs Free Energy=	0.388791
Sum of electronic and zero-point Energies=	-962.474085
Sum of electronic and thermal Energies=	-962.449711
Sum of electronic and thermal Enthalpies=	-962.448767
Sum of electronic and thermal Free Energies=	-962.533481

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.537	90.503	178.296

C,0,1.9871922011,-0.8460887035,1.841496618
C,0,1.8943454287,-2.3792649957,1.8511410075
C,0,1.4846233556,-2.9297903375,0.4783925451
C,0,2.4769569361,-2.5080368179,-0.6080473744
C,0,3.0921810815,-1.2528925727,-0.4536414388
C,0,2.6242810342,-0.2731982589,0.5556887283
O,0,2.7263631064,-3.3238359288,-1.5527339979
O,0,1.6480304573,0.3173001781,-0.3317881537
O,0,0.8016662272,1.6013035823,0.42157712
C,0,1.1236400565,2.8357799235,-0.23272268
C,0,2.6162005772,3.1590328019,-0.0704180533
C,0,0.7403378825,2.7881240327,-1.7212402669
C,0,0.2732225564,3.8878556554,0.5055846274
H,0,3.8063307508,-0.9209240592,-1.2039645643
H,0,3.3832530567,0.4821598466,0.7933630018
H,0,2.559168789,-0.5051255698,2.7133346085
H,0,0.9896521735,-0.4047324239,1.9358611155
H,0,2.8726687268,-2.8040196022,2.1132322195
H,0,1.1913459105,-2.7087668226,2.6277649116
H,0,1.4373998714,-4.0248216273,0.4844703777
H,0,0.4811845726,-2.5674751107,0.2110922505
H,0,0.9893378619,3.7327723798,-2.2174783766
H,0,1.2788026146,1.9796083716,-2.2223040782
H,0,-0.3363088794,2.6203386601,-1.8393699628
H,0,2.8463208776,4.1437108883,-0.4925974763
H,0,2.8921489179,3.1637671829,0.9892393534
H,0,3.2262828537,2.4129867722,-0.5863325951
H,0,0.4555239946,4.8828113278,0.0834036333

H,0,-0.7947318393,3.6675789217,0.406563145
H,0,0.528266574,3.9117813564,1.5699065443
H,0,-0.5992427379,0.6914923691,-0.029719101
N,0,-1.4360735842,0.1229476288,-0.2805933446
C,0,-1.4488782636,-0.5577141309,-1.5773893165
C,0,-2.8824845097,-0.618579895,-2.0943885035
H,0,-0.7924585965,-0.002891032,-2.2498122255
H,0,-1.0290021802,-1.565528241,-1.4642250988
C,0,-2.4486377827,0.0841765698,0.5687162684
N,0,-3.571110818,-0.5848923938,0.2903194364
C,0,-4.700787158,-0.6924860115,1.2169063854
C,0,-3.784784726,-1.2266484151,-1.0257781673
H,0,-5.4926158909,0.0149187908,0.9438621053
H,0,-5.0995845554,-1.7087885556,1.1536885521
H,0,-4.3923712399,-0.5133476656,2.2445381245
H,0,-3.6050828129,-2.3044966246,-0.9189628292
C,0,-2.2857023329,0.8175583655,1.8698308365
H,0,-3.2294573309,0.390478774,-2.3469713294
H,0,-2.9345380026,-1.2274400296,-3.0018092201
H,0,-4.8392321448,-1.0878576043,-1.2858163996
H,0,-3.1078189779,1.5213403537,2.0279012282
H,0,-2.271290271,0.1148286373,2.7096539188
H,0,-1.3423776181,1.3641477777,1.8621784811

tsAxMeoutGaucheB3 DBU model – 6-31G*

E(RB+HF-LYP) = -962.820402562

Zero-point correction= 0.453043 (Hartree/Particle)
Thermal correction to Energy= 0.476616
Thermal correction to Enthalpy= 0.477560
Thermal correction to Gibbs Free Energy= 0.400048
Sum of electronic and zero-point Energies= -962.367360
Sum of electronic and thermal Energies= -962.343787
Sum of electronic and thermal Enthalpies= -962.342843
Sum of electronic and thermal Free Energies= -962.420354

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.081	89.260	163.137

C,0,-1.5318480328,2.2492504134,1.310174344
C,0,-0.2013863006,2.1428523152,2.065514524
C,0,0.9626916449,2.723670573,1.2506511531

C,0,0.9967274084,2.2615377466,-0.218611864
C,0,-0.2368796847,1.9621060162,-0.826771409
C,0,-1.4353800731,1.6986147779,-0.1026741545
O,0,2.1186998799,2.2349519972,-0.8002337283
O,0,-1.6478620577,-0.0124510679,0.1998599098
O,0,-2.0101398078,-0.5971813404,-1.0871304695
C,0,-3.2534642447,-1.321223621,-0.9641071808
C,0,-3.1022631903,-2.459302078,0.0541756782
C,0,-4.3951732046,-0.374725312,-0.5752692767
C,0,-3.4534625288,-1.8728044577,-2.381200519
H,0,-0.2374599191,1.776643524,-1.8974982065
H,0,-2.3615594491,1.7989344664,-0.6684782085
H,0,-1.8207413974,3.3074434604,1.2261278145
H,0,-2.3330572106,1.7455705012,1.8639112502
H,0,-0.280123392,2.6428296436,3.040735255
H,0,-0.008408835,1.0832143717,2.2804010738
H,0,0.893665187,3.8223032984,1.2436347068
H,0,1.932270982,2.4879516238,1.7080787388
H,0,-5.3452283925,-0.9184327418,-0.5148203506
H,0,-4.1942512752,0.0819708341,0.3972140263
H,0,-4.5014659519,0.4224057145,-1.3190110928
H,0,-4.0191287209,-3.0572121452,0.1120597433
H,0,-2.2774904904,-3.1209462074,-0.2351109474
H,0,-2.8897366732,-2.0516369032,1.0461301537
H,0,-4.3791195599,-2.4560510782,-2.4353044593
H,0,-3.5153771863,-1.0549194076,-3.1063925354
H,0,-2.6183132488,-2.522610467,-2.6637646283
H,0,-0.1386487313,-0.8470574541,0.1974894197
N,0,0.8246289878,-1.2155379401,0.3973982288
C,0,1.1021022829,-1.5652867962,1.7882860709
C,0,2.3776402416,-0.8701576745,2.256089272
H,0,0.2345494678,-1.2629756005,2.3794787002
H,0,1.1994062362,-2.6558507199,1.875429836
C,0,1.7819897832,-0.9186355493,-0.4709300199
N,0,3.0760477573,-0.9473765246,-0.13031415
C,0,4.0978165968,-0.4219869797,-1.047234667
C,0,3.5054502668,-1.1499584284,1.2671034725
H,0,4.0331460178,0.6719409269,-1.0679679819
H,0,5.0779905062,-0.7457918049,-0.6912882782
H,0,3.9568638516,-0.8159500311,-2.0544551407
H,0,3.8796404262,-2.177143915,1.3735007872
C,0,1.3884922646,-0.5872974654,-1.8772305175
H,0,2.2026061438,0.2081808957,2.3158620272
H,0,2.6682313518,-1.2221676013,3.2509985985

H,0,4.3430981301,-0.4724326369,1.4544985572
H,0,1.6979748473,0.4443121235,-2.0863826012
H,0,1.8834044146,-1.2758847365,-2.5719944739
H,0,0.3086221636,-0.6787142739,-1.990425469

tsAxMeoutGaucheB3BB DBU model – 6-31+G**

E(RB+HF-LYP) = -962.897285038

Zero-point correction= 0.450208 (Hartree/Particle)
Thermal correction to Energy= 0.473932
Thermal correction to Enthalpy= 0.474876
Thermal correction to Gibbs Free Energy= 0.396692
Sum of electronic and zero-point Energies= -962.447077
Sum of electronic and thermal Energies= -962.423353
Sum of electronic and thermal Enthalpies= -962.422409
Sum of electronic and thermal Free Energies= -962.500593

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	297.397	89.900	164.553

C,0,-1.6417667502,2.2198364349,1.2647475416
C,0,-0.3723778897,2.1222387601,2.1209270556
C,0,0.8452038499,2.7132095211,1.3959005447
C,0,0.9952921093,2.250819771,-0.0641670495
C,0,-0.1822878012,1.9437009658,-0.7690976623
C,0,-1.4344145981,1.6593293378,-0.1332661925
O,0,2.1651918111,2.2233543127,-0.556403363
O,0,-1.6209814257,-0.0306896228,0.1577773553
O,0,-2.0065967819,-0.6508424774,-1.1048516107
C,0,-3.2960248046,-1.3018516494,-0.9754366054
C,0,-3.2236808259,-2.4109835198,0.0823899169
C,0,-4.3894193047,-0.2818654075,-0.636095788
C,0,-3.5083187289,-1.8897410548,-2.3762108921
H,0,-0.0974258879,1.7546841362,-1.8351033234
H,0,-2.3137940103,1.7571635985,-0.7692392317
H,0,-1.9228156694,3.2763349813,1.1479936575
H,0,-2.4822047192,1.7186688724,1.7579071774
H,0,-0.5286859957,2.6245890047,3.0848284079
H,0,-0.1867457007,1.0648826736,2.352487355
H,0,0.7651160284,3.8102109288,1.3727222942
H,0,1.7775432252,2.4920993385,1.9290545466
H,0,-5.3654423347,-0.7760398788,-0.5775107593
H,0,-4.1845328917,0.1911841531,0.3273613351

H,0,-4.4433331203,0.49601725,-1.4042822308
H,0,-4.1744297856,-2.9526719969,0.1370207742
H,0,-2.4333458648,-3.126660333,-0.1684678247
H,0,-3.0111224283,-1.984802892,1.0661443281
H,0,-4.4665286194,-2.4175947909,-2.419184852
H,0,-3.51494821,-1.0969378159,-3.1305089784
H,0,-2.7120531054,-2.5986015901,-2.6246696771
H,0,-0.0755880946,-0.8731166417,0.1814356552
N,0,0.8919931465,-1.2167444372,0.3783352516
C,0,1.2038873041,-1.5312670553,1.771224448
C,0,2.4694238539,-0.7911014415,2.1963606735
H,0,0.342104831,-1.2399225567,2.3753287923
H,0,1.3325683142,-2.6166657477,1.8774412498
C,0,1.8318573626,-0.9320172341,-0.5145013343
N,0,3.1307485718,-0.9483582674,-0.1975306272
C,0,4.1450807146,-0.4862459244,-1.154319404
C,0,3.589454478,-1.0762050348,1.2008699764
H,0,4.1422044968,0.6093275342,-1.1887972278
H,0,5.1188834012,-0.8534987761,-0.8247983183
H,0,3.9534413583,-0.884775655,-2.1502851492
H,0,4.0006876299,-2.0845358951,1.3414727985
C,0,1.4085003776,-0.6389492361,-1.9204531935
H,0,2.2701940066,0.2834966113,2.2232820992
H,0,2.7825238057,-1.104525016,3.1968056735
H,0,4.4039738574,-0.3603525366,1.3417129774
H,0,1.7483080381,0.3645585807,-2.1916659925
H,0,1.8494615476,-1.3760483008,-2.6005966013
H,0,0.3234289618,-0.6887694067,-1.9989325899

tsAxMeoutGaucheB3PCM DBU model – PCM Dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.838975684

Zero-point correction= 0.451263 (Hartree/Particle)
Thermal correction to Energy= 0.475426
Thermal correction to Enthalpy= 0.476370
Thermal correction to Gibbs Free Energy= 0.395813
Sum of electronic and zero-point Energies= -962.387713
Sum of electronic and thermal Energies= -962.363550
Sum of electronic and thermal Enthalpies= -962.362606
Sum of electronic and thermal Free Energies= -962.443163

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.334	89.629	169.547

C,0,-1.3941410854,2.6197879512,1.2183860244
C,0,0.0907269146,2.7195179512,1.5882610244
C,0,0.9068949146,3.3506629512,0.4535430244
C,0,0.6193699146,2.7476139512,-0.9300529756
C,0,-0.6611650854,2.1795979512,-1.1448509756
C,0,-1.5900460854,1.9438099512,-0.1202329756
O,0,1.5053379146,2.8486589512,-1.8184289756
O,0,-1.5245430854,0.1339429512,0.4912610244
O,0,-2.0505650854,-0.6410140488,-0.6237809756
C,0,-3.1305910854,-1.4844530488,-0.1709799756
C,0,-2.6234540854,-2.4684650488,0.8921370244
C,0,-4.2860130854,-0.6328310488,0.3697750244
C,0,-3.5432260854,-2.2221450488,-1.4504789756
H,0,-0.8803470854,1.8222209512,-2.1498309756
H,0,-2.6247540854,1.7865369512,-0.4143789756
H,0,-1.8264070854,3.6313209512,1.1527910244
H,0,-1.9554150854,2.0863929512,1.9933360244
H,0,0.2155259146,3.2907709512,2.5176120244
H,0,0.4721169146,1.7096389512,1.7870800244
H,0,0.6844489146,4.4283079512,0.3922210244
H,0,1.9844469146,3.2714929512,0.6423710244
H,0,-5.1188310854,-1.2672330488,0.6952330244
H,0,-3.9460550854,-0.0373860488,1.2209910244
H,0,-4.6549110854,0.0475529512,-0.4062489756
H,0,-3.4217060854,-3.1502960488,1.2075930244
H,0,-1.7959500854,-3.0659490488,0.4923920244
H,0,-2.2641800854,-1.9208070488,1.7676100244
H,0,-4.3760090854,-2.9037390488,-1.2456429756
H,0,-3.8600420854,-1.5094660488,-2.2195889756
H,0,-2.7061670854,-2.8076790488,-1.8462159756
H,0,-0.0335640854,-0.5036380488,0.4519980244
N,0,0.9388589146,-0.9308870488,0.5497890244
C,0,1.3803839146,-1.2498330488,1.9085810244
C,0,2.8895259146,-1.0688710488,2.0238310244
H,0,0.8410199146,-0.5910490488,2.5952960244
H,0,1.0924279146,-2.2820060488,2.1483600244
C,0,1.7172399146,-1.0184400488,-0.5128609756
N,0,2.9996389146,-1.4037900488,-0.4207559756
C,0,3.8445449146,-1.5972000488,-1.6016759756
C,0,3.5784519146,-1.8019590488,0.8764200244
H,0,4.8829999146,-1.4151810488,-1.3153129756
H,0,3.7626499146,-2.6205670488,-1.9890559756
H,0,3.5824809146,-0.8911750488,-2.3893279756

H,0,3.4871589146,-2.8907890488,0.9931310244
C,0,1.1201599146,-0.6628970488,-1.8448839756
H,0,3.1430959146,-0.0029600488,1.9838470244
H,0,3.2501899146,-1.4633860488,2.9789580244
H,0,4.6446719146,-1.5584370488,0.8506240244
H,0,1.4690149146,0.3280579512,-2.1634969756
H,0,1.3950319146,-1.4012800488,-2.6031259756
H,0,0.0337659146,-0.6326100488,-1.7543619756

tsAxMeoutGaucheB3BBPCM DBU model – PCM Dichloroethane – 6-31+G**

E(RB+HF-LYP) = -962.921673226

Zero-point correction=	0.447355 (Hartree/Particle)
Thermal correction to Energy=	0.471892
Thermal correction to Enthalpy=	0.472836
Thermal correction to Gibbs Free Energy=	0.390338
Sum of electronic and zero-point Energies=	-962.474319
Sum of electronic and thermal Energies=	-962.449781
Sum of electronic and thermal Enthalpies=	-962.448837
Sum of electronic and thermal Free Energies=	-962.531335

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.117	90.569	173.633

C,0,-2.1503100427,2.0673620061,1.2675990366
C,0,-0.7943060427,2.6780060061,1.6398630366
C,0,-0.3307390427,3.6772430061,0.5728850366
C,0,-0.4676170427,3.1703720061,-0.8657049634
C,0,-1.3687670427,2.1098270061,-1.1230779634
C,0,-2.1138200427,1.4651850061,-0.1180039634
O,0,0.1822859573,3.7780140061,-1.7679929634
O,0,-1.3615060427,-0.2348869939,0.3793590366
O,0,-1.6992790427,-1.1728519939,-0.6789699634
C,0,-2.5286880427,-2.2460859939,-0.1673369634
C,0,-1.7716210427,-3.0323299939,0.9111100366
C,0,-3.8547660427,-1.6994209939,0.3765220366
C,0,-2.7631150427,-3.1107839939,-1.4120799634
H,0,-1.4780270427,1.7881650061,-2.1578329634
H,0,-3.0122320427,0.9416720061,-0.4305159634
H,0,-2.9242450427,2.8513750061,1.2757070366
H,0,-2.4568800427,1.3113090061,1.9971830366
H,0,-0.8485920427,3.1652260061,2.6213980366
H,0,-0.0567300427,1.8702060061,1.7262650366

H,0,-0.9273270427,4.6003780061,0.6401390366
H,0,0.7125159573,3.9760530061,0.7299870366
H,0,-4.4867100427,-2.5194749939,0.7356750366
H,0,-3.6705140427,-1.0143279939,1.2080870366
H,0,-4.4015380427,-1.1633069939,-0.4065629634
H,0,-2.3659410427,-3.8874369939,1.2520320366
H,0,-0.8226770427,-3.4069649939,0.5123420366
H,0,-1.5603410427,-2.3914259939,1.7710280366
H,0,-3.3897190427,-3.9725319939,-1.1590919634
H,0,-3.2685060427,-2.5336139939,-2.1932149634
H,0,-1.8132280427,-3.4797879939,-1.8122829634
H,0,0.2154559573,-0.4439929939,0.4043480366
N,0,1.2597499573,-0.6466009939,0.5178360366
C,0,1.7589509573,-0.8988339939,1.8701910366
C,0,3.2038169573,-0.4230369939,1.9788520366
H,0,1.1061879573,-0.3711939939,2.5706700366
H,0,1.6856769573,-1.9717409939,2.0933230366
C,0,2.0403019573,-0.6406789939,-0.5470149634
N,0,3.3602079573,-0.8600989939,-0.4558339634
C,0,4.2538949573,-0.9086449939,-1.6148669634
C,0,4.0259039573,-1.0383449939,0.8512080366
H,0,4.8402149573,0.0149050061,-1.6867899634
H,0,4.9400309573,-1.7519789939,-1.4919499634
H,0,3.6993509573,-1.0528229939,-2.5396029634
H,0,4.1889039573,-2.1114329939,1.0183550366
C,0,1.3955979573,-0.3845219939,-1.8803719634
H,0,3.2411589573,0.6708110061,1.9128920366
H,0,3.6318739573,-0.7141959939,2.9427420366
H,0,5.0079839573,-0.5586989939,0.7854640366
H,0,1.8631229573,0.4666440061,-2.3835459634
H,0,1.4945999573,-1.2627939939,-2.5268439634
H,0,0.3361139573,-0.1761929939,-1.7412219634

VITA

Chad F. Christian received his Bachelor of Arts degree in Chemistry from Texas A&M University in College Station, TX in 2000. He entered the Ph.D. program in Chemistry at Texas A&M University in September 2000. He received his Ph.D. in May 2007 working under the direction of Dr. Daniel A. Singleton. His research interests include physical organic chemistry and organometallic chemistry.

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