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This again? Logic loops and catalytic cycles

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This again? Logic loops and catalytic cycles

by

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The student author, whose presentation of the scholarship herein was approved by the program of study committee, is solely responsible for the content of this dissertation. The Graduate College will ensure this dissertation is globally accessible and will not permit alterations after a degree is conferred.

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ABSTRACT

This dissertation is composed of chapters that are published, in preparation for journal submission or currently unpublished. Chapter 2 covers the development of a prototype Hartree-Fock Self-Consistent Field code using a distributed task based task manager. Chapter 3 is a computational study of the extensive reaction mechanisms of the zirconium catalysis of 4-penteneamine into 2-methylpyrrolidine. Chapters 4-7 describe the synthesis of various catalysts from experimental collaborators, the characterization of which includes some computational results obtained by me.

CHAPTER 1. GENERAL INTRODUCTION

1 General Overview

A goal of computational chemistry is to predict properties of interest for a chemical system. Our most accurate *ab initio* calculations, while providing excellent results, have historically been computationally intractable on any but the smallest systems. To get useful answers we need to find approximations that capture the features we're interested in and discard computationally expensive calculations that don't provide value for us. There are some promising new theories being developed that extend *ab initio* calculations to larger systems including an entire class of methods known as Fragmentation Methods[1].

Once accurate and affordable methods are identified, computational chemistry provides a number of advantages over traditional bench chemistry. Computations can allow quick feasibility testing for multiple reactions when physical experiments might take quite a long time. Computations can allow a look at reaction intermediates for reactions that happen too quickly for analysis. There is no concern about chemical safety with computations (although it's questionable which is better ergonomically).

2 Dissertation Organization

This dissertation is composed of chapters that are published, in preparation for journal submission or currently unpublished. Chapter 2 covers the development of a prototype Hartree-Fock Self-Consistent Field code using a distributed task based task manager. Chapter 3 is a computational study of the extensive reaction mechanisms of the zirconium catalysis of 4-penteneamine into 2-methylpyrrolidine. Chapters 4-7 describe the synthesis of various catalysts from experimental collaborators, the characterization of which includes some computational results obtained by me.

3 Theoretical Background

3.1 Schrodinger equation

In the first half of 1926 Erwin Schrodinger published a series of papers that developed a wave equation for time independent systems, solutions to quantum harmonic oscillators, rigid rotors and diatomic molecules and finally the time dependent wave equation for non-relativistic particles[2] (1.1).

$$\frac{\delta\Psi\left(\vec{r},t\right)}{\delta t}=\frac{-i}{\hbar}\hat{H}\Psi\left(\vec{r},t\right) \tag{1.1}$$

Where $\hat{H}$ is the Hamiltonian operator, $\vec{r}$ is the position, t is time, i is $\sqrt{-1}$ and $\hbar$ is the Planck constant divided by 2π. Ψ is the wavefunction for the system, contains all information about the system, is antisymmetric to satisfy the Pauli exclusion principle[3], and is normalized so that $\langle\Psi|\Psi\rangle=1$. This equation can be difficult to solve, so if the evolution of the system over time is not a concern (i.e. looking for a single point energy, minimum energy configuration, etc.), this equation can be simplified to:

$$\hat{H}\Psi=E\Psi \tag{1.2}$$

E is an eigenvalue of the Hamiltonian operator and is the energy of the system. The Hamiltonian operator is a function of the kinetic (T) and potential (V) energy of the system that can be expressed:

$$\hat{H}=\hat{T}_e+\hat{T}_n+\hat{V}_{ee}+\hat{V}_{en}+\hat{V}_{nn} \tag{1.3}$$

$\hat{T}_e$ and $\hat{T}_n$ are the kinetic energies of the electrons and nuclei, respectively. $\hat{V}_{ee}$, $\hat{V}_{en}$, $\hat{V}_{nn}$ are the electron-electron repulsion, electron-nucleus attraction, and nucleus-nucleus repulsion potential energy terms, respectively. Expanding the operators yields

$$\hat{H}=-\sum_{e}^{N_e}\frac{\nabla_e^2}{2}-\sum_{n}^{N_n}\frac{\nabla_n^2}{2M_n}-\sum_{e<f}^{N_e}\frac{1}{\vec{r}_{ef}}-\sum_{e}^{N_e}\sum_{n}^{N_n}\frac{Z_n}{\vec{r}_{en}}-\sum_{n<l}^{N_n}\frac{Z_nZ_l}{\vec{r}_{nl}} \tag{1.4}$$

∇_e^2, ∇_n^2 are Laplacian operators for electron e and nucleus n respectively

$$\nabla^2 = \left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2} \right) \tag{1.5}$$

M_n and Z_n are the mass and charge of nucleus n. $\vec{r}_{ab}$ is the distance between particles a and b. N_e and N_n are the numbers of electrons and nuclei, respectively.

3.2 The Born-Oppenheimer Approximation

The Born-Oppenheimer approximation allows for the reduction of complexity of this system by treating the nuclei as having fixed positions and the electrons as moving in a field of the fixed nuclei[4]. This approximation is usually a very good one because nuclei are much heavier than electrons allowing the electrons to be considered as instantly adjusting to the position of the nuclei. Consequently, we may separate the terms with no dependence on the electron positions and treat them as a constant. $\hat{T}_n$ can be set to zero and $\hat{V}_{nn}$ becomes a pseudo-constant in that it dependends only on the fixed positions of the nuclei. The remaining three terms make up the electronic Hamiltonian.

$$\hat{H}_e \Psi = \left(\hat{T}_e + \hat{V}_{ee} + \hat{V}_{en} \right) \Psi = E_e \Psi \tag{1.6}$$

Where E_e is the electronic energy. The total energy under the Born-Oppenheimer approximation then becomes

$$E_{tot} = E_e + V_{nn} \tag{1.7}$$

Because $\hat{V}_{ee}$ isn't separable, there is no analytic solution for equation 1.6 for systems with more than one electron. Various approximations for this term have led to the field of theoretical chemistry. One approximation is to treat all electrons as though they do not interact. This approximation, called the Independent Particle Model, yields the Hartree product wavefunction.

$$\Psi_{HP}(\vec{r}) = \Phi_1(\vec{r}_1)\Phi_2(\vec{r}_2)\dots\Phi_n(\vec{r}_n) \tag{1.8}$$

Where $\Phi(\vec{r}_a)$ is the wave function for electron a or (more commonly) the a^{th} molecular orbital. This equation does not satisfy the antisymmetry requirement because interchanging any two func-

tions does not yield a sign change. However, the Slater determinant of this wave function does satisfy this requirement, and when applied yields the Hartree-Fock wave function.

$$\Psi_{HF}(\vec{r}) = |\Phi_1(\vec{r}_1)\Phi_2(\vec{r}_2)\dots\Phi_n(\vec{r}_n)| \tag{1.9}$$

3.3 Hartree-Fock method

The difficulty of solving $\hat{V}_{ee}$ remains. One of the earliest approximations was the Hartree-Fock approximation in which each electron is treated as interacting with an average field of the other electrons rather than each electron individually[5]. This yields

$$\begin{aligned} E_{HF} &= \left\langle \Psi_{HF}|\hat{H}_e|\Psi_{HF} \right\rangle \\ &= 2\sum_{i}^{N_\phi} h_{ii} + \frac{1}{2}\sum_{ij}^{N_\phi}(2J_{ij} - K_{ij}) \end{aligned} \tag{1.10}$$

Note that instead of explicitly summing over the electrons, this equation sums over orbitals that represent the electrons, so the indices have changed. h_{ii} is the one electron integral

$$\begin{aligned} h_{ij} &= (\phi_i|h_1|\phi_j) \\ &= \int \phi_i(\vec{r}_1)\left(\frac{-\nabla^2}{2} - \sum_{n}^{N_n}\frac{Z_n}{\vec{r}_{n1}}\right)\phi_j(\vec{r}_1)d\vec{r}_1 \end{aligned} \tag{1.11}$$

where $\vec{r}_{n1}$ is the distance between the nucleus n and the electron. J_{ij} is the Coulomb term

$$J_{ij} = (ij|ij) \tag{1.12}$$

K_{ij} is the exchange term

$$K_{ij} = (ij|ji) \tag{1.13}$$

Using integral notation

$$(ij|kl) = \int\int \phi_i^*(\vec{r}_1)\phi_j(\vec{r}_1)\frac{1}{r_{12}}\phi_k^*(\vec{r}_2)\phi_l(\vec{r}_2)d\vec{r}_1 d\vec{r}_2 \tag{1.14}$$

where $\vec{r}_a$ are the coordinates of electron a. Because J and K require the position of the other electrons, this system must be solved iteratively using the orbitals produced by the previous

iteration. This process is repeated until the orbitals (density) and the energies change by less than some threshold. This iterative process is called the Self Consistent Field (SCF) method[6] and it yields a one determinant wavefunction with a set of optimized orbitals.

The Hartree-Fock assumption that electrons are moving in an average field of the other electrons means that the result of this method does not fully capture the effects of interactions between individual electrons. This electron correlation is quite important for understanding many chemical systems and a number of methods have been devised to capture some of its effects. This paper will only discuss those used in other sections.

3.4 Density Functional Theory (DFT)

Because the ground state of any system has a unique electron density, the correlation energy can be recovered from the electronic density[7]. Unfortunately, there is no known universal function to produce the electronic density of all chemical systems.

The most common formulation of DFT is the Kohn-Sham formulation which approximates the one electron integrals as an electron moving in an external potential[8].

$$\hat{h}_{KS} = \frac{-\nabla^2}{2} + \sum_{n}^{N_n} \frac{Z_n}{\vec{r}_{n1}} + \int \frac{\rho(\vec{r}')}{|\vec{r}_1 - \vec{r}'|} d\vec{r}' + \hat{V}_{XC}(\vec{r}) \tag{1.15}$$

Where $\rho(\vec{r})$ is the electronic density at $\vec{r}$ given by the function

$$\rho(\vec{r}) = \sum_{i}^{N} |\phi_i(\vec{r})|^2 \tag{1.16}$$

The orbitals ϕ_i are different from the orbitals found in the Hartree-Fock method above although they are optimized in a similar fashion using the Kohn-Sham equations. $\hat{V}_{XC}$ is the exchange correlation functional which is unknown. One common technique for developing useful approximations for $\hat{V}_{XC}$ is to split the term into exchange and correlation components and then fit the relative amounts of different exchange and correlation functions to experimental data or the results of high level theoretical calculations. For instance B3LYP[9][10], a widely used functional that was fitted to the G1[11] set of neutral and ionic atoms and molecules, has an exchange correlation term which is given by

$$\begin{aligned}\hat{V}_{XC} = \; & 0.2Ex(HF) + 0.8Ex(LDAorLDSA) + 0.72Ex(B88) \\ & + 0.81Ec(LYP) + 0.19Ec(VWN)\end{aligned} \tag{1.17}$$

where $Ex(HF)$, $Ex(LDAorLDSA)$, and $Ex(B88)$ are the exchange functions from Hartree-Fock, Local Density Approximation(LDA) or Local Spin-Density Approximation(LSDA) (depending on whether the system is open or closed shell), and Becke 88[12], respectively. $Ec(LYP)$, and $Ec(VWN)$ are the correlation functions LYP[10] and VWN[13], respectively. It is worth noting that the coefficients for the exchange potentials don't add up to one. This is because the Becke 88 exchange potential uses a correction that comes from either the LDA or LSDA exchange potential. This fitting process can allow for fairly accurate calculations of systems that are similar to the set used for the fitting. However, care must be taken not to treat any functional as a "black box" that applies to all systems. Generally, one should use a benchmarking study to verify that a given functional is appropriate for the system being studied. This principle is illustrated (somewhat incidentally) in the zirconium catalysis project in chapter 2.

3.5 Møller-Plesset Perturbation Theory

Another way to capture some of the correlation energy is through Møller-Plesset Perturbation Theory(MPPT)[14]. This is accomplished by treating excitations (replacing occupied orbitals with virtual orbitals in the Slater determinant) of the ground state Hartree-Fock wave function Ψ_0 (Ψ_{HF} from equation 1.9) as perturbations to the wave function. The order of perturbation is the number of excitations, so a first order perturbed wave function would be Ψ_i^a, where the electron in orbital ϕ_i has been excited to orbital ϕ_a Brillouin's theorem[15] shows that the first order perturbation is zero when using the HF wave function as the zero order wave function. So the second order perturbation, referred to as MP2[16], is the first level to provide a useful result.

The Slater-Condon[17][18] rules tell us that the single electron contribution of a doubly (or more) excited wavefunction will be zero, so all that is left is the variation in the two electron contribution.

$$E_{MP2} = 2\sum_{ijab}^{N_\phi} \frac{\langle\phi_i\phi_j|\,\hat{v}\,|\phi_a\phi_b\rangle\,\langle\phi_a\phi_b|\,\hat{v}\,|\phi_i\phi_j\rangle}{\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b} - \sum_{ijab}^{N_\phi} \frac{\langle\phi_i\phi_j|\,\hat{v}\,|\phi_a\phi_b\rangle\,\langle\phi_a\phi_b|\,\hat{v}\,|\phi_j\phi_i\rangle}{\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b} \tag{1.18}$$

Where $\hat{v}$ is an excitation operator moving the electrons in ϕ_i and ϕ_j to unoccupied orbitals ϕ_a and ϕ_b and ϵ_n is the energy of the n^{th} molecular orbital energy. Because the excited wave function has not been been minimized with respect to energy, MPx doesn't provide an upper bound to the energy of the chemical system for any x greater than 1.

MP2 requires recalculating all of the two electron integrals for every unique pair of virtual orbitals, so it can be computationally intensive. Using Møller-Plesset perturbation theory with more than double excitations is more computationally expensive and, more importantly, tends to diverge and produce worse results[19]. Other theories like Coupled Cluster[20] and Configuration Interaction [21] are more efficient and, for full CI at least, produce variational wave functions.

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CHAPTER 2. DAG IT ALL

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1 Background

Equations describing the physical properties of one and two-body systems are fairly straightforward and can be solved analytically. Adding a third body produces an interdependency in the system that can't be solved analytically. Instead, such systems have to be solved numerically, often with the use of approximations.

One such approximation comes about because nuclei are thousands of time more massive than electrons, they don't move as quickly as electrons. It is very common to treat the nuclei as stationary, an approach known as the Born-Oppenheimer approximation[1]. However, even with the Born-Oppenheimer approximation, most chemical systems can't be solved analytically because most chemical systems have more than one electron.

Electrons are the source of most of the interesting properties of molecules and, in a given chemical system, each of the electrons interacts to some extent with all of the other electrons. Numerically solving for all of these N-body interactions is computationally expensive and, depending on the system and property being studied, may not have a significant impact on the result. In chemical systems, this effect becomes more extreme as the size of the system (i.e. the number of electrons or basis functions) increases. Mathematically, these interactions all take the form of integrating products of wave functions. Usually atomic electron wave functions are assumed to contain a term like $Ae^{-\alpha r}$ that can be impossible to solve analytically. Numerical solutions being costly, an almost universal way to reduce the computational cost of these interactions is to approximate the wave functions for each electron as a linear combination of Gaussian functions[2] of the form $Ae^{-\alpha r^2}$ which can be solved analytically. These functions are considered the basis

set for a given system. Even with the use of Gaussians, the number of functions with significant interactions can still be computationally intractable. Further approximations are needed.

Many quantum mechanical approximations require a wave function containing all the information about the system. Of course, approximate methods often use approximate wave functions, and many algorithms for generating these approximate wave functions follow a similar pattern. They start with a particular guess and then iterate over the components of the wave function (usually made of basis sets[2]) to produce a set of optimized coefficients (weights) under the assumption that all the other coefficients are correct. The trial wave function with updated weights is then used to compute the energy of the system until subsequent iterations result in insignificant changes. Ultimately, this process produces a wave function whose coefficients have been minimized with respect to energy. This is a variational method[3] and so this wave function represents an upper bound for the energy of the system it represents.

1.1 Hartree-Fock method

The Hartree-Fock(HF) Self Consistent Field(SCF) method is one of the oldest such algorithms and is shown in Scheme 2.1. The SCF method approximates individual electron-electron interaction by treating each electron as though it were interacting with an electric field made up of the average of all of the other electronic interactions rather than each electron individually[4]. This approximation means that the HF wave function doesn't capture information related to the correlation between individual electrons. However, the HF wave function is commonly used as a starting point for other methods which capture some of this correlation energy.

The SCF method shown in Scheme 2.1 iteratively solves the Hartree-Fock equations using a wave function made up of the Slater determinant[5] of the basis set representing the electrons in the system[6]. These functions in the input basis set are centered on atomic nuclei and are called atomic orbitals (AOs). The overlap between each pair of AOs is stored in $\boldsymbol{S}$ and computed as

$$\mathbf{S}_{mn} = \int \phi_m^*(\vec{r})\phi_n(\vec{r})d\vec{r} \tag{2.1}$$

where ϕ_a and ϕ_a^* are the function representing orbital a and it's complex conjugate, respectively. $\vec{r}_1$ is position. $\boldsymbol{S}$ is diagonalized and it's eigenvectors are multiplied by the inverse square root of

```
for (m, n) in AO:
  OEI(m,n) = (m|n) // The one electron integrals
  S =overlap_of_atomic_orbitals
X =eigenvectors(S) · (eigenvalues(S))^(-1/2)
P = Initial guess at density
repeat {
  for (m, n) in AO:
    TEI(m,n) = 0.0
    for (o, p) in AO:
      TEI(m,n)+ = P(o,p) * (mn|op)
    F(m,n) = OEI(m,n) + TEI(m,n)
  ee = P · F // electronic energy
  de = ee − ee_prev
  // Store P and ee
  P_prev = P
  ee_prev = ee
  // Transform F from AO to MO basis
  F' = X^t · F · X
  // Diagonalization to solve the MO basis
  C' =eigenvectors(F')
  // Partial transform of MO basis to AO basis
  C = X · C'
  // Use C to create a new density matrix
  P =updated_P(C)
  dp = (P − P_prev) · (P_prev − P)
} until ((dp <threshold) && (de <energy threshold))
```

Scheme 2.1: Outline of the Hartree-Fock SCF algorithm. $\boldsymbol{S}, \boldsymbol{X}, \boldsymbol{OEI}, \boldsymbol{TEI}, \boldsymbol{F}, \boldsymbol{F'}, \boldsymbol{P}, \boldsymbol{P_{prev}}$ and $\boldsymbol{C}$ are NxN matrices where N is the number of equations representing the system's electrons. $(m|n)$ is an integral capturing the effect of delocalizing a single electron over two centers (eq 2.2). $(mn|op)$ is an integral capturing the interaction between two electrons that have been delocalized over as many as four centers (eq 2.5).

its eigenvalues. The result ($\boldsymbol{S^{-1/2}}$) is stored in $\boldsymbol{X}$. Linear combinations of AOs produce molecular orbitals (MOs). Diagonalizing the overlap matrix produces a transformation matrix that is used to remove linear dependencies in the MO basis set. Some calculations such as the one and two electron integrals are greatly simplified by working in the atomic orbital basis, while other calculations, such as actually finding the molecular orbitals, have to be done in the molecular orbital basis. The Fock matrix $\boldsymbol{F}$ is then built by adding the one and two electron contributions to the electronic energy. The one electron contributions are calculated as

$$(m|n) = \int \phi_m^*(\vec{r}_1) \left(-\frac{\nabla^2}{2} - \sum_n^{N_n} \frac{Z_n}{r_{n1}} \right) \phi_n(\vec{r}_1) d\vec{r}_1 \tag{2.2}$$

where

$$\nabla^2 = \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2} \tag{2.3}$$

and $\vec{r}_1$ is the position of electron 1 and r_{n1} is the distance between the electron and nucleus n. N_n is the total number of nuclei and Z_n is the charge on nucleus n.

The two electron contributions to each orbital pair are found by adding the density weighted contribution from every other orbital pair.

$$\boldsymbol{TEI}(m,n) = \sum_{o,p}^{N_\phi} \boldsymbol{P}(o,p) \left((mn|op) - (mn|po) \right) \tag{2.4}$$

where o and p are the indices being summed over from the total set of orbitals, N_ϕ. $\boldsymbol{P}(o,p)$ is the density of the pair. The effect of the interaction is captured via the two electron integrals:

$$(mn|op) = \int \int \phi_m^*(\vec{r}_1) \phi_n(\vec{r}_1) \frac{1}{r_{12}} \phi_o^*(\vec{r}_2) \phi_p(\vec{r}_2) d\vec{r}_1 d\vec{r}_2 \tag{2.5}$$

where r_{12} is the distance between electrons 1 and 2.

The weights of the two electron integrals aren't known *a priori* so a guess at the density must be made with the density matrix $\boldsymbol{P}$. The two electron integrals are much easier to compute in the atomic orbital basis set as, in that basis, they are computed in terms of the center of the atoms on which the atomic orbitals are centered. Once $\boldsymbol{F}$ is built however, it needs to be converted to the molecular orbital basis so that linear dependencies in the molecular orbitals can be removed and a new density matrix formed.

Once converted to the MO basis set, the Hartree-Fock equations are solved by diagonalizing $\boldsymbol{F}$. These eigenvectors $\boldsymbol{C'}$ are the linearly independent molecular orbitals. A new guess at the density matrix is made by setting the coefficients of the unoccupied molecular orbitals to zero and multiplying $\boldsymbol{P} = \boldsymbol{C'C'^t}$. This density matrix is still in the MO basis set, so it needs to be transformed back to the AO basis set before the next iteration. The AO result of this process is $\boldsymbol{P} = \boldsymbol{XC'C'^tX^t}$. In fact, the density in the MO basis set is never used and so it is very common to

save some computations by using a matrix $\boldsymbol{C} = \boldsymbol{X}\boldsymbol{C}'$ to directly form the AO basis density matrix as $\boldsymbol{P} = \boldsymbol{C}\boldsymbol{C}^t$. This new density matrix and electronic energy are compared to the old ones to find out if further refinement is needed. If not, the process is complete.

Traditionally, parallel implementations of this algorithm have multiple global sync operations. At worst, there might be one at the end of each of the nested for loops. There may be one or two at the end of the general matrix multiplications (GEMM) during the transformation of the Fock matrix. There may be several during the diagonalization of $\boldsymbol{F}'$ and another when the $\boldsymbol{C}'$ is multiplied by the transformation matrix $\boldsymbol{X}$. There is another potential sync after the GEMM that creates the updated density matrix, $\boldsymbol{P}$. Often the evaluation criteria at the end of each loop represents something like a sync in that every process will wait until it's done before the next iteration starts.

All of these syncs and delays exist because the algorithm that performs each function usually comes from a highly optimized math library that requires the entire input (or matrix/vector) to be available before the function is called. This isn't a requirement of the math operation though. Each element of the result of a GEMM, for instance, requires only that a particular row and column from the inputs be available to perform a dot product operation. Even then, it's not necessary to have the entire row and column available because the dot product is just the sum of the products of corresponding elements. So all that's strictly necessary to progress the GEMM is the pair of elements from the input matrices. Of course, modern processors are highly optimized to do these kinds of operations in bulk so actually implementing a GEMM one multiplication at a time would be extremely inefficient. However, it has long been the case that GEMMs are decomposed into optimized dot product operations to make use of cached memory and processor optimizations. GEMMs are such a common use for dot products that it's worth while for makers of basic linear algebra subroutines (BLAS [7]) libraries to optimize the GEMM by using optimized dot products. GEMMs, however, are used in so many diverse applications that it's not practical for BLAS libraries to provide optimal ways of doing the GEMM for each application. That task is up to the application developer and, for most applications, simply getting their input together in the format required by the optimized BLAS libraries and using those will provide immediate performance boosts. There may be some penalty for having to have all the data available and formatted correctly, but this penalty is usually substantially smaller than having to write and optimize linear algebra functions.

As the size of data increases and the number of these linear algebra operations increases, the syncing operations necessarily take longer. Mostly this is an issue of load balancing (when one process sits idle while another process works through a backlog of tasks) and partly because there is more data that needs to be collected. Because of this, there may be some benefit to be had by reformulating the linear algebra operations in such a way that some of the granularity of the actual data requirements of the underlying optimized operations are made available to the application developer. One way to do this is to express the algorithm as a set of tasks with data dependencies.

1.2 Task graph

PaRSEC [8] is a software framework that does just this. Algorithms that can be expressed as a directed acyclic graph (DAG) whose edges indicate data dependencies can be put into PaRSEC and the need for global syncs between tasks disappears [9]. The PaRSEC framework tracks which tasks produce which blocks of data and starts each task as the data it needs becomes available. Eliminating the need to collect all of the data in between tasks allows an idle process to move on to the next task even if another process is still working on the original task.

Scheme 2.2 shows an example of a DGEMM implemented in PaRSEC. When the PaRSEC DAG parser processes this task, it will produce one C function for each unique combination of m, n, and k. Each of these functions will contain information about which functions will produce the correct data for A, B, and C. For instance, the function that's created for $m = 0, n = 0$, and $k = 0$ will receive data labelled A from GET_A(0, 0). The indices for GET_A don't have to be called m and k, but they must span at least the same range as m and k in the DGEMM. If they span more than m and k in DGEMM, then the data flow control structure in GET_A must contain some instructions about what to do when there is no corresponding value to m and k in DGEMM. B similarly comes from some data labelled B in GET_B(0, 0). The READ directive before A and B tell the task manager that the data in A and B will not be sent on to another task once the DGEMM tasks are complete. C must be read in from GET_C(m, n) when k is zero and will be sent to PUT_C(m, n) after $k = nt - 1$. Otherwise, it comes from the instance of DGEMM with the same m and n values, but whose k is one less than the current task. In this case, C is a matrix

```
DGEMM(m, n, k)
  m = 0 .. mt - 1
  n = 0 .. nt - 1
  k = 0 .. nt - 1
: descC(m, n)

READ A <- A GET_A(m, k)
READ B <- B GET_B(k, n)
RW C <- (k == 0) ? C GET_C(m, n)
                 : DGEMM(m, n, k - 1)
     -> (k == nt - 1) ? C PUT_C(m, n)
                      : DGEMM(m, n, k + 1)
BODY
  cblas_dgemm(CblasRowMajor,
              CblasNoTrans, CblasNoTrans,
              lda, ldb, ldc,
              alpha, (double *)A, lda
              (double *)B, ldb,
              (k == 0) ? 0.0 : 1.0, (double *)C, ldc);
END
```

Scheme 2.2: Sample implementation of an DGEMM in PaRSEC. m, n, and k are the indices that serve to denote each unique dgemm task when the parser turns this into C code. : $descC(m, n)$ tells the task scheduler to run on the process that originally owned the data $desc(m, n)$. READ and RW instruct the task engine about the flow of data into and out of the task. The task itself is code written in C between the BODY and END delimiters.

composed of mt tiled rows and nt tiled columns and the indices for m and n will iterate over all of the tiles. Each of the unique tasks generated by the task manager will execute on the process that owns the data $descC(m, n)$. k will also iterate over the number of tiled rows, and is used to iterate among the tiles of A's row m. Similarly, k iterates over the tiles in B's column n. The code in the BODY makes $\mathbf{C}_{mn} = \sum_{k=0}^{nt-1} \mathbf{A}_{mk}\mathbf{B}_{kn}$.

The relative simplicity of the SCF algorithm makes it an ideal model system for testing variations intended to address these bottlenecks for more complex algorithms. For example, the entire class of multi-reference methods use a wave function composed of combinations of Hartree-Fock wave functions. Each of these has to be optimized via an SCF calculation and then the combined wave function also has to be optimized via an SCF calculation. However, the SCF is also complicated enough that it traditionally doesn't scale in parallel as well as correlation methods - in part, due to the number of syncs in the algorithm and the smaller amount of computational work. The

elimination of the global syncs for more complex algorithms may produce substantial performance improvements.

Expressing the algorithm as a set of data dependencies between tasks also has the advantage of shifting the burden of load balancing the tasks to the developers of the task framework from the developers of the physical theory. Likewise, communication and memory management between processes can also be pushed to the task manager. Ideally, the theoretician just tells the task scheduler which task is generating the data and which is using it and the task framework takes care of making sure that the tasks happen in the right order and that the data is available to the process handling the task.

2 Proof of concept - a diagonalizer

PaRSEC includes the source code for DAG implementations of many BLAS functions[10]. Some of these, like GEMMs, can used like a template; grafted into a task graph replacing the variable, task names and process locations found in the library code. However, other standard BLAS functions, including an eigenvalue and eigenvector solver have not yet been implemented. Because diagonalizing matrices is necessary for the SCF procedure, an eigensolver had to be developed. A diagonalizer using a modified Jacobi algorithm[11] was chosen because parallel versions of the Jacobi eigensolver algorithm can be implemented as a DAG task graph. Most modern eigensolvers rely on QR decomposition which is very fast, but requires decomposing the input matrix in a particular order and can't proceed until the entire matrix has been processed. This does not lend itself to the process of DAG implementation.

2.1 Jacobi eigenvalue algorithm

2.1.1 Serial algorithm

The Jacobi eigenvalue algorithm starts by finding the non-diagonal element m_{ij} of symmetric matrix $\boldsymbol{M}^{(0)}$ with the greatest magnitude.

$$\boldsymbol{M}^{(0)} = \begin{bmatrix} m_{11} & \dots & m_{1i} & \dots & m_{1j} & \dots & m_{1n} \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ m_{i1} & \dots & m_{ii} & \dots & m_{ij} & \dots & m_{in} \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ m_{j1} & \dots & m_{ji} & \dots & m_{jj} & \dots & m_{jn} \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ m_{n1} & \dots & m_{ni} & \dots & m_{nj} & \dots & m_{nn} \end{bmatrix} \tag{2.6}$$

Then a rotation matrix, $\boldsymbol{G}^{(0)}$, is formed

$$\boldsymbol{G}^{(0)} = \begin{bmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \dots & c & \dots & -s & \dots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \dots & s & \dots & c & \dots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{bmatrix} \tag{2.7}$$

such that

$$\boldsymbol{G}^{(0)}\boldsymbol{M}^{(0)}\boldsymbol{G}^{(0)\mathsf{T}} = \begin{bmatrix} m'_{11} & \dots & m'_{1i} & \dots & m'_{1j} & \dots & m'_{1n} \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ m'_{i1} & \dots & m'_{ii} & \dots & 0 & \dots & m'_{in} \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ m'_{j1} & \dots & 0 & \dots & m'_{jj} & \dots & m'_{jn} \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ m'_{n1} & \dots & m'_{ni} & \dots & m'_{nj} & \dots & m'_{nn} \end{bmatrix} = \boldsymbol{M}^{(1)} \tag{2.8}$$

$\boldsymbol{G}^{(0)}$ rotates $\boldsymbol{M}^{(0)}$ by θ where $c = cos\theta$ and $s = sin\theta$ and the rotation makes $m'_{ij} = m'_{ji} = 0$. Once $\boldsymbol{M}^{(1)}$ is found, the element with the greatest magnitude is found and the process of rotation $\boldsymbol{M}^{(1)}$ begins. This process is repeated for N iterations until all of the non-diagonal elements of $\boldsymbol{M}^{(N)}$ are 0. Because c and s will both be less than or equal to one, each iteration will result in a decrease of the total magnitude of the non-diagonal elements of $\boldsymbol{M}$.

2.1.2 Parallel algorithm

The serial method requires comparing every non-diagonal element for each iteration and results in a diagonal matrix $\boldsymbol{M}^{(N)} = \boldsymbol{G}\boldsymbol{M}^{(0)}\boldsymbol{G}^{\intercal}$ where $\boldsymbol{G} = \boldsymbol{G}^{(N)}\boldsymbol{G}^{(N-1)}\dots\boldsymbol{G}^{(0)}$.

If the matrix is distributed over multiple processors then the communication overhead for such a comparison can be significant. To eliminate this overhead, instead of choosing the largest element one may simply choose any convenient element. This will likely result in the process requiring more iterations, but eliminates costly communication overhead. Because the matrix that will rotate any given element to zero is linearly independent from any matrix that zeros out an element whose row and column indices are different, a rotation matrix that zeros out several elements simultaneously can be constructed[11]. To take advantage of data locality and algorithmic simplicity, every other off-diagonal element is selected for elimination so that the rotation matrix for iteration i is

$$\boldsymbol{G}^{(i)} = \begin{bmatrix} c_1 & -s_1 & 0 & \dots & 0 \\ s_1 & c_1 & \vdots & & \vdots \\ 0 & \dots & \ddots & \dots & 0 \\ \vdots & & \vdots & c_{n/2} & -s_{n/2} \\ 0 & \dots & 0 & s_{n/2} & c_{n/2} \end{bmatrix} \tag{2.9}$$

and will zero out n elements.

This matrix undergoes round robin reordering of rows and columns so that the now zeroed elements are moved away from the diagonal and new elements are brought next to the diagonal. The process repeats itself for the new ordering until all the non-diagonal elements have magnitudes less than the desired threshold.

2.1.3 DAG algorithm

Implementing the parallel Jacobi as a DAG requires breaking the relevant matrices into tiles. This creates data pipelines that eliminates the need for syncing operations. In the parallel implementation of the traditional algorithm above, the whole process must wait for the entire rotation matrix to be constructed and the entire rotation GEMM must complete before construction of the next rotation matrix can begin.

If the matrices are split into tiles, each tile can be operated on independently from the others creating data pipelines. If $M^{(0)}$ and $G^{(0)}$ can be split up into tiles like

$$M^{(0)} = \begin{bmatrix} \mathbf{M}_{11}^{(0)} & \dots & \mathbf{M}_{1N}^{(0)} \\ \vdots & \ddots & \vdots \\ \mathbf{M}_{N1}^{(0)} & \dots & \mathbf{M}_{NN}^{(0)} \end{bmatrix} \quad G^{(0)} = \begin{bmatrix} \mathbf{G}_{11}^{(0)} & \dots & \mathbf{G}_{1N}^{(0)} \\ \vdots & \ddots & \vdots \\ \mathbf{G}_{N1}^{(0)} & \dots & \mathbf{G}_{NN}^{(0)} \end{bmatrix} \tag{2.10}$$

then $\mathbf{M}_{ij}^{(1)}$ only depends on three tiles.

$$\mathbf{M}_{ij}^{(1)} = \mathbf{G}_{ii}^{(0)} \mathbf{M}_{ij}^{(0)} \mathbf{G}_{jj}^{(0)} \tag{2.11}$$

If the number of rows and columns of the tiles of $M^{(0)}$ are even, then $\mathbf{G}_{ii}^{(0)}$ will only depend on $\mathbf{M}_{ii}^{(0)}$ and $\mathbf{G}_{ij} = \mathbf{0}$ when $i \neq j$. Similarly, during the round robin tournament reordering, each tile is dependent only on the adjacent tiles having finished their rotation operation.

2.2 Implementation

Currently PaRSEC has limited functionality for combining DAGs. Task graph composition currently consists of macros that automate the process of running multiple task pools sequentially. However, each pool must complete successfully before the next begins, so this approach loses the advantage of global sync removals. To recapture that advantage, it's up to the developer to generate a single DAG containing all the tasks. This is fairly straightforward if there are only a few unique DAGs being put together, but requires significant effort if the final task graph is made of several DAGs, especially if any of the component DAGs are reused.

In the Jacobi diagonalizer for example, there are 11 to 17 tasks. For debugging it's helpful to group these tasks into separate DAGs that can be unit tested. During testing, some of these unit DAGs may need tasks for initializing and finalizing the data that they'll operate on, but these tasks are removed when the DAGs are merged and are not included in the task counts listed here. The generation of the pseudo-Givens matrix G and DGEMMs are simple one task DAGs. The algorithm for round robin shuffling a matrix is a four task DAG. If the order of the eigenvalues and eigenvectors is important, the sorter can be another DAG made up of some number of

tasks depending on the complexity of the sorting and layout of the data being sorted. Most eigenvalue solvers return the solutions sorted by eigenvalue, which takes a five task DAG, while simply returning the two matrices ordered the same way as the input matrix requires two tasks.

Thus the complete diagonalizer requires the composition of five or six unit DAGs depending on whether a sorter is needed. Each task in a DAG needs to be provided with the names of the tasks that send or receive the incoming and outgoing blocks of data and what label that data had or will have in the other task. This requires manually updating the input and output of each of the unit DAGs. Also, each task has to have a unique identifier in the final DAG, so unit DAGs that are reused like the DGEMMs and matrix shuffler may have to have all of their tasks renamed each time they are inserted into the final graph.

In some cases, an alternative to duplicating a task is available. The PaRSEC DAG parser expands each task in the graph into a collection of uniquely named inline functions in C. So the DGEMM in Scheme 2.2 would be algorithmically turned into $mt * nt * nt$ uniquely named tasks, one for each unique combination of values in $m, n,$ and k. Another index can be added to the task and used in the data flow control to specify the origin and destination of the data as in Scheme 2.3.

Because the process location (: $location(m, n)$) in Scheme 2.3 depends only on indices m and n, each DGEMM task that shares the same m and n value will run on the same process regardless of the k or key index value. The location of the process must be specified for the task scheduler so this technique can only be used to reuse tasks that can share a process location. For the diagonalizer, this is desirable as aligning the tiles of the eigenvalue and eigenvector matrix eliminates the need to send $\mathbf{G}_{ij}^{(n)}$ to two different processes. However, forcing process alignment between unrelated tasks can introduce additional load imbalances.

This technique has the advantage of reducing the number of tasks that need to be modified if the code in the task changes. However, it has the notable disadvantage of making data flow somewhat more difficult to read.

Finally, because the diagonalizer is an iterative process, each task has to have a unique identifier for each iteration. This is accomplished by adding another index to track the iteration. For example, if the DGEMM in Scheme 2.3 were to be used iteratively then the first line would be-

```
DGEMM(m, n, k, key)
  m = 0 .. mt - 1
  n = 0 .. nt - 1
  k = 0 .. nt - 1
  key = 1 .. 2
:location(m, n)

READ A <- (key == 1) ? A READ_A(m, k) : D READ_D(m, k)
READ B <- (key == 1) ? B READ_B(k, n) : E READ_E(k, n)
RW C <- (k != 0) ? C DGEMM(m, n, k - 1, key)
     <- ((k == 0) && (key == 1)) ? C READ_C(m, n)
     <- ((k == 0) && (key == 1)) ? F READ_F(m, n)
     -> (k != nt - 1) ? C DGEMM(m, n, k + 1, key)
     -> ((k == nt - 1) && (key == 1)) ? C PUT_C(m, n)
     -> ((k == nt - 1) && (key == 2)) ? F PUT_F(m, n)

BODY
  cblas_dgemm(CblasRowMajor,
              CblasNoTrans, CblasNoTrans,
              lda, ldb, ldc,
              alpha, (double *)A, lda
              (double *)B, ldb,
              (k == 0) ? 0.0 : 1.0, (double *)C, ldc);
END
```

Scheme 2.3: Introduction of an index to the DGEMM from scheme 2.2 to reuse the code body. In this example, if $key == 1$, the task will do the same thing as in 2.2. If $key == 2$, This task will multiply data D and E from READ_D and READ_E respectively. The ultimate product will be sent on as F to PUT_F.

come $DGEMM(m, n, k, key, iter)$, another index $iter = 1..maxiter$ would be added to the list of unique identifiers and an $iter$ index added to the tasks in the data flow description. This does not significantly complicate the data flow control for most tasks, it's just tedious.

3 Prototype SCF

The full SCF was implemented as described in Scheme 2.1 except for one modification. It sometimes happens that the density matrix $\boldsymbol{P}$ will oscillate between two states and so the residual of the difference between two iterations' density matrices never changes and the algorithm fails to converge. To prevent this, a technique called "oscillation damping" was used[12]. This means that

if an element of the density matrix changes by more than some threshold then instead of using the new value, the old value will just be shifted by the threshold amount in the direction of the new value. That is, if $|P_{ij}^{new} - P_{ij}^{old}| > threshold$ then $P_{ij}^{new} = P_{ij}^{old} + sign(P_{ij}^{new} - P_{ij}^{old}) * threshold$. This process can increase the number of iterations the SCF takes to converge depending on how large the selected threshold is. However, some method is needed to ensure convergence of these oscillating cases.

Code for computing the integrals shown in 2.2 and 2.5 have been implemented in several open source packages. This SCF implementation uses Aces III[13] to compute the one electron integrals and Simint[14] to compute the two electron integrals.

The final task graph was composed of 56 tasks made from about 15 unique unit DAGs. Some of these units (like the diagonalizer) had multiple subunits not included in this tally. About half of the tasks were inside the iterative portion of the SCF and required the addition of an index to track that.

4 Results and Conclusions

An iterative diagonalizer was successfully implemented with PaRSEC. This demonstrates that in at least some cases, pipelining data can remove the need for expensive syncing operations in a cyclic process.

Expanding on this, a prototype SCF code was made that correctly calculates the energy of test systems compared to similar calculations performed by NWChem. Simple energy calculations were performed on water and peroxide molecules using geometries optimized in NWChem[15] using the STO-3G[16] basis set provided by the Basis Set Exchange[17][18][19] and the resulting energies matched the results of similar calculations performed with NWChem within chemical accuracy (see Table 2.1).

Table 2.1: Results of SCF energy calculations on water and peroxide with the DAG SCF and NWChem. The difference in energy between the two runs is well within chemical accuracy (typically 0.1 kcal/mol).

Molecule	DAG SCF (ht)	NWChem (ht)	ΔE (ht)	ΔE (kcal/mol)
H_2O	-74.951408	-74.951407	0.000001	0.006
H_2O_2	-148.669133	-148.669081	0.000052	0.032

The code is not yet suitable for general use and lacks optimizations commonly available in most other computational chemistry packages (more on this below).

There are two main problems with using PaRSEC to implement these cyclic algorithms. The first is the issue of composing multiple unit DAGs into one larger task graph as discussed in the section on implementing the diagonalizer. More robust task composition is on the PaRSEC development roadmap, but for now such composition all has to be done by hand.

The second issue is that there is currently no way for a task inside the graph to signal to the task manager whether a future task needs to be run. For the diagonalizer, this means that the number of iterations has to be set before the task graph is executed. It will run for the set number of iterations regardless of when (or if) the diagonalization converges. The same problem exists with the number of iterations of the SCF algorithm itself as well. The number of SCF iterations is set before the task pool is executed and can't be modified from within the algorithm.

This problem is exacerbated when the iterative diagonalizer is run as a part of the iterative SCF algorithm. In Scheme 2.1, the number of iterations for the diagonalization of $\boldsymbol{F'}$ has to be set before the SCF and remains constant from one SCF iteration to the next. Currently, this means setting the number of iterations for each iterative process for each chemical system being run.

A method to cancel future tasks is also on the PaRSEC development roadmap but this may be significantly more complicated than the DAG composition process (not least because of difficulties arising from the composition of multiple DAGs that self-terminate).

4.1 Future Direction

4.1.1 Diagonalizer

The Jacobi diagonalizer only works on symmetric matrices. For simplicity sake, the diagonalizer as written does not take advantage of this symmetry and so some of the operations are unnecessarily duplicated. Specifically, if the matrix being diagonalized was stored and operated on as a triangular matrix, $(N^2 - N)$ tasks could be removed from the multiplications of the eigenvalue collector during each iteration where N is the number of rows of tiles. For each tile $\mathbf{M}_{ij}^{(n)}$, $\mathbf{M}_{ji}^{(n)} = \mathbf{M}^{\mathbf{t}}{}_{ij}^{(n)}$ for $i \neq j$ so there is no need to compute both tiles.

4.1.2 SCF

Because of the need to set so much of the SCF task graph for the specific chemical being studied, information about the test chemical systems is hard-coded. This makes running new systems very cumbersome. A parser that can read the coordinates and basis functions for each atom needs to be incorporated.

The main difficulty with (and entire point of) this project was implementing a fundamentally cyclic algorithm in an acyclic task manager. The process of pipelining the data for a cyclic algorithm is currently only possible when the number of cycles required can be determined before the task graph is constructed. This can be worked around by passing an instruction to a given task determining whether the task should do anything or just exit successfully. This carries some computational and communication overhead as every task in the graph still has to be initiated, but may improve performance if there are a lot of useless iterations happening.

Finally, a DAG may not be well suited for implementing the entire SCF algorithm. Most computational chemistry packages incorporate methods to accelerate the SCF convergence process. The most common of these, Direct Inversion of the Iterative Subspace (DIIS) extrapolates the difference in the Fock matrix between iterations and attempts to project an error-free Fock matrix onto a basis set made of previous guesses at the Fock matrix. It's a very good accelerator, but requires the solution of a very small set of equations to get the coefficients for the linear combinations of the previous Fock matrices. Because of this, there is a bottleneck in the task graph while these equations are solved. Using a DAG for every other part of the cycle may still yield performance improvements. The reduction in the number of SCF iterations may be worth the introduction of a once-per-iteration sync.

4.2 Acknowledgements

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CHAPTER 3. ZIRCONIUM CATALYED CYCLOAMINATION OF 4-PENTENAMINE, A MODEL SYSTEM

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Abstract

Cycloamination reactions proceed by mechanisms that are not well understood. While several mechanisms have been proposed, this work examines in detail the complex reaction landscape for the {$PhB(C_5H_4)(2\text{-oxazoline})_2$}Zr catalyzed cycloamination of 4-penteneamine to 2-methylpyrrolidine. After considering different reaction environments and relevant thermodynamics, two linked cyclization mechanisms are suggested, an olefin insertion and a [2π+2π] cycloaddition. The accuracy of B3LYP and M06-L density functionals compared to MP2 for this system is also discussed.

Introduction

Optically active cyclic amines have important industrial and pharmaceutical applications, however stereochemical control of the synthesis of these compounds is currently limited.[1] Typically, such isomer-producing reactions have poor enantioselectivity because the molecular symmetry of the starting amine does not allow a

thermodynamically favored product isomer; however some progress has been made on this front using asymmetric transition metal complexes as catalysts[2] with zirconium complexes proving to be particularly effective for stereospecific synthesis.[3,4,] Understanding the mechanistic impact of these catalysts on the enantioselectivity requires an understanding of the reaction mechanisms which has not yet fully emerged.

This paper examines the role of a model system, {PhB(C_5H_4)(2-oxazoline)$_2$}Zr (Figure 1) (herein represented by [Zr]), in the catalytic cyclization of the symmetric model compound 4-penteneamine to 2-methylpyrrolidine via three proposed mechanisms. [5,6,7] A better understanding of the cyclization mechanisms, although entirely symmetric in the model system, will open the way to further examination of the stereospecific reactions.

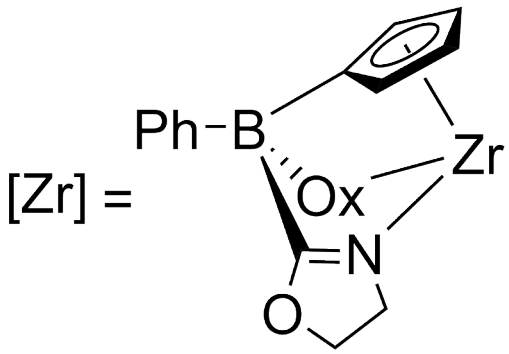

Figure 1: Model system catalyst. Experimental catalysts for similar reactions have substitutions on the oxazoline rings (Ox) that make the catalyst asymmetric.

These types of cyclization reactions are thought to proceed by one of three mechanisms (Figure 2): (A) olefin insertion in which the carbon-carbon double bond inserts across a zirconium-nitrogen single bond essentially replacing the zirconium-nitrogen bond with a zirconium-carbon bond;[8,9,10] (B) [2π+2π] cycloaddition in which the C=C inserts across the Zr=N to produce a dual ring system;[11] and (C) concerted ring formation and

hydrogen transfer.[12] Replacing the amine hydrogens with deuterium increases the stereoselectivity of the reaction indicating that the rate limiting step will involve a hydrogen transfer and the cyclization must occur prior or concurrently to that hydrogen transfer.[12] Unfortunately, due to similar experimental characteristics (e.g. rate law and primary isotope effects), isolating a mechanism solely from experimental data may not be possible.

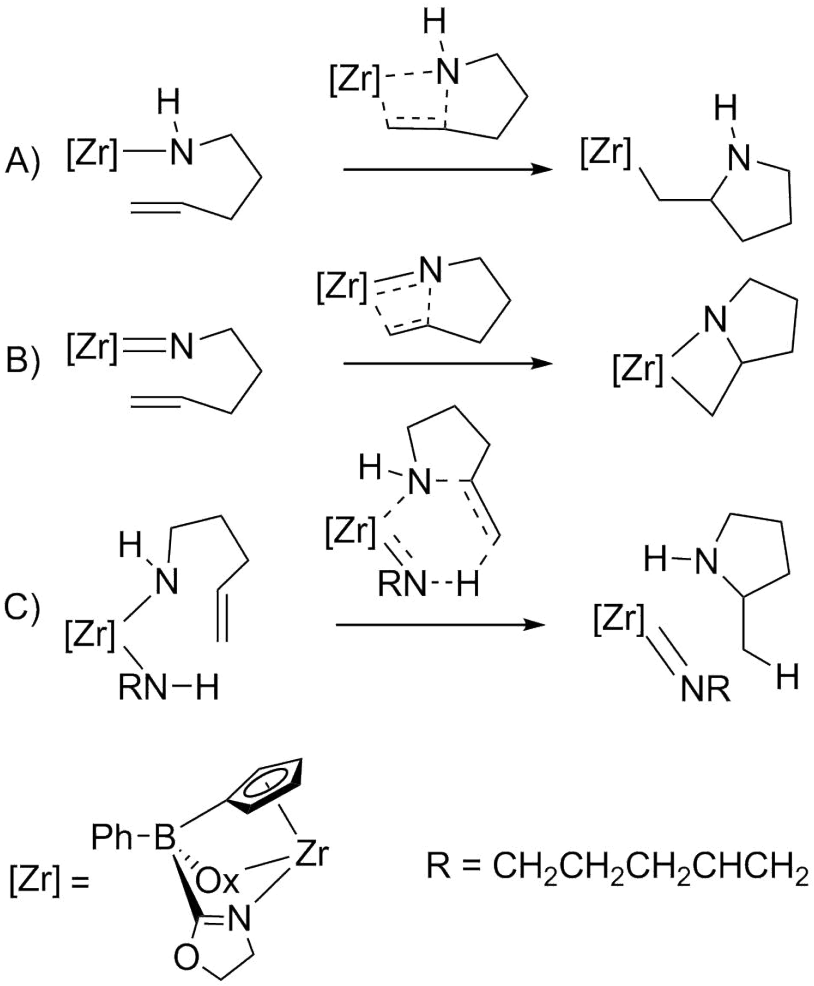

Figure 2: Three potential cyclization reactions. A) olefin insertion in which the carbon-carbon double bond inserts across the zirconium-nitrogen single bond forming new zirconium-carbon and nitrogen-carbon single bonds. B) [2π+2π] cycloaddition in which the C=C inserts across the Zr=N leaving a dual-ring system. C) a concerted reaction in which the ring closure is accompanied by a hydrogen transfer.

Previous computational work on hydroamination reactions with catalytic cyclopentadienyltitanium complexes suggested that a [2π+2π] cycloaddition of an unsaturated C=C bond across a Ti=N bond was an energetically plausible mechanism.[7] Further, a more recent computational study[6] comparing hydroamination cyclization catalytic cycles proceeding through [$Cp_2Zr(NHR)_2$] and [Cp_2Zr=NR] intermediates suggested that the [2π+2π] cycloaddition should be the kinetically favored product although the olefin insertion does not have prohibitively high energetic barriers. The current study fleshes out this understanding by showing that both mechanisms may come into play with different concentrations of amine substrate.

The most likely pathway(s) must be energetically favorable[7] and explain why experiments show that similar reactions have first-order rate dependence at low substrate concentrations and zero-order at high substrate concentrations. This dependence of the rate order on substrate concentration suggests that the irreversible step happens after a reversible substrate-catalyst interaction.[12]

Computational Methods

All calculations were performed with NWChem.[13] Initial geometry optimizations were performed with a "tight" convergence criteria with B3LYP[14,15] and with the 3-21G[16] basis set for light atoms and LANL2DZ ECP for zirconium.[17] The geometries thus located were further optimized and Hessians obtained with B3LYP using the 6-311G(d,p) basis set[18] for light atoms and Stuttgart 1997 RSC with ECP[19] for zirconium. The Hessian calculations were performed on optimized geometries to verify that there was only one

imaginary frequency for saddle points and none for the minima, and to obtain the zero-point energy (ZPE) corrections.

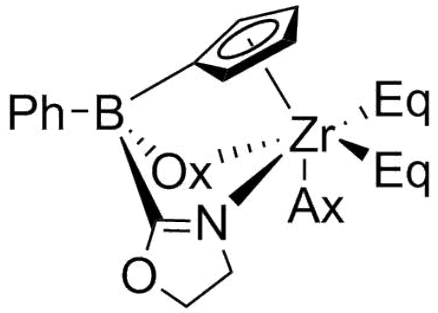

Figure 3: Model system catalyst with backbone indicating the position of equatorial(Eq) and axial(Ax) ligand positions.

The catalyst backbone leaves enough space for about three ligands to be coordinated to the zirconium, two “equatorial” positions across from the oxazolines and one “axial” position across from the cyclopentadienyl (Figure 3). If one of these positions is unoccupied and the reaction doesn’t involve a coordinated amine it may occur with or without a spectator amine coordinated to the open spot. For example, any of the three cyclizations shown in Figure 2 could happen whether there is a spectator amine nearby or not. Where possible, these reactions with spectator amines were considered to find whether their presence impacted the barrier heights. However, several of the these located minima and transition states had multiple imaginary frequencies associated with the motion of the coordinated amine. The potential energy surface associated with small changes in the coordinated amines is very flat and so elimination of these additional imaginary frequencies was impractical even with the tightest criteria for saddle point or optimization convergence. For these pseudo-minima, all the imaginary frequencies were verified to be associated with minute

translations of the coordinated amine rather than motion of part of the system that would be reacting. For transition states with these coordinated amines the largest imaginary frequency was verified to be the desired reaction coordinate of the transition state and any other imaginary frequencies were verified to correspond to these small substrate translations. Single point energy calculations were performed with MP2, B3LYP and M06-L[20] theories with the larger basis set and corrected with the B3LYP ZPE. Entropies were computed from the Hessian calculations and Gibbs free energies were calculated assuming room temperature (a common temperature for the experimental reactions[7]).

A complete set of the reactions studied in this work is given in Figure 4. Cyclization reactions are labeled with a "C" (C1 and C1-S are olefin insertions, C2 and C2-S are 2π+2π cycloadditions, C3 and C3-S are concerted). Hydrogen transfer reactions are labeled with an "H." Substrate association reactions are labeled with an "A" and product dissociations are labeled with a "D." Reactions with a coordinated spectator amine have a "-S" suffix while those with a formed but not yet dissociated product have a "-P" suffix.

When searching for minima, the atoms involved in the transition states were nudged from their positions in the located saddle point along both directions of the transition state vibrational mode and then the NWChem geometry optimization driver was allowed to find a local minima. Thus, the final geometry of each elementary reaction typically must undergo a slight rearrangement to get into position for the start of the next elementary reaction. For example, in Figure 4 the cyclization depicted by reaction C1 precedes the hydrogen transfer H6. The minimum after the cyclization may not have the amine or the ring in the ideal position for the

subsequent hydrogen transfer. To align the hydrogen and carbon might require rotations along the Zr-C or Zr-N bond. Transition states associated with these rotations typically have very low barrier heights relative to the other reactions depicted and these syntheses occur in solutions where a thermal bath provides energy for low barrier height reactions. As such, the transition states associated with these conformer rearrangements were not sought. Because the differences in energy between minima in the same basin are mostly small compared to the barrier heights required to move out of the basin, the minima are treated as though they are in equilibrium. The one exception to this trend is that the product of D1 is significantly lower in energy (15-18 kcal/mol) than any of the minima needed to move the reaction forward (reactions C1, C3, H1 reverse, or A1). This minima is still treated as being in equilibrium with the other minima because the rearrangement of the dissociation product to any of the other reaction's reactants can be accomplished by a sequence of C-C rotations. The larger energy gap may cause a delay for the next reaction, but should not stop it. The energies listed in the paper and tables are the energy differences from the conformer that is required for the reaction. So, in the example of the cyclized product of C1 needing its ligands to rotate to get into position for H6, the C1 cyclization reaction energy would use the minima before the rotation while the H6 transfer energy would use the minima after the rotation. Because all minima within a basin are considered to be in equilibrium, the most likely path out of each basin is likely to be the reaction with the lowest barrier height, even if that reactant is higher in energy than a reactant for a competing pathway. More information about the specific minima for each reaction is available in the supplemental information. Additionally, association and dissociation transition states were not sought due to time constraints.

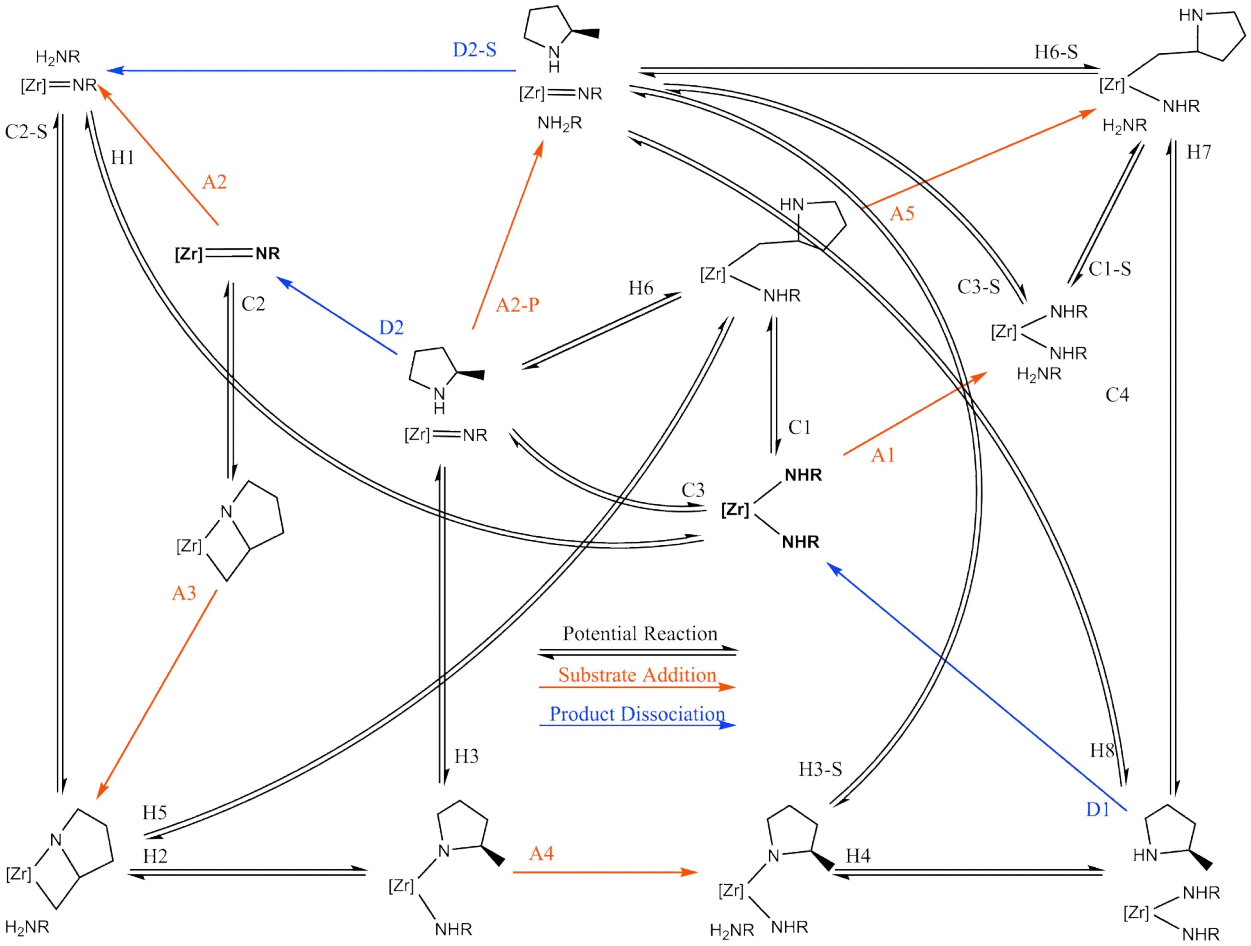

Figure 4: Complete set of all 2-methylpyrrolidine producing reactions studied. Double arrows indicate a reaction where a transition state was located and the "forward" and "reverse" reactions were both considered. Reactions with suffix -S and -P indicate the presence of a coordinated spectator substrate amine or product ring respectively. Reactions whose labels starts with a "C" are cyclization reactions. The molecules depicted with bold type are likely entry points for the cycle. C1 and C1-S are olefin insertion cyclizations. C2 and C2-S are [2π+2π] cycloadditions. C3, C3-S and C4 are concerted cyclization and hydrogen transfer reactions. Reactions starting with an "H" are hydrogen transfers. Labels beginning with an "A" or "D" are substrate addition and product dissociations, respectively. To avoid graphical clutter, rather than picturing the free substrate and product molecules adding or subtracting, the addition and dissociation reactions have been indicated by orange and blue reaction lines respectively.

Unlike the experimental systems this model's catalyst and substrate amines have C_s symmetry. Because of the symmetry, every studied geometry has an enantiomer with identical energy. Consequently, no conclusions about which enantiomer is preferred can be drawn from this work. Rather, the purpose of these calculations was to identify likely reaction pathways. Even within this highly symmetric system, each reaction has multiple possible arrangements for the ligands. For example, Figure 5 shows the transition states for a sample olefin insertion reaction and a sample hydrogen transfer reaction. The arrangement of the reacting ligands can be axial

(5A, 5C), when at least one directly involved atom is coordinated to the zirconium opposite to the cyclopentadienyl ring, or equatorial (5B, 5D), where all directly involved atoms are roughly opposite to the oxazolines. For each reaction with an examined transition state at least one equatorial and one axial transition state configuration were found. However, time constraints prevented calculation of all such possible states (for example, in the axial olefin insertion cyclization pictured in (Figure 5a) one might imagine the zirconium bound nitrogen in the axial position and the zirconium bound carbon in the equatorial position).

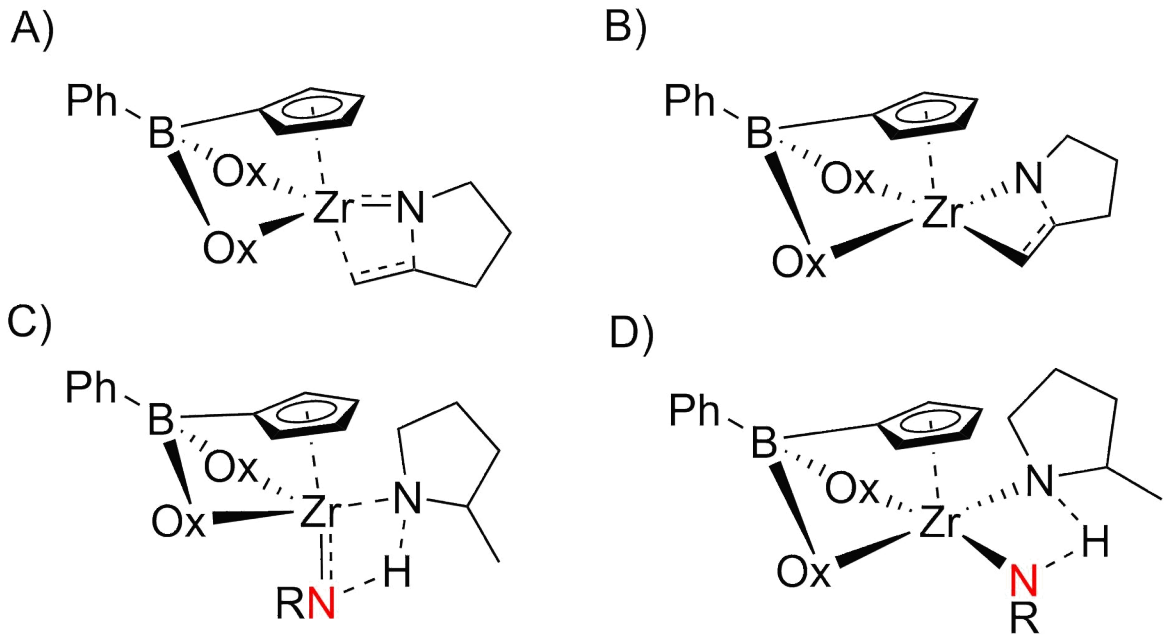

Figure 5: A) Cyclization where the carbon is in the axial position and the nitrogen is on the equatorial position. B) Cyclization where the carbon and nitrogen are both in equatorial positions. C) Hydrogen transfer between the axial nitrogen (shown in red) and an equatorial nitrogen. D) Hydrogen transfer between an equatorial nitrogen (in red) to the equatorial ring nitrogen.

Results

This catalytic cycle is experimentally thought to begin with either the formation of [Zr](NHR)$_2$ or the formation of [Zr]NR (denoted in bold in Figure 4). Depending on reaction conditions, the reaction may proceed to product dissociation at D1, D1-S, D2, or D2-S.

There are many possible reaction paths providing many possible catalytic cycles such as A1 to C1-S to H7 to D1. For reactions using the D1 or D1-S dissociation, the catalytic cycle starts anew at C1 or C1-S. The other cycle (discussed below) goes through either C2 or C2-S and ends with D2 or D2-S. Properties of the elementary reactions will be discussed first in order to explain why only two of the many potential catalytic cycles are likely.

Cyclization trends

The MP2 Gibbs free energies of the cyclization barrier heights for both axial and equatorial cyclizations are given in Table 1. For the olefin insertion cyclizations, there isn't a very significant difference between the barrier heights of the equatorial vs. axial cyclizations. However, the 2π+2π cycloaddition had substantially lower barrier heights when the reaction occurred along the equatorial positions compared to the axial configurations. Axial cyclizations in the presence of a spectator amine had lower barriers than the same reaction without the spectator. This was especially pronounced for reactions C3 and C3-S, but this is probably because the C3 concerted transition state has a significantly higher barrier height to begin with. Looking at the more plausible barriers of the C1 and C2 axial reactions, adding a spectator amine in the equatorial position lowered the barrier height by 1-5 kcal/mol. For equatorial cyclizations, there was not a clear trend in the impact of a spectator amine being added to the axial position. Also equatorial olefin insertion decyclizations (C1 and C1-S) are the only exothermic decyclization reactions.

The equatorial cyclizations had an average barrier height of 15.0 kcal/mol compared to the axial cyclizations average of 20.5 kcal/mol. Most of this is an artifact of the high barriers of the

concerted reactions, however. Just considering the C1 and C2 reactions with and without substrate, the preference for equatorial cyclization becomes more pronounced with an average barrier height of 5.6 kcal/mol compared to the average axial cyclization barrier height of 12.2 kcal/mol.

The olefin insertion reactions C1 and C1-S have low barriers in a narrow range of 9.1 to 11.5 kcal/mol. The [2π+2π] cycloadditions C2 and C2-S have even lower barriers with only the axial cyclization C2 barrier height of 8.8 kcal/mol falling outside the otherwise very low range of 1.0 to 3.5 kcal/mol. The concerted reactions C3 and C3-S all have barriers exceeding 30 kcal/mol. The saddle point of the concerted reaction C4 was not found but is assumed to have a similarly high barrier. However, if this assumption doesn't hold and the concerted cyclization with a coordinated substrate has a much lower barrier, the likely overall reaction mechanism will only change if the barrier for that concerted cyclization is less than 14.5 kcal/mol because C4 is in "competition" with H7. If the cyclization barrier is significantly lower than 14.5 kcal/mol, then the two step cyclization and hydrogen transfer C1-S followed by H7 would be replaced by a single step reaction C4. This might impact the kinetics of the reaction but not the likely pathways.

In general, both the olefin insertion and [2π+2π] cycloaddition had low enough barrier heights for the cyclization and decyclization reactions to be in an equilibrium favoring the cyclized product. The concerted reactions had high enough energetic barriers that they were unlikely to occur. Removal of these concerted cyclizations leaves the two cycles shown in Figure 6, with cycle A proceeding via a 2π+2π cycloaddition and cycle B via an olefin insertion. Both cycles may

be active and the degree to which one is preferred over the other is determined by substrate availability. More discussion on this below.

Table 1: MP2 Gibbs free energy barrier heights of the cyclization reactions in kcal/mol. The labeled reactions can be seen in Figure 4. Reactions with labels ending in "-S" have a spectator amine. Barrier heights for the d- reactions are those in which the amine hydrogens are replaced by deuterium when calculating the zero point energy.

Cyclization type	Label	Direction	Axial	Equatorial	d-Axial	d-Equatorial
olefin insertion	C1	cyclizing	6.0	9.3	5.9	9.1
olefin insertion	C1	de-cyclizing	14.9	7.7	15.2	7.9
[2π+2π]	C2	cyclizing	8.8	1.3	7.0	1.3
[2π+2π]	C2	de-cyclizing	19.7	7.1	20.7	7.1
concerted	C3	cyclizing	39.4	29.9	39.6	31.3
concerted	C3	de-cyclizing	44.2	37.5	45.0	39.2
olefin insertion	C1-S	cyclizing	5.6	10.8	5.3	14.9
olefin insertion	C1-S	de-cyclizing	20.6	1.8	20.8	2.0
[2π+2π]	C2-S	cyclizing	3.5	0.9	4.8	-0.9
[2π+2π]	C2-S	de-cyclizing	18.0	5.8	18.0	3.9
concerted	C3-S	cyclizing	32.5	31.0	32.8	32.1
concerted	C3-S	de-cyclizing	32.5	36.3	34.6	37.9

Hydrogen Transfers

The MP2 Gibbs free energies for all the hydrogen transfers in Figure 4 can be found in Table 2. The barrier heights are generally lower than 25 kcal/mol. Axial hydrogen transfers tended to have lower barrier heights than the equatorial reactions, averaging 14.1 kcal/mol for the axial transfers compared to 19.1 kcal/mol for equatorial transfers.

Taken in isolation, each hydrogen transfer reaction can be considered to be an equilibrium, albeit one that may be reactant or product favored. Because of this, the reaction direction that moves the overall system toward a product elimination is considered to be the "forward" direction while the other direction is the "reverse." In fact, the plausibility of each hydrogen transfer being an equilibrium rather than an irreversible reaction causes some unexpected

results. For example, H6 may be the product elimination step even though it is in competition with H5 reverse, a reaction with a lower barrier height. The reason is that if the reaction proceeds via H5, the eventual bottleneck will be H3, the barrier height of which is 2.6 to 8.3 kcal/mol higher than that of H6.

Table 2: MP2 Gibbs free energy barrier heights of the hydrogen transfer reactions in kcal/mol. The labelled reactions can be seen in Figure 4. The "forward" and "reverse" direction indicate whether the overall system is moved closer to or further away from the final product elimination. Barrier heights for the d- reactions are those in which the amine hydrogens are replaced by deuterium during the zero point energy calculation.

Label	Direction	Axial	Equatorial	d-Axial	d-Equatorial
H1	Forward	14.5	14.5	17.0	16.7
H1	Reverse	23.4	20.7	25.5	22.3
H2	Forward	10.1	13.4	12.2	15.7
H2	Reverse	17.7	30.7	19.2	32.1
H3	Forward	21.6	20.5	23.4	22.1
H3	Reverse	10.6	11.8	12.6	14.0
H4	Forward	4.5	10.0	6.5	11.9
H4	Reverse	4.3	13.0	6.0	14.8
H5	Forward	6.1	18.6	8.1	20.6
H5	Reverse	-0.6	10.0	1.3	11.9
H6	Forward	18.9	17.8	20.3	21.7
H6	Reverse	19.7	17.8	21.4	19.4
H7	Forward	14.5	20.4	15.5	22.6
H7	Reverse	23.6	24.1	23.8	25.5
H8	Forward	6.1	16.6	8.3	17.9
H8	Reverse	19.7	22.6	21.3	24.4
H3-S	Forward	18.7	23.1	17.4	19.7
H3-S	Reverse	4.1	13.9	2.8	15.7
H6-S	Forward	18.3	29.6	23.9	28.1
H6-S	Reverse	20.8	33.2	22.5	32.3

Substrate coordination and product dissociation

The coordination of either a substrate or product tends to lower the overall system energy compared to the dissociated system. However, as seen in Table 1 and Table 2, there doesn't seem to be a particular trend with regard to whether the transition state or minima is more stabilized. Reactions that happen with a coordinated amine (those with a "-S" label suffix) may

or may not have lower barrier heights than the same reaction without the coordinated amine. Reactions with an "A" label indicate the association of 4-penteneamine and the "D" label indicates the dissociation of 2-methylpyrrolidine, the product. Table 3 shows that the associations are all exothermic and the product dissociations are endothermic.

Table 3: MP2 Gibbs free energy reaction energies in kcal/mol of substrate association (A) and product dissociation(D) reactions. Note that all associations are exothermic and all dissociations are endothermic.

Reaction	Equatorial	Axial
A1	-7.9	-13.2
A2	-14.8	-14.9
A3	-19.2	-17.0
A4	-6.8	-8.1
A5	-3.8	-16.6
D1	5.0	3.3
D2	15.9	14.1

Likely catalytic cycles

The very large number of pseudo-minima with similar energies makes an exhaustive search of possible reactions impossible (or at least absurdly expensive). As such, a detailed kinetic model isn't practical. However, with the calculations performed, two experimental conditions can be approximated. One is a condition with very low concentrations of substrate (Figure 6A), such that the system has time to reach a steady state between association reactions. The other is a condition with abundant substrate (Figure 6B). In both cases, the overall reaction starts at [Zr] $(NHR)_2$ ready to undergo either cyclization C1 or association A1.

There are several likely pathways depending on the concentration of amine. If the substrate is scarce the energetically favored path from the starting material becomes C1-H6-D2. The reaction will proceed as far as it can until an amine is required, halting until an amine

coordinates to the reaction site (the reactions with orange arrows in Figure 6a). The low energy barriers of the reactions will not be the limiting factor and the 2π+2π cycloaddition becomes the dominant cyclization mechanism. This is a somewhat more complicated cycle than the situation with abundant substrate amine because the reactions involved have low enough forward and reverse barriers to be considered a kind of three minima equilibrium H3-H2-H5-H6 Thermodynamically favored reactions H5 and H2 all form equilibria as shown in Figure 6a, but H3 and H6 become the only exits. After the product dissociates the reaction pauses at the product favored 2π+2π cycloaddition cyclization equilibrium until another amine associates at either A2 or A3 and then the cycle repeats.

In the case of abundant substrate, it is anticipated that every time the association of an amine is possible it will occur because the association process is nearly barrierless and exothermic. This results in the cycle shown in Figure 6b. The first step is either association A1 followed by the olefin insertion cyclization C1-S or cyclization C1 followed by association A5. With abundant substrate, the exothermic association reaction is preferable to the hydrogen transfer H6 which has an actual barrier. After this, the substrate addition/hydrogen transfer/product elimination of H7 is kinetically preferred over H6-S by either 3.8 kcal/mol or 7.9 kcal/mol depending on whether the system has an axial or equatorial orientation. H7 is the rate limiting step having a barrier height of either 14.5 for the equatorial transfer or 19.0 kcal/mol for the axial transfer. The result of H7 may reverse the product elimination through H4. However H4 is a low barrier equilibrium, so eventually the product amine will dissociate via D1 leaving the reaction ready to cyclize another amine at C1. With abundant substrate, the 2π+2π cycloaddition doesn't usually

happen because the reactions required to produce the starting material C3 or C3-S forward, or H1 reverse have higher barrier heights than the olefin insertion cyclizations.

Of course, as the reaction proceeds the substrate will become more scarce and the kinetically dominant cycle will shift from B to A. The system has to "wait" at the product of C1 and entry to cycle A becomes likely through direct elimination via H6 or entering the three minima equilibrium discussed above via H5 reverse. This explains the rate order dependence on substrate concentration. At higher substrate concentrations the rate determining step is an intra-molecular reaction with a rate that is zero-order with respect to substrate concentration. Lower substrate concentrations are diffusion limited and have a first-order dependence on the substrate concentration.

Axial vs. Equatorial reactivity

In all the reactions studied, the catalyst has C_s symmetry, so neither R- nor S- products are expected to be the thermodynamic nor kinetic product of any of the cyclizations shown in Figure 5. However, for the equatorial reactions, a standard orientation for the reacting ligand relative to the catalyst was chosen. Specifically, the ligand was oriented so that the product ring would be facing away from the cyclopentadienyl ring on the catalyst backbone. The importance of this is not that it predicts which product is more likely to form, but which orientation the cyclization step is likely to take. The axial hydrogen transfer reactions generally require less energy than the equatorial hydrogen transfers and equatorial cyclizations generally require less energy than axial cyclizations.

For the olefin insertion cycle (Figure 6b) two different versions of each axial reaction was studied. These were reactions in which one of the two zirconium coordinated atoms was in the axial position. For the cyclization, these two atoms were the nitrogen and the methyl carbon on the newly formed ring. For the hydrogen transfers, these were the hydrogen donating nitrogen and the hydrogen receiving carbon or nitrogen. The different orientations of the six axial reactions thus studied had an average difference between zero point energy corrected barrier height enthalpies of only -0.58 kcal/mol and average difference of reaction energy of -0.64 kcal/mol. There was no clear trend and the enthalpic differences were so small that the sterics of an asymmetric or substituted amine or catalyst will likely have more of an impact on which geometries are preferred. Because the model system has no asymmetries there isn't a kinetic or thermodynamic preference and no such duplicate reactions were sought for the 2π+2π cycle. A full report of the resulting barrier heights and reaction energies is available in the SI, but only the axial reaction with the lowest forward barrier height is discussed here.

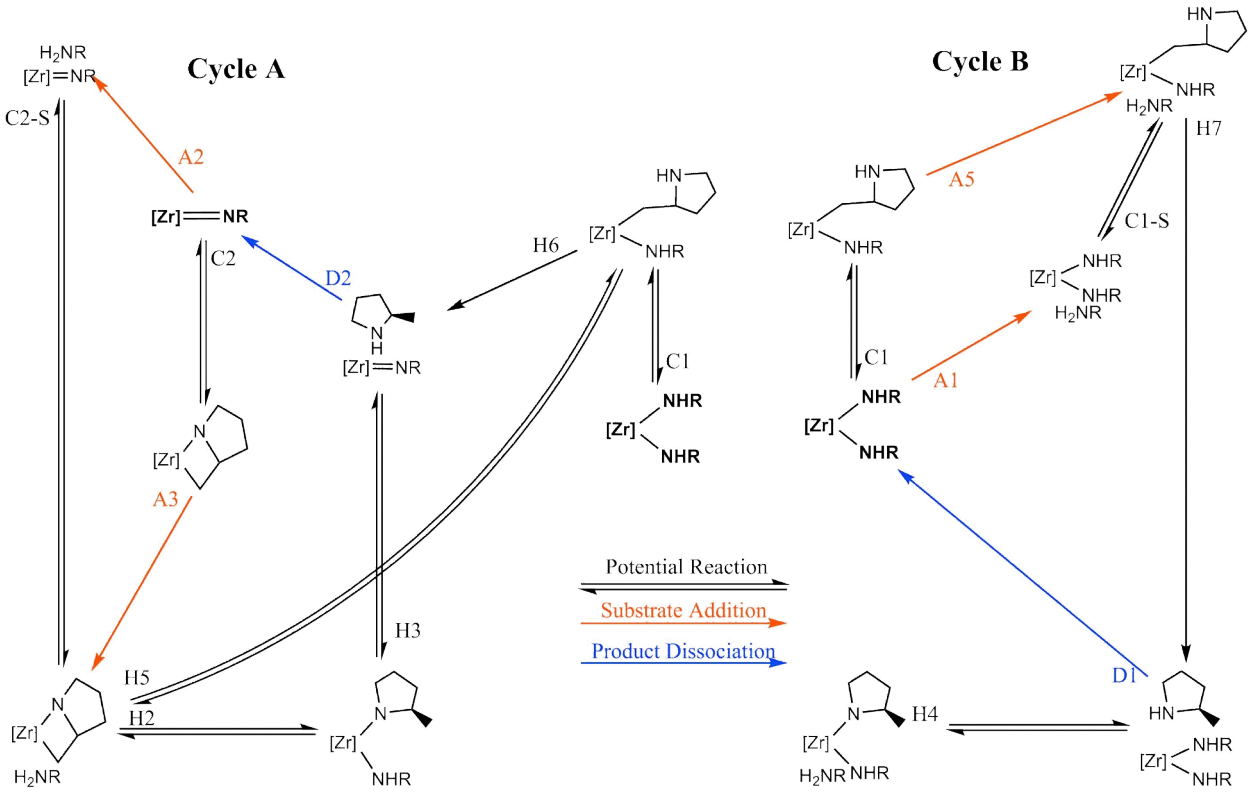

Figure 6: Two most likely catalytic cycles. A) the 2π+2π cycloaddtion is the dominant cycle when the substrate amine is sparse. C2 and C2-S have comparable barrier heights and are both product favored, so it doesn't matter whether the the association or the cyclization happens first. Either way, the reaction is held up by the amine association and not the cyclization. B) the olefin insertion is the dominant cycle when the substrate amine is abundant. The bold molecules are the likely entry points for the catalytic cycles.

Isotope Effect

Experimentally, the enantiomeric yield is slightly increased when using a deuterated amine substrate. The stereospecific yield, already above 90% for similar undeuterated reactions increases by a few percent when the substrate amine is deuterated[7]. Again, due to the symmetry of the model catalyst there can be no identifiable trends between R- and S- products from this work. However, there is a trend with deuteration among reaction types. For cyclization reactions that do not include a hydrogen transfer (C1, C1-S, C2, C2-S), there is no significant impact on likely reactions (Table 1). Even if there were, it probably would not be kinetically significant as the cyclization barrier heights are lower than most of the hydrogen transfer

reaction barriers. The barrier heights of the concerted cyclizations are so high they are unlikely to occur regardless of deuteration.

For non-cyclizing hydrogen transfer reactions, the barrier height is increased via deuteration (Table 2) by an average of 1.4 kcal/mol. The increase tends to be about the same magnitude for both the axial and equatorial barrier heights. Because reaction rates at constant temperature scales as $k \propto e^{-E_a}$, increases in the absolute barrier heights will shift the product towards the lower barrier reaction even if the difference between the enantiomers barrier heights remains about the same. The computed barrier heights increasing by about the same magnitude with amine deuteration is consistent with the experimentally observed slight increases in stereoselectivity.

Conclusions

Based on the calculations and reasoning presented in this paper, there are two likely mechanisms by which the reaction may proceed. With abundant substrate, an olefin insertion is the likely enantiomer selecting step while the subsequent hydrogen transfer is the rate limiting step. With scarce substrate, the cyclization is more likely to proceed via a [2π+2π] cycloaddition and the rate will be limited by the diffusion of the amine in solution. In either case, the reaction path with the lowest barrier tends to be an equatorial cyclization followed eventually by the rate limiting axial hydrogen transfer. Generally, equatorial cyclizations have lower barrier heights than axial cyclizations and axial hydrogen transfers are energetically preferable to equatorial hydrogen transfers. The consistent positive impact of amine deuteration on the enantiomeric yield is consistent with an increase in absolute but not relative barrier heights.

Acknowledgments

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Calculations were performed on the Condo and Cyence clusters of the High Performance Computing facility at Iowa State University.

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CHAPTER 4. OXYGEN INSERTION REACTIONS OF MIXED N-HETEROCYCLIC CARBENE-OXAZOLINYLBORATO ZINC ALKYL COMPLEXES

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[William Everett contributed the computational results. All experimental data was obtained by members of the Sadow group.]

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Abstract

We report the synthesis of a new mixed oxazoline–carbene scorpionate ligand, bis(4,4-dimethyl-2-oxazolinyl)(1-mesitylimidazolyl)phenylborate (PhB(Ox^{Me2})$_2$$Im^{Mes}$). Reactions of the protonated form PhB(Ox^{Me2})$_2$(Im^{Mes}H) with dialkylzinc compounds provide four-coordinate zinc alkyl complexes, and X-ray diffraction studies of the {PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnR (R = Me, Et) compounds show significant structural distortions involving the R groups shifting away from the carbene donor. The reaction of {PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnEt (**3**) and O_2 provides an isolable mononuclear zinc alkylperoxide {PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnOOEt (**4**), which has been characterized by single crystal X-ray diffraction and ^{17}O NMR spectroscopy.

Introduction

Reactions of metal–carbon bonds and O_2 are important potential components of new approaches to green oxidative catalysis. Often these reactions can be complicated by unselective product formation from overoxidation rather than formation of metallo-alkylperoxides that might be used as mediators of selective oxidation. This challenge affects organozinc chemistry, and the vigorous reactions of zinc alkyl compounds and oxygen are often difficult to control.[1] For example, reactions of $ZnEt_2$ and O_2 give $Zn(OEt)_2$ or EtZnOEt, while $ZnMe_2$ and O_2 provide MeZnOMe, rather than [Zn]OOR.[2–4] Lithium zincates, which can show enhanced reactivity in metalation in comparison to zinc alkyls,[5] also react with O_2 to give bridging alkoxides.[6,7] Only recently, the interaction of organozinc compounds and oxygen provided isolable and crystallographically characterized zinc alkylperoxide products, and this isolation often required carefully controlled preparative conditions.[3,8–13] In addition, the products are generally multimetallic species with bridging alkoxide or alkylperoxide groups.

Recently, the synthesis of To^MZnOOR (To^M = tris(4,4-dimethyl-2-oxazolinyl)phenylborate) by reaction of To^MZnR (R = Et, *n*-C_3H_7, *i*-C_3H_7, *t*-Bu) and O_2 was described.[14] In contrast to these alkylzinc compounds, To^MZnMe and To^MZnH are inert to oxygen up to 120 °C and 100 psi of O_2, even in the presence of reacting To^MZnEt–O_2 mixtures. In addition, tris(pyrazolyl)borato zinc alkyls are inert to O_2,[15,16] while $Tp^{t\text{-Bu}}MgR$ ($Tp^{t\text{-Bu}}$ = tris(3-*tert*-butyl)pyrazolylborate) react to give magnesium

alkylperoxides.[17,18] $To^{M}MgMe$ reacts with O_2 to give $To^{M}MgOMe$ species.[19] {HB(3-*t*Bupz)$_2$(5-*t*-Bupz)}$AlEt_2$ (*t*-Bupz = $N_2C_3H_2$*t*-Bu) forms uncharacterized products upon addition of excess O_2.[20] On the basis of the pattern that suggests that To^{M} enhances the reactivity of Mg and Zn relative to $Tp^{t\text{-}Bu}$, we considered approaches to further enhance the reactivity of {L_2X}ZnMe or {L_2X}ZnH toward reaction with O_2 through modification of the ancillary ligand's electronic properties. However, strategies for this are not entirely straightforward. First, the To^{M} ligand is currently the only ancillary ligand that has provided monometallic zinc alkylperoxides from zinc alkyls and O_2. Second, in a comparative study, the infrared stretching frequencies of Tp*Re(CO)$_3$ and $To^{M}Re(CO)_3$ suggest To^{M} is the stronger donor of the two, while the $E_{1/2}$ data indicates that Tp*Re(CO)$_3$ is more easily oxidized than $To^{M}Re(CO)_3$.[21] Furthermore, the electron-donating ability of tris(pyrazolyl)borates, at least in comparison to isoelectronic cyclopentadienide, is known to vary across the periodic table.[22]

Some direction comes from the proposed pathway for O_2 insertion into Zn–C bonds. Kinetic evidence supporting a radical chain mechanism in the reaction of $To^{M}ZnEt$ and O_2 suggests that the inertness of $To^{M}ZnMe$ toward O_2 is related to the lack of interaction of $To^{M}ZnMe$ and $^{\cdot}OOR$.[14] We hypothesized that increasing the electron density on the zinc center could further increase the reactivity of zinc methyl and zinc hydride moieties. N-heterocyclic carbenes (NHCs) are strong donors and should

increase the electron density on the zinc center.[23–26] Moreover, tris(carbene)borates[27,28] are sufficiently strong donors to allow access to high oxidation state 3d metal complexes,[29] such as a monometallic Fe(V) nitrido,[30] and bis(carbene)borates have been shown to stabilize low coordinate Ni(II) centers[31] and catalytic calcium and strontium centers.[32] Mixed oxazolinylcarbene-coordinated rhodium complexes catalyze carbonyl hydrosilylation,[33–35] and the combination of oxazolines and N-heterocyclic carbenes may offer new possibilities in catalysis. Furthermore, an N-heterocyclic carbene zinc dihydride complex was recently isolated and shown to react with carbon dioxide, whereas ZnH_2 is unstable with respect to its elemental components and reportedly inert toward CO_2.[36]

Hence, a modified tridentate monoanionic scorpionate ligand in which one oxazoline ring in To^M was replaced with a N-heterocyclic carbene, generated from N-substituted imidazolium, was sought to affect the aforementioned reactivity of [Zn]–Me toward oxygen. Typically, N-heterocyclic carbenes coordinate to zinc(II) centers as neutral L-type ligands.[23,24] However, N-borylation gives an overall uninegative charge to the bis(oxazolinyl)(carbene)phenylborate, and the reaction of the imidazolium borate and dialkylzinc results in a metalation reaction to give zwitterionic complexes. Recently, a bis(carborane)-substituted NHC provided an interesting dianionic carbene ligand.[37]

The present study describes the synthesis of the first example of a mixed oxazoline–carbene borate ligand, bis(oxazolinyl)(carbene)phenylborate, its metalation chemistry with alkylzinc reagents to give tetracoordinate $\{L_2X\}ZnR$, and the reactions of $\{L_2X\}ZnR$

and O_2 to give the second example of an ancillary ligand that supports an isolable monomeric zinc alkylperoxide.

Experimental

General synthetic procedures

All reactions were performed under a dry argon atmosphere using standard Schlenk techniques or under a nitrogen atmosphere in a glovebox, unless otherwise indicated. Benzene, toluene, and pentane were dried and deoxygenated using an IT PureSolv system. Benzene-d_6 was heated to reflux over Na/K alloy and vacuum transferred. Acetonitrile-d_3 was heated to reflux over CaH_2 and vacuum transferred. $[PhB(Ox^{Me2})_2]_n$,[38] and 1-mesitylimidazole[39] were synthesized according to literature procedures. Dimethylzinc solution (2.0 M in toluene) was purchased from Sigma-Aldrich and transferred to a flask equipped with a resealable Teflon valve for storage inside a glovebox. Diethylzinc was purchased from Strem Chemicals, Inc., and stored inside a glovebox in its original Swagelok cylinder.

^1H, $^{13}C\{^1H\}$, ^{11}B, and ^{17}O NMR spectra were collected on an Avance II 600 MHz NMR spectrometer. ^{15}N chemical shifts were determined by ^1H–^{15}N HMBC experiments on an Avance II 600 MHz NMR spectrometer. ^{15}N chemical shifts were originally referenced to an external liquid NH_3 standard and recalculated to the CH_3NO_2 chemical shift scale by adding −381.9 ppm. Infrared spectra were recorded on a Bruker Vertex spectrometer. Elemental analyses were performed using a Perkin-Elmer 2400 Series II CHN/S in the Iowa State Chemical Instrumentation Facility.

$PhB(Ox^{Me2})_2(Im^{Mes}H)LiCl$ (**1**·LiCl). $[PhB(Ox^{Me2})_2(LiCl)]_n$ (1.175 g, 3.598 mmol) was suspended in toluene (15 mL), and 1-mesitylimidazole (0.625 g, 3.36 mmol) was added to give a transparent brown solution. The reaction mixture was stirred at room temperature overnight. The product, as a white precipitate, was observed after 6 h. The suspension was allowed to settle in a centrifuge over 7 min at 4000 rpm, and the top clear brown solution was decanted. The precipitate was washed with toluene (3 × 5 mL) and dried *in vacuo* to afford the product as a white solid (1.144 g, 2.232 mmol, 66.8%). ^{1}H NMR (acetonitrile-d_3, 600 MHz): δ 8.15 (s, 1 H, 2H-$N_2C_3H_3Mes$), 7.31–7.18 (m, 7 H, C_6H_5, 4- and 5H-$N_2C_3H_3Mes$), 7.07 (s, 2 H, *m*-$C_6H_2Me_3$), 3.74 (m, 4 H, $CNCMe_2CH_2O$), 2.33 (s, 3 H, *p*-$C_6H_2Me_3$), 2.01 (s, 6 H, *o*-$C_6H_2Me_3$), 1.33 (s, 6 H, $CNCMe_2CH_2O$), 1.24 (s, 6 H, $CNCMe_2CH_2O$). $^{13}C\{^1H\}$ NMR (acetonitrile-d_3, 150 MHz): δ 179.53 (br, $CNCMe_2CH_2O$), 146.96 (br, *ipso*-C_6H_5), 139.95 (2C-$N_2C_3H_3Mes$), 135.85 (*ipso*-$C_6H_2Me_3$), 133.33 (*o*-C_6H_5), 132.79 (*o*-$C_6H_2Me_3$), 130.18 (*m*-$C_6H_2Me_3$), 129.92 (*p*-$C_6H_2Me_3$), 128.49 (*m*-C_6H_5), 127.09 (4,5C-$N_2C_3H_3Mes$), 126.26 (*p*-C_6H_5), 123.12 (4,5C-$N_2C_3H_3Mes$), 78.30 ($CNCMe_2CH_2O$), 68.14 ($CNCMe_2CH_2O$), 28.72 ($CNCMe_2CH_2O$), 28.52 ($CNCMe_2CH_2O$), 21.17 (*p*-$C_6H_2Me_3$), 17.51 (*o*-$C_6H_2Me_3$). ^{11}B NMR (acetonitrile-d_3, 128 MHz): δ −9.2. $^{15}N\{^1H\}$ NMR (acetonitrile-d_3, 71 MHz): δ −139 ($CNCMe_2CH_2O$), −180 ($N_2C_3H_3Mes$), −202 ($N_2C_3H_3Mes$). IR (KBr, cm^{-1}): 3164 w, 2962 m, 2927 w, 1658 s (CN), 1546 m, 1461 w, 1135 s, 990 m, 969 m, 767 m. Anal.

Calcd for $C_{28}H_{35}BClLiN_4O_2$: C, 65.58; H, 6.88; N, 10.93. Found: C, 67.76; H, 7.04; N, 10.56. Mp, 127–130 °C.

{PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnMe (**2**). PhB($Ox^{Me2}$)$_2$($Im^{Mes}$H)LiCl (**1·LiCl**, 0.351 g, 0.684 mmol) was suspended in benzene (10 mL), and a 2.0 M solution of $ZnMe_2$ (0.380 mL, 0.760 mmol) in toluene was added. The white suspension was stirred at room temperature overnight. The suspension was filtered, and the solvent was removed under reduced pressure to afford a white solid, which was triturated with pentane (2 × 10 mL) and dried *in vacuo* (0.336 g, 0.611 mmol, 89.3%). ^{1}H NMR (benzene-d_6, 600 MHz): δ 8.45 (d, $^3J_{HH}$ = 7.2 Hz, 2 H, *o*-C_6H_5), 7.55 (t, $^3J_{HH}$ = 7.2 Hz, 2 H, *m*-C_6H_5), 7.40 (t, $^3J_{HH}$ = 7.2 Hz, 1 H, *p*-C_6H_5), 6.75 (s, 2 H, *m*-$C_6H_2Me_3$), 6.62 (s, 1 H, $N_2C_3H_2$Mes), 6.06 (s, 1 H, $N_2C_3H_2$Mes), 3.55 (d, $^2J_{HH}$ = 7.8 Hz, 2 H, $CNCMe_2CH_2O$), 3.53 (d, $^2J_{HH}$ = 7.8 Hz, 2 H, $CNCMe_2CH_2O$), 2.09 (s, 3 H, *p*-$C_6H_2Me_3$), 1.97 (s, 6 H, *o*-$C_6H_2Me_3$), 1.08 (s, 6 H, $CNCMe_2CH_2O$), 1.03 (s, 6 H, $CNCMe_2CH_2O$), −0.52 (s, 3 H, $ZnCH_3$). ^{13}C{^{1}H} NMR (benzene-d_6, 150 MHz): δ 188.56 (br, $CNCMe_2CH_2O$), 186.02 (br, 2C-$N_2C_3H_2$Mes), 143.39 (*ipso*-C_6H_5), 138.29 (*p*-$C_6H_2Me_3$), 137.40 (*o*-$C_6H_2Me_3$), 137.01 (*o*-C_6H_5), 135.26 (*ipso*-$C_6H_2Me_3$), 129.47 (*m*-$C_6H_2Me_3$), 127.75 (*m*-C_6H_5), 127.23 (*p*-C_6H_5), 124.61 (4,5C-$N_2C_3H_2$Mes), 119.01 (4,5C-$N_2C_3H_2$Mes), 80.46 ($CNCMe_2CH_2O$), 66.14 ($CNCMe_2CH_2O$), 28.40 ($CNCMe_2CH_2O$), 28.31 ($CNCMe_2CH_2O$), 21.36 (*p*-$C_6H_2Me_3$),

18.19 (*o*-$C_6H_2Me_3$), −16.91 ($ZnCH_3$). ^{11}B NMR (benzene-d_6, 128 MHz): δ −9.9. $^{15}N\{^1H\}$ NMR (benzene-d_6, 71 MHz): δ −148 ($CNCMe_2CH_2O$), −171 (3N-$N_2C_3H_2Mes$), −190 (1N-$N_2C_3H_2Mes$). IR (KBr, cm^{-1}): 3123 w, 3076 w, 2956 s, 2926 m, 2891 m, 2824 w, 1594 s (CN), 1491 m, 1461 m, 1268 s, 1193 m, 1183 m, 1158 s, 1108 w, 1015 w, 951 m, 819 m, 704 m, 669 m, 640 m, 523 w. Anal. Calcd for $C_{29}H_{37}BN_4O_2Zn$: C, 63.55; H, 6.78; N, 10.19. Found: C, 63.77; H, 6.72; N, 10.77. Mp, 173–176 °C.

{$PhB(Ox^{Me2})_2Im^{Mes}$}ZnEt (**3**). $PhB(Ox^{Me2})_2(Im^{Mes}H)LiCl$ (**1·LiCl**, 0.740 g, 1.44 mmol) was suspended in benzene (10 mL), and $ZnEt_2$ (0.165 mL, 1.61 mmol) was added. The white suspension was stirred at room temperature overnight. The suspension was filtered, the solvent was removed under reduced pressure, and the resulting white solid was triturated with pentane (2 × 10 mL), and dried *in vacuo* (0.754 g, 1.34 mmol, 92.7%). ^1H NMR (benzene-d_6, 600 MHz): δ 8.45 (d, $^3J_{HH}$ = 7.2 Hz, 2 H, *o*-C_6H_5), 7.55 (t, $^3J_{HH}$ = 7.2 Hz, 2 H, *m*-C_6H_5), 7.40 (t, $^3J_{HH}$ = 7.2 Hz, 1 H, *p*-C_6H_5), 6.79 (s, 2 H, *m*-$C_6H_2Me_3$), 6.61 (s, 1 H, $N_2C_3H_2Mes$), 6.05 (s, 1 H, $N_2C_3H_2Mes$), 3.54 (m, 4 H, $CNCMe_2CH_2O$), 2.12 (s, 3 H, *p*-$C_6H_2Me_3$), 1.96 (s, 6 H, *o*-$C_6H_2Me_3$), 1.31 (m, 3 H, $ZnCH_2CH_3$), 1.07 (s, 6 H, $CNCMe_2CH_2O$), 1.04 (s, 6 H, $CNCMe_2CH_2O$), 0.44 (m, 2 H, $ZnCH_2CH_3$). $^{13}C\{^1H\}$ NMR (benzene-d_6, 150 MHz): δ 188.53 (br, $CNCMe_2CH_2O$), 186.24 (2C-$N_2C_3H_2Mes$), 143.83 (br, *ipso*-C_6H_5), 138.47 (*p*-$C_6H_2Me_3$), 137.75 (*o*-$C_6H_2Me_3$), 136.90 (*o*-C_6H_5), 135.56 (*ipso*-$C_6H_2Me_3$), 129.44 (*m*-$C_6H_2Me_3$), 127.74 (*m*-

C_6H_5), 127.20 (*p*-C_6H_5), 124.81 (4,5C-$N_2C_3H_2$Mes), 118.89 (4,5C-$N_2C_3H_2$Mes), 80.34 ($CNCMe_2CH_2O$), 66.09 ($CNCMe_2CH_2O$), 28.50 ($CNCMe_2CH_2O$), 28.28 ($CNCMe_2CH_2O$), 21.37 (*p*-$C_6H_2Me_3$), 18.06 (*o*-$C_6H_2Me_3$), 14.45 ($ZnCH_2CH_3$), −1.48 ($ZnCH_2CH_3$). ^{11}B NMR (benzene-d_6, 128 MHz): δ −10.0. ^{15}N{^{1}H} NMR (benzene-d_6, 71 MHz): δ −148 ($CNCMe_2CH_2O$), −170 (3N-$N_2C_3H_2$Mes), −190 (1N-$N_2C_3H_2$Mes). IR (KBr, cm^{-1}): 3132 w, 3008 w, 2971 s, 2927 s, 2885 s, 2852 m, 1592 s (CN), 1492 m, 1464 m, 1398 w, 1366 w, 1269 s, 1193 m, 1183 m, 1157 s, 1109 w, 1010 w, 963 s, 822 w, 744 m, 704 m, 672 m, 641 m. Anal. Calcd for $C_{30}H_{39}BN_4O_2Zn$: C, 63.90; H, 6.97; N, 9.94. Found: C, 64.07; H, 6.81; N, 10.32. Mp, 199–201 °C.

{PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnOOEt (**4**). A benzene solution (15 mL) of {PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnEt (**3**, 0.700 g, 1.24 mmol) was degassed with “freeze–pump–thaw” cycles (3×), and then oxygen was added (1 atm). The solution was allowed to stir at room temperature overnight. Evaporation of the mixture to dryness gave a white solid. The crude product was dissolved in a minimal amount of toluene, and the solution was cooled to −30 °C to produce colorless crystals. The crystals were isolated by filtration, washed with pentane (2 × 2 mL) and dried *in vacuo* (0.621 g, 1.04 mmol, 84.0%). ^{1}H NMR (benzene-d_6, 600 MHz): δ 8.4 (2 H, *o*-C_6H_5), 7.5 (m, 2 H, *m*-C_6H_5), 7.4 (m, 1 H, *p*-C_6H_5), 6.7 (s, 2 H, *m*-$C_6H_2Me_3$), 6.6 (s, 1 H, $N_2C_3H_2$Mes), 6.0 (s, 1 H, $N_2C_3H_2$Mes), 3.8 (m, 2 H, $ZnOOCH_2CH_3$), 3.6 (m, 4 H, $CNCMe_2CH_2O$), 2.1 (s, 3 H, *p*-$C_6H_2Me_3$), 2.0 (s, 6 H, *o*-$C_6H_2Me_3$), 1.3 (s, 6 H, $CNCMe_2CH_2O$), 1.2 (s, 6 H,

CNC*Me*$_2$CH$_2$O), 1.1 (m, 3 H, ZnOOCH$_2$C*H*$_3$). ^{13}C{^{1}H} NMR (benzene-d_6, 150 MHz): δ 188.77 (br, *C*NCMe$_2$CH$_2$O), 181.45 (2C-N$_2$C$_3$H$_2$Mes), 142.44 (br, *ipso*-C$_6$H$_5$), 138.38 (*p*-*C*$_6$H$_2$Me$_3$), 136.93 (*o*-*C*$_6$H$_2$Me$_3$), 136.84 (*o*-C$_6$H$_5$), 135.23 (*ipso*-C$_6$H$_2$Me$_3$), 129.44 (*m*-C$_6$H$_2$Me$_3$), 127.74 (*m*-C$_6$H$_5$), 127.32 (*p*-C$_6$H$_5$), 124.99 (4,5C-N$_2$C$_3$H$_2$Mes), 119.48 (4,5C-N$_2$C$_3$H$_2$Mes), 80.77 (CNCMe$_2$*C*H$_2$O), 71.29 (ZnOO*C*H$_2$CH$_3$), 65.9 (CN*C*Me$_2$CH$_2$O), 28.18 (CNC*Me*$_2$CH$_2$O), 28.04 (CNC*Me*$_2$CH$_2$O), 21.21 (*p*-C$_6$H$_2$*Me*$_3$), 18.00 (*o*-C$_6$H$_2$*Me*$_3$), 14.62 (ZnOOCH$_2$*C*H$_3$). ^{11}B NMR (benzene-d_6, 128 MHz): δ −10.0. ^{15}N{^{1}H} NMR (benzene-d_6, 71 MHz): δ −150 (CNCMe$_2$CH$_2$O), −169 (N$_2$C$_3$H$_2$Mes), −190 (N$_2$C$_3$H$_2$Mes). ^{17}O NMR (benzene-d_6, 81 MHz): δ 328 (Zn*O*OCH$_2$CH$_3$), 165 (ZnO*O*CH$_2$CH$_3$). IR (KBr, cm^{-1}): 3133 w, 2966 s, 2927 m, 2888 m, 1610 s (CN), 1462 m, 1276 w, 1179 m, 1154 s, 1065 m, 968 s, 853 w, 849 w, 734 m, 704 m. Anal. Calcd for C$_{30}$H$_{39}$BN$_4$O$_4$Zn: C, 60.47; H, 6.60; N, 9.40. Found: C, 60.98; H, 6.64; N, 8.92. Mp, 138–141 °C.

X-ray crystallography

Single-crystal X-ray diffraction experiments for **1–4** were carried out on a Bruker diffractometer with an APEX II CCD detector using graphite monochromated MoKα radiation with a detector distance of 50.6 mm. Full-sphere data collection with exposures of 30 s per frame were made with ω scans in the range 0–180° at φ = 0, 120, and 240°. A semi-empirical absorption correction was based on a fit of a spherical

harmonic function to the empirical transmission surface as sampled by multiple equivalent measurements[40] using SADABS software.[41] The experiment was optimized to collect data to a resolution of 0.71 Å, however, the datasets have been truncated to obtain the statistically relevant resolution. The positions of metal atoms were found by direct methods. The remaining atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined in the full-matrix anisotropic approximation. All hydrogen atoms were placed in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. All calculations were performed using the BRUKER APEX II software suite.[42]

SQUEEZE was used to treat diffuse electron density in solvent accessible voids for structures **1–3**.[43] Crystallographic data and structure refinement parameters for **1–4** are summarized in Table 1.

DFT calculations

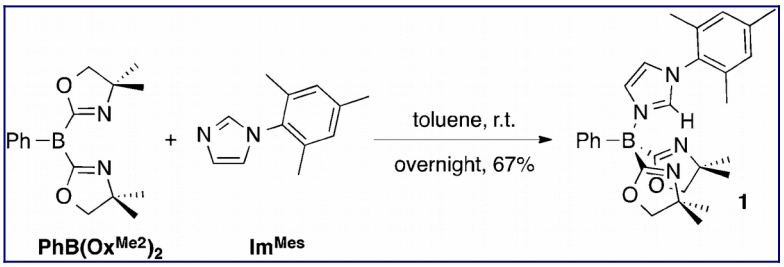
All calculations were performed with the NWChem computational chemistry software.[44] Density functional theory with the B3LYP functional was used for single point energy calculations, geometry optimization and frequency calculations.[45–47] The 6-311G(d,p) basis set was used for H, C, N, O, and B.[48] The Stuttgart 1997 relativistic small core basis set with effective core potential was used for Zn.[49]

Table 1 Crystallographic data for compounds **1–4**

	1·LiCl	**2**	**3**	**4**
Chemical formula	$C_{37}H_{44}BClLiN_4O_4$	$C_{29}H_{37}BN_4O_2Zn$	$C_{32.5}H_{45}BN_4O_2Zn$	$C_{33.5}H_{47}BN_4O_4Zn$
Formula weight	629.96	549.81	599.91	645.93
Crystal system	Triclinic	Trigonal	Trigonal	Monoclinic
Unit-cell dimensions	a = 11.152(1) Å	$a = b$ = 29.159(2) Å	$a = b$ = 28.780(3) Å	a = 9.497(1) Å
	b = 12.661(1) Å	c = 19.403(3) Å	c = 20.259(2) Å	b = 26.859(3) Å
	c = 13.378(1) Å	$\alpha = \beta$ = 90°	$\alpha = \beta$ = 90°	c = 13.405(2) Å
	α = 85.243(2)°	γ = 120°	γ = 120°	$\alpha = \gamma$ = 90°
	β = 69.278(1)°			β = 96.814(2)°
	γ = 88.683(2)°			
Volume	1760.5(3) Å^3	14 287(2) Å^3	14 542(2) Å^3	3395.0(7) Å^3
Space group	P	R	R	$P12_1/n1$
Z	2	18	18	4
Reflections collected	19 082	53 056	53 004	44 529
Independent reflections	8984	8974	8740	7785
R_{int}	0.0261	0.0303	0.0356	0.0327
R $I > 2\sigma(I)$	R_1 = 0.0424	R_1 = 0.0415	R_1 = 0.0314	R_1 = 0.0448
	wR_2 = 0.0963	wR_2 = 0.1480	wR_2 = 0.0839	wR_2 = 0.1329
R_{all}	R_1 = 0.0610	R_1 = 0.0553	R_1 = 0.0432	R_1 = 0.0537
	wR_2 = 0.1062	wR_2 = 0.1602	wR_2 = 0.0878	wR_2 = 0.1398

Results and discussion

The compound $PhB(Ox^{Me2})_2(Im^{Mes}H)$ (**1**; $Im^{Mes}H$ = 1-mesitylimidazolium; Ox^{Me2} = 4,4-dimethyl-2-oxazoline) is synthesized in 67% yield by the reaction of bis(4,4-dimethyl-2-oxazolinyl)phenylborane ($PhB(Ox^{Me2})_2$) and 1-mesitylimidazole (Im^{Mes}) in toluene (eqn (1)).[38,39] Previously, a related strategy for the synthesis of heteropodal multidentate oxazolinylborate ligands involved addition of sodium cyclopentadienide to $PhB(Ox^{Me2})_2$ to provide the compound $Na[PhB(Ox^{Me2})_2(C_5H_5)]$.[50] It appears that this ligand synthesis approach has some versatility in varying donor groups linked to oxazolines through a borate center.



(1)

This material is poorly soluble in toluene and benzene, but dissolves readily in acetonitrile. The ^{1}H NMR spectrum of the substance, acquired in acetonitrile-d_3, contained a diagnostic downfield singlet at 8.15 ppm, which was assigned to the 2-H on the imidazolium ring. Signals at 1.24 (6 H) and 1.33 ppm (6 H) were assigned to oxazoline methyl groups and two singlets at 2.01 (6 H) and 2.33 ppm (3 H) were assigned to the mesityl group. For comparison, the ^{1}H NMR chemical shifts of Im^{Mes} appear at 7.06 (2-H), 1.58 (*ortho*-Mes), and 1.97 ppm (*para*-Mes) in acetonitrile-d_3. These signals are distinct from those of **1**, and this provides convincing evidence that the imidazole is coordinated to the boron center even in a donor-solvent such as acetonitrile. Inequivalent oxazoline methyl groups indicate that the C_{2v}-symmetry of PhB(Ox^{Me2})$_2$ is disrupted by coordination of the imidazole to the boron center. The ^{11}B NMR spectrum, also acquired in acetonitrile-d_3, showed one singlet at −9.2 ppm. This result is consistent with a four-coordinate boron center. The ^{13}C{^{1}H} NMR spectrum, acquired in acetonitrile-d_3, showed a sharp peak at 139.95 ppm and a broad peak at 179.53 ppm, which were assigned to the 2-C on the imidazolium ring and the 2-Cs on the oxazoline rings, respectively. Interestingly, the ^{15}N NMR chemical shifts for oxazoline and both imidazolium nitrogen atoms were obtained through ^{1}H–^{15}N HMBC

experiments. The oxazoline chemical shift (−139 ppm) was easily identified by correlations to its methyl groups; both imidazolium nitrogen atoms correlated with the imidazolium 2-H, 4-H, and 5-H. One of the signals, at −202 ppm, is similar to the ^{15}N NMR values of 1-alkyl substituted imidazolium salts. The other ^{15}N NMR chemical shift (−180 ppm) is further downfield than the signals from alkyl and aryl-substituted imidazoles,[51] although this signal is similar to that reported for silver-coordinated N-heterocyclic carbenes.[52] For comparison, the ^{15}N NMR chemical shifts of Im^{Mes} are −206 and −121 ppm for the 1-N and 3-N, respectively.

Crystals obtained from a concentrated toluene solution cooled to −30 °C were subjected to an X-ray diffraction study, verifying the connectivity of compound **1** as containing an imidazole coordinated to the boron center. A trace amount of benzene facilitates the crystallization, and two benzene molecules are included in the unit cell. The molecular structure is shown to be the centrosymmetric dimer (**1**·LiCl)$_2$ (Fig. 1); the two oxazolines of **1** are coordinated to a lithium cation, and each half of the dimer are related by a crystallographically imposed inversion center. As a result, the two imidazolium rings are located on opposite faces of the (LiCl)$_2$ parallelogram.

The Li centers are four coordinate, and the N1–Li1–N2 angle of 93.7(1)° and Cl1–Li1–Cl1# angle of 95.12(8)° are much smaller than the N1–Li1–Cl1 or N2–Li1–Cl1 angles that range from 112.8(1)° to 123.3(1)°. As expected based on VSEPR considerations, the Li1–Cl1–Li1# angles are acute (84.88(8)°).

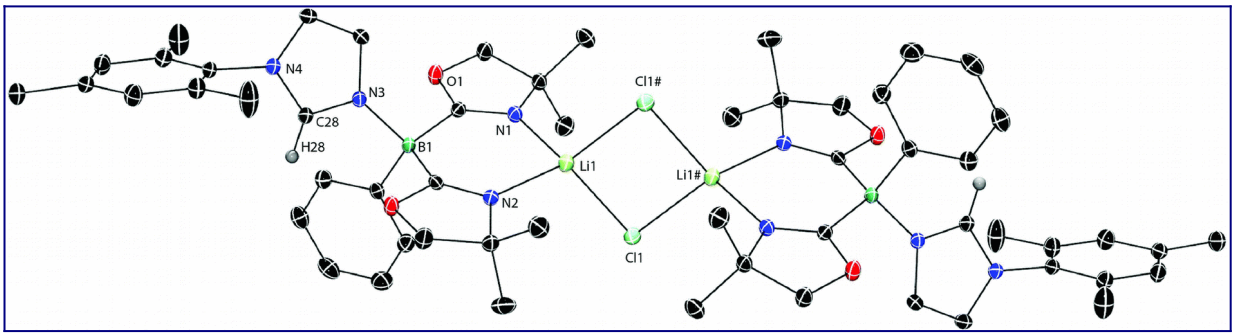


Fig. 1 Rendered thermal ellipsoid diagram of $(1{\cdot}LiCl)_2$ with ellipsoids plotted at 35% probability. H28 atoms are illustrated, but all other H atoms and two co-crystallized benzene molecules are not depicted for clarity. Atoms with designator # related to the basic atom with transformation 2 − *x*, 2 − *y*, 2 − *z*. Selected interatomic distances (Å): Li1–N1, 2.070(3); Li1–N2, 2.079(3); Li1–Cl1, 2.371(2); Li1–Cl1#, 2.439(2). Selected interatomic angles (°): N1–Li1–N2, 93.7(1); Cl1–Li1–Cl1#, 95.12(8); N1–Li1–Cl1, 119.3(1); N1–Li1–Cl1#, 112.8(1); N2–Li1–Cl1, 114.7(1); N2–Li1–Cl1#, 123.3(1), Li1–Cl1–Li1#, 84.88(8).

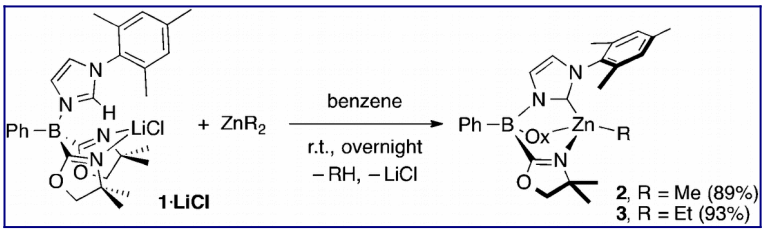
LiCl is carried over in variable amounts from the reaction of 2-LiOx^{Me2} and $PhBCl_2$ for preparation of $[PhB(Ox^{Me2})_2]_n$, although $[PhB(Ox^{Me2})_2]_n$ may be purified from LiCl by repeated extractions with benzene or by column chromatography. The solution phase NMR spectroscopy above describes **1**·LiCl, likely with acetonitrile-d_3 coordinated to the lithium center. The presence of LiCl does not interfere in later metalation chemistry with dialkylzinc compounds, and $(\mathbf{1}{\cdot}LiCl)_2$ may be used in further reactions described here. Although LiCl sometimes enhances metalation chemistry,[5,53,54] typically the LiCl is associated with the base rather than the substrate. In fact, LiCl must be removed from $(\mathbf{1}{\cdot}LiCl)_2$ for the successful deprotonation of **1** by more aggressive bases, such as $PhCH_2K$. That work will be described elsewhere. In addition, elemental analysis data for $(\mathbf{1}{\cdot}LiCl)_2$ was consistently high for carbon which may reflect slightly variable quantities of LiCl and coordinated donor in **1**.

Compound **1** is readily metalated at the imidazolium 2-H by reaction with dialkylzinc compounds to give $\{PhB(Ox^{Me2})_2Im^{Mes}\}ZnR$ (R = Me (**2**), Et (**3**)) in 89 and 93% yield,

respectively (eqn (2)). The most convenient preparation involves the reaction of (**1**·LiCl)$_2$ as a suspension in benzene with $ZnMe_2$ or $ZnEt_2$. As the reaction proceeds and **2** or **3** are formed, LiCl is eliminated and the cloudy suspension becomes less opaque. Methane or ethane by-products are formed, and these species are detected by ^{1}H NMR spectroscopy in micromolar scale reactions performed in benzene-d_6.

A singlet resonance at −0.52 ppm in the ^{1}H NMR spectrum of **2** in benzene-d_6 was assigned to a zinc methyl group on the basis of its upfield chemical shift and integration (3 H). The downfield imidazolium 2-H signal in (**1**·LiCl)$_2$ was not observed in the spectra of **2** or **3**, which suggested that the 2-C on the imidazolium had been metalated in both cases. The oxazoline groups are equivalent, as are the *ortho*-methyl groups on the mesityl ring. These data indicate that the compounds have effective C_s symmetry. For compound **2** for example, two singlets in the alkyl region at 1.03 (6 H) and 1.08 ppm (6 H) assigned to the methyl groups on the oxazoline rings correlated in a ^{1}H–^{15}N HMBC experiment to a ^{15}N NMR signal at −148 ppm (referenced to nitromethane). The zinc methyl ^{1}H NMR resonances also correlated with the oxazoline nitrogen, proving that both oxazolines are coordinated to the zinc center in solution. Three additional crosspeaks in the ^{1}H–^{15}N HMBC experiment showed correlations between the imidazole 1-N (−190 ppm) and the ^{1}H NMR resonances assigned to *meta*-$C_6H_2Me_3$ (6.75 ppm) and the imidazole 4-H and 5-H (6.68 and 6.08 ppm). Two more crosspeaks between a ^{15}N NMR signal at −171, assigned to the 3-N bonded to the boron center,

and the imidazole 4-H and 5-H completed the assignment of the nitrogen centers in **2**. Thus, the ^{15}N NMR chemical shift values for both oxazoline and imidazole groups change from those of (**1**·LiCl)$_2$ upon metalation with zinc. In the $^{13}C\{^1H\}$ NMR spectrum, a signal at 186.02 ppm was assigned to the zinc-coordinated N-heterocyclic carbene. This chemical shift is essentially identical to that reported for HB(Im$^{t\text{-Bu}}$)$_3$MgBr.[28] Similar ^{15}N and ^{13}C NMR data describing the ancillary mixed oxazoline–carbene borate ligand were obtained for compound **3**.



(2)

Compounds **2** and **3** are readily crystallized from concentrated benzene solutions at room temperature. Results from single crystal X-ray diffraction studies are presented in Fig. 2 and 3. Interestingly, both **2** and **3** are solved in the space group *R* (trigonal crystal system).

The distinguishing feature of the molecular structures of both compounds **2** and **3** is a distortion of the zinc alkyl group from the pseudo tetrahedral position where the ligand–zinc–carbon angles would be similar and the boron–zinc–carbon angles would be 180°. Instead, the B1–Zn1–C23 and B1–Zn1–C29 angles in **2** and **3** are 166.8(1) and 164.8(1)°, respectively. The large obtuse carbene–zinc–alkyl angles in **2** and **3** are 138.1(1) and 140.01(6)°, while the nitrogen–zinc–carbon angles range from 116–120°.

The three angles from the donors on the ancillary ligand are similar in both mixed carbene–oxazolinylborato zinc methyl and ethyl compounds (ranging from 88–92°).

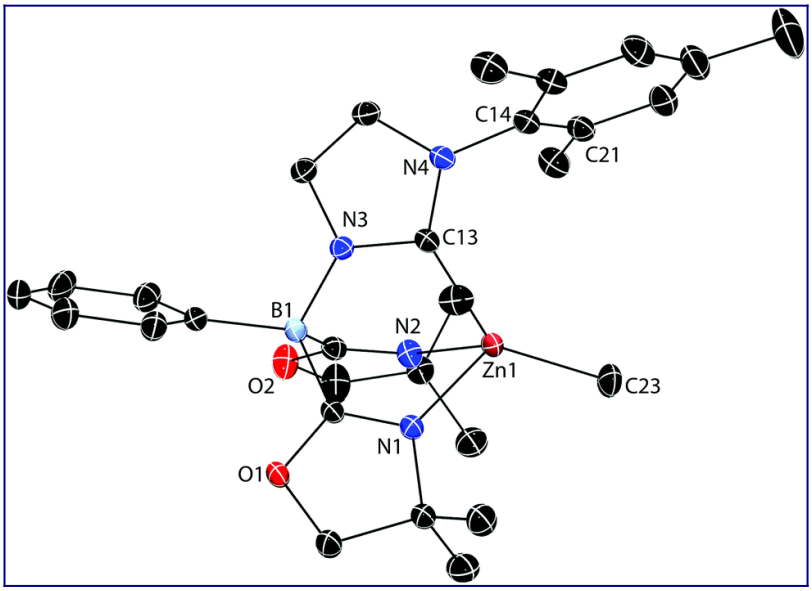


Fig. 2 Rendered thermal ellipsoid diagram of {PhB(Ox^{Me2})$_2$Im^{Mes}}ZnMe (2) with ellipsoids at 35% probability. H atoms are not depicted for clarity. Selected interatomic distances (Å): Zn1–C13, 2.043(2); Zn1–N1, 2.104(2); Zn1–N2, 2.193(2); Zn1–C23, 1.978(2). Selected interatomic angles (°): B1–Zn1–C23, 166.8(1); C13–Zn1–C23, 138.1(1); N1–Zn1–C23, 116.08(9); N2–Zn1–C23, 120.1(1); N1–Zn1–N2, 88.79(7); C13–Zn1–N1, 92.74(7); C13–Zn1–N2, 88.27(7); C13–N4–C14–C21, 60.1(3).

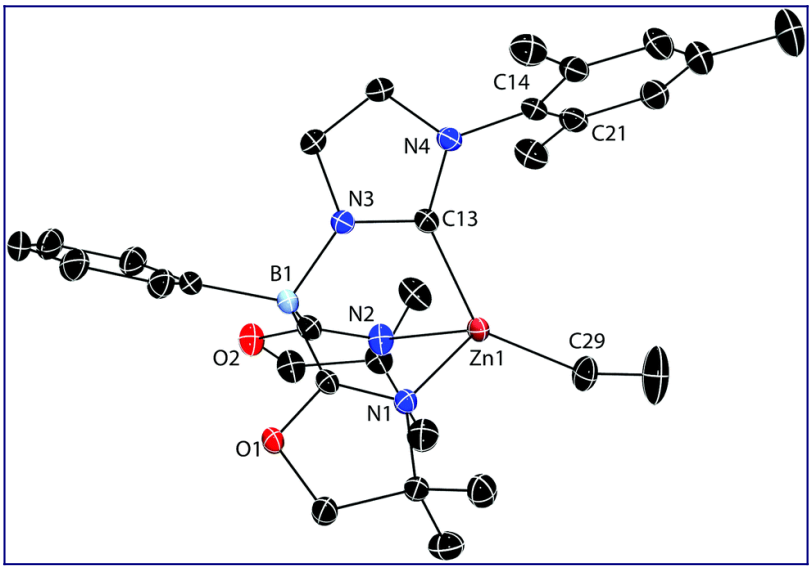


Fig. 3 Rendered thermal ellipsoid diagram of {PhB(Ox^{Me2})$_2$Im^{Mes}}ZnEt (3) with ellipsoids at 35% probability. H atoms and 0.5 disordered pentane are not depicted for clarity. Selected interatomic distances (Å): Zn1–C13, 2.043(1); Zn1–N1, 2.125(1); Zn1–N2, 2.165(1); Zn1–C29, 1.979(2). Selected interatomic angles (°): B1–Zn1–C29, 164.8(1); C13–Zn1–C29, 140.01(6); N1–Zn1–C29, 118.04(6); N2–Zn1–C29, 115.94(6); N1–Zn1–N2, 88.61(5); C13–Zn1–N1, 92.25(5); C13–Zn1–N2, 88.36(5); C13–N4–C14–C21, 63.5(3).

The mesitylcarbene donor is much larger than the oxazoline donors, and the steric properties of $PhB(Ox^{Me2})_2Im^{Mes}$ (solid angle, 6.26 steradians, 49.9%) are greater than those of To^M (solid angle, 5.51 steradians, 43.9%).[55,56] The steric bulk of the mesitylcarbene donor might be responsible for the distortion. However, a few features argue against sterics as responsible for the unusual geometry. First, there are no unfavorable interligand interactions, as determined by the above solid angle calculations. Second, the zinc–oxazoline and zinc–alkyl distances in **2** and **3** are similar to those in the C_{3v}-symmetric, undistorted To^MZnMe and To^MZnEt.[14,57] For example, the $Zn–C_{alkyl}$ interatomic distances in **2** and **3** are 1.978(2) and 1.979(2) Å, whereas the distances are 1.972(1) and 1.994(2) Å in To^MZnMe and To^MZnEt, respectively. The Zn–N interatomic distances in **2** and **3** range from 2.10–2.19 Å, whereas the Zn–N distances in To^MZnEt and To^MZnMe range from 2.06–2.10 Å. Thus, the coordination environment at zinc appears unremarkable with the exception of the unexpected alkyl ligand position.

Additionally, the mesityl group is twisted with respect to the imidazole ring by approximately 60° in both **2** and **3**. The shortest H···H distance in **2** between a mesityl *ortho*-methyl and the zinc methyl is 2.83 Å (the C···C distance is 3.877 Å), and these are greater than the sum of the van der Waals radii of H and Me groups. In compound **3**, the ethyl ligand is oriented with the methyl group pointing into the open space resulting from the canted mesityl group. It is unreasonable that the mesityl ring would twist to form close contacts to an alkyl group on zinc, and then subsequently push the alkyl group into a distortion.

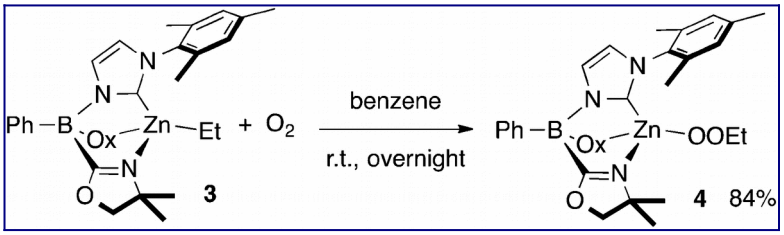
However, an electronic effect for the alkyl groups' unusual positions would also be surprising in the context of a metal-centered electronic distortion because compounds **2** and **3** are closed-shell, d^{10} complexes and unlikely to be distorted, even though the structural distortion of **2** and **3** is reminiscent of the tetragonal distortion of Cu(II) in spinels.[58] In addition, bending the ligand from a pseudo-tetrahedral position does not lower the overall symmetry of the complex.

To further probe these unusual structural features, the full structure of **2** was computationally optimized. In the gas-phase minimized structure, the methyl distortion is maintained (carbene–zinc–carbon angle, 139.4°), while the imidazole-mesityl torsion angle rotates to 84.3° (in comparison to 60.1° in the structure obtained by X-ray diffraction). From this, we conclude that the canted mesityl group does not relate to the distortion of the zinc's coordination sphere.

To further emphasize this point, the methyl position was straightened with both gas-phase and X-ray mesityl torsion angles of 84.3° and 60.1°. In both cases, the energy of the linear B–Zn–Me structures are higher by 0.9 and 1.2 kcal mol^{-1}, respectively, than structures with the observed B–Zn–Me angle of 167°. This small energy change related to the methyl position suggests that there are subtle electronic effects rather than steric effects in play and, indeed, it is difficult to identify any single electronic feature that is responsible for the distortion from pseudo-C_{3v} symmetry.

Compound **3** and O_2 (1 atm) react at room temperature overnight to give $\{PhB(Ox^{Me2})_2Im^{Mes}\}ZnOOEt$ (**4**) (eqn (3)), which is isolated as a white solid in 84%

yield. Other possible products, including zinc ethoxy {PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnOEt or 2-*O*-imidazolone, were not detected in ^{1}H NMR spectra of crude reaction mixtures.



(3)

The reaction at the [Zn]–CH_2CH_3 is readily assessed by changes in the ^{1}H and $^{13}C\{^1H\}$ NMR spectra acquired in benzene-d_6. The ^{1}H NMR signals for the CH_2CH$_3$ appeared at 0.44 ppm in **3** and 3.8 ppm in **4**. The $^{13}C\{^1H\}$ NMR signals for the *C*H$_2$CH$_3$ was upfield of tetramethylsilane in the zinc alkyl starting material **3** at −1.48 ppm, and the signal in **4** was downfield in the ether region at 71.29 ppm. The 2-C signal in the $^{13}C\{^1H\}$ NMR spectra of **3** (186.24 ppm) and **4** (181.45 ppm) were barely affected by exposure to oxygen. In addition, **3** was allowed to react with ^{17}O-labelled O_2 to give **4**-$^{17}O_2$. An ^{17}O NMR spectrum acquired in benzene-d_6 contained two broad peaks at 328 and 165 ppm. The downfield resonance was assigned to the oxygen bonded to zinc (O_α), and the upfield resonance was then assigned to ZnO*O*Et (O_β); the difference Δ(δO) is 163 ppm (Δ(δO) = $\delta O_\alpha - \delta O_\beta$). For comparison, the ^{17}O NMR signals for To^{M}ZnOOEt were detected at 319 and 169 ppm and have a smaller difference in chemical shift (Δ(δO) = 150 ppm),[14] while the signals for Tp$^{t\text{-Bu}}$MgOOEt are even more separated (Δ(δO) = δO_α

− δO_β = 407 − 130 = 277 ppm).[17,18] Thus, the ^{17}O chemical shifts of **4**-$^{17}O_2$ are upfield for O_α and downfield for O_β with respect to the corresponding shifts in To^{M}ZnOOEt.

Compound **4** crystallizes from a concentrated toluene solution at −30 °C. The solution to the single crystal X-ray diffraction study confirmed that O_2 inserted into the Zn–C bond (Fig. 4). Most importantly, the formation of a ZnOOEt moiety is confirmed, and the zinc–carbene interaction is intact. The OOEt ligand is disordered over two positions, and the interatomic distances and angles must be cautiously interpreted; however, it is worth noting that the model places O3a and O3b at the same position, and this position gives the same type of distortion observed and described above for compounds **2** and **3**. In addition, the C22–N4–C19–C12 torsion angle (72.3(2)°) that describes the mesityl group position is larger than in **2** and **3**.

As noted above, the alkyl ligands of **2** and **3** are distorted with respect to ideal positions. However, this distortion apparently did not translate into enhanced reactivity for the zinc methyl, at least with respect to the interaction of **2** and oxygen. In fact, compound **2** is stable under O_2 (1–3 atm) up to 60 °C. The inert nature of the zinc methyl in **2** follows the reactivity of To^{M}ZnMe and To^{M}ZnH, which, as noted above, also are inert toward reaction with O_2.

We were unable to isolate {PhB(Ox^{Me2})$_2$Im^{Mes}}ZnO*t*-Bu from the reaction of **3** and *t*-BuOOH. Even though a small amount of ethane was detected by ^1H NMR spectroscopy in micromolar scale reactions performed in benzene-d_6, the majority of **3** remained unreacted at room temperature over 1 day. After 2 days at room temperature, a signal

at 10.86 ppm assigned to a 2H-imidazolium moiety was observed as part of the major product suggesting protonation of the carbene.

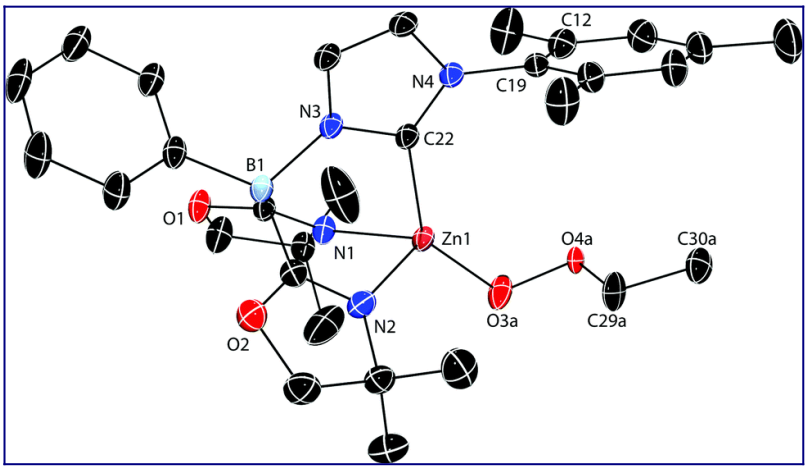


Fig. 4 Rendered thermal ellipsoid diagram of {PhB(Ox^{Me2})$_2$Im^{Mes}}ZnOOEt (4) with ellipsoids plotted at 35% probability. The OOCC heavy atom positions are disordered over two positions, and only O3a, O4a, C29a, C30a atoms of the alkyl peroxide moiety are shown. The two positions for the OOEt group were refined using similarity restraints. However, O3a and O3b positions are identical. H atoms and a disordered toluene solvent molecule are not depicted for clarity.

Conclusions

We have described the preparation of a new heteroleptic monoanionic scorpionate ligand that contains two oxazoline donors and one N-heterocyclic carbene donor. There are some similarities between the tris(oxazolinyl)borate To^{M} and the bis(oxazolinyl)(carbene)borate in the facile metalation reactions of H[ligand] by dialkylzinc reagents. Both ligands support four-coordinate monoalkyl zinc compounds. In addition, both To^{M}ZnMe and {PhB(Ox^{Me2})$_2$Im^{Mes}}ZnMe compounds are inert toward O_2, whereas both To^{M}ZnEt and {PhB(Ox^{Me2})$_2$Im^{Mes}}ZnEt react with O_2 to give isolable zinc alkylperoxides. Unlike To^{M}ZnEt, {PhB(Ox^{Me2})$_2$Im^{Mes}}ZnEt does not provide an isolable [Zn]OO*t*-Bu in its reaction with *t*-BuOOH. The ancillary ligand PhB(Ox^{Me2})$_2$Im^{Mes} is only the second example of a ligand that supports a monometallic zinc alkylperoxide formed

from O_2. Notably, the carbene moiety is inert toward O_2 as well as any $^{\cdot}OOR$ present during the radical chain process that gives {PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnOOEt. Additionally, a significant and systematic structural distortion of the compounds {PhB(Ox^{Me2})$_2$$Im^{Mes}$}ZnX has been observed, where the X group (Me, Et, OOEt) is distorted away from the carbene ligand in three structures determined by X-ray crystallographic diffraction studies. However, this distortion, or the substitution of an oxazoline in the To^{M}ZnR compounds with a carbene donor does not appear to affect the reactivity of zinc methyl or ethyl toward O_2, either by increasing the reactivity of the zinc methyl or decreasing the reactivity of the zinc ethyl toward O_2.

Acknowledgements

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Footnote

† Electronic supplementary information (ESI) available: Experimental data and spectra for compounds **1**·LiCl, **2–4**. CCDC 995354–995357. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c4dt01011f

CHAPTER 5. CERIUM-CATALYZED HYDROSILYLATION OF ACRYLATES TO α-SILYL ESTERS

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[William Everett contributed the computational results. All experimental data was obtained by members of the Sadow group.]

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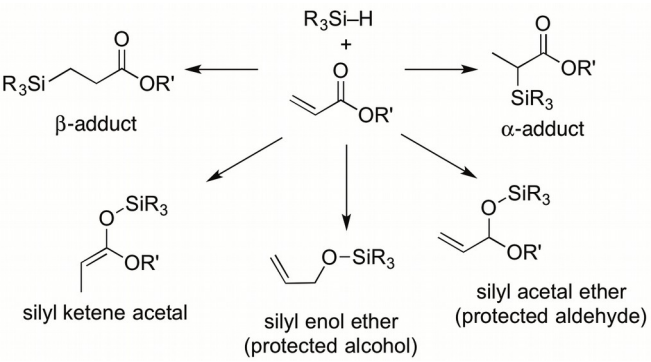
Abstract

The homoleptic organocerium complex $Ce\{C(SiHMe_2)_3\}_3$ (**1**) reacts with $B(C_6F_5)_3$ to produce a zwitterionic bis(alkyl) hydridoborato $Ce\{C(SiHMe_2)_3\}_2HB(C_6F_5)_3$ (**2**). NMR and IR spectroscopy and X-ray crystallography indicate that each alkyl ligand contains two bridging Ce←H-Si interactions in compounds **1** and **2**. Compound **2** is a precatalyst for the hydrosilylation of acrylates to give α-silyl esters at room temperature with a turnover number of 2200.

Catalytic hydrosilylation enables synthetic chemistry to impact wide ranging technological applications such as adhesives, electronics, and medical devices.[1] In many synthetic applications, the SiH functionality is important. For example, SiH-containing organosilanes from hydrosilylation may be transformed by oxidation or cross-coupling.[2] Late transition-metal catalysts have been extensively employed in hydrosilylations,[3] and earth abundant first row metal based catalysts have recently attracted attention.[4] While early metal complexes are active for such additions to olefins, these oxophilic systems typically have limited functional group tolerance.[5]

Carbonyl hydrosilylations catalyzed by reducible titanocene-based complexes notably overcome this limitation.[6] Alternatively, hypervalent silane intermediates are proposed in a calcium-catalyzed ketone hydrosilylation.[7]

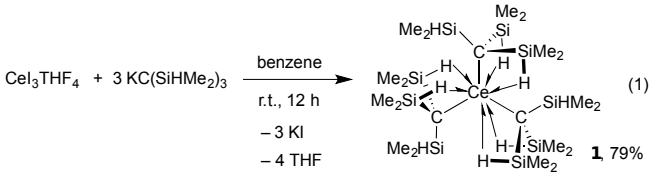
A further challenge in metal-catalyzed hydrosilylations of α,β-unsaturated esters involves unselective conversions providing mixtures of silyl ketene acetals, silyl ethers, α- and β-adducts, or polyacrylates (Scheme 1).[8] These selectivity challenges may be addressed by new reaction pathways and new catalysts. Recently, $B(C_6F_5)_3$ was discovered to catalyze the addition of α,β-unsaturated esters and tertiary silanes, giving silyl ketene acetals that isomerize to α-silyl esters through a $B(C_6F_5)_3$-catalyzed retro-Brook rearrangement.[9] This system is best with substituted esters, while acrylates and methacrylates conversions are not reported. Alternatively, a scandium hydridoborate catalyzes CO_2 reductive hydrosilylation,[10] and we observed that a zwitterionic magnesium hydridoborate complex produces silyl ketene acetals, without subsequent rearrangement.[11] These catalysts' hydridoborate functionality appeared to be important, and this motivated consideration of



Scheme 1. Possible products from acrylate hydrosilylations. Polymerization (not shown) is also a common pathway with oxophilic early metal centers.

other [M]HB(C_6F_5)$_3$ complexes in catalytic hydrosilylations. We hypothesized that larger rare earth centers might influence the selectivity in these hydrosilylation and thus targeted compounds of the type Ln[H(BC_6F_5)$_3$].

Abstraction of a β-H by reaction of early main-group metal or rare earth alkyl compounds and B(C_6F_5)$_3$ provides a straightforward route to [M]HB(C_6F_5)$_3$].[12] We therefore synthesized a suitable precursor Ce{C($SiHMe_2$)$_3$}$_3$ (**1**) by reaction of $CeI_3(THF)_4$ and 3 equiv. of KC($SiHMe_2$)$_3$ [Eq. (1)].



The ^{1}H NMR spectrum of **1** (298 K) contained broad signals at 4.9 (9 H, SiH) and 1.1 (53 H, SiMe) in the diamagnetic region, whereas a spectrum acquired at 206 K showed three sharp methyl resonances at –11.6, 9.3 and 10.6 ppm (18 H each). In addition, peaks at –19.7 (6 H) and 24.5 (3 H) ppm were assigned to Ce←H-Si and terminal SiH groups. The IR spectrum of **1** contained bands at 2107 and 1829 cm^{-1} assigned to ν_{SiH} of terminal and bridging groups. Crystallography revealed a trigonal planar geometry for the CeC_3 core (Figure 1), long Ce-C distances (2.651(2), 2.659(2), and 2.672(2) Å), and short Ce-H and Ce-Si distances.[13] Trigonal coordination of the carbon centers contrasts the pyramidal structures and much shorter Ce-C distances of Ce{$CH(SiMe_3)_2$}$_3$ (2.475(7) Å). That compound and Ce{$N(SiMe_3)_2$}$_3$ are notable for their pyramidal (non-VSEPR) geometries.[14]

Compound **1** and B(C_6F_5)$_3$ yield the desired zwitterionic Ce{C($SiHMe_2$)$_3$}$_2$HB(C_6F_5)$_3$ (**2**) and 0.5 equiv. of the disilacyclobutane [(Me_2HSi)$_2$C–$SiMe_2$]$_2$ [Eq. (2)]. Formation of

$HB(C_6F_5)_3^-$ rather than $(Me_2HSi)_3C\text{-}B(C_6F_5)_3^-$ suggests that the reaction proceeds by an intermolecular β-hydrogen abstraction.[12] Colorless crystals are obtained from toluene at –40 °C.

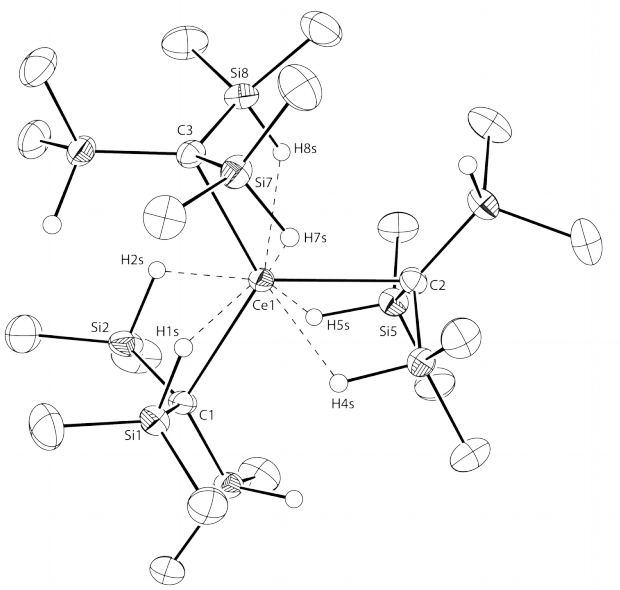
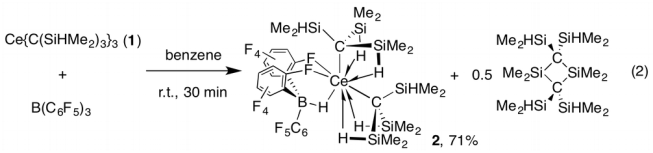


Figure 1: ORTEP diagram of $Ce\{C(SiHMe_2)_3\}_3$ (1) plotted at 50% probability. The only H atoms included in the image are bonded to Si which were objectively located.



The ^1H NMR spectrum of **2** contained one signal at 3.99 ppm, and unlike **1**, this peak could not be resolved at low temperature. A broad signal at –45 ppm in the ^{11}B NMR spectrum indicated that the hydridoborate anion coordinated to the Ce center. Peaks at 2117 and 1795 cm^{-1} in the IR spectra of **2** were assigned to the two Si-H in classical and bridging groups.

A single crystal X-ray diffraction study of **2** reveals that the two $C(SiHMe_2)_3$ coordinate to the Ce center in a fashion similar to **1** (Figure 2).[16] The third ligand is the tridentate

$HB(C_6F_5)_3$. The sum of C-Ce-C and C-Ce-centroid angles is 360° (with the centroid defined as the average position of the H1b, F1, and F6 atoms) suggesting that the three ligands are arranged in a trigonal planar geometry similar to **1**. The only other structurally characterized cerium hydridoborate compound reported in the CCDC is $[1,2,4\text{-}t\text{Bu}_3C_5H_2]_2Ce(H)BPh_3$).[17] The Ce-C, Ce-Si, and Ce-H distances in **2** are shorter than in **1**. For example, the Ce1-C1 and Ce1-C2 distances are 2.582(3) and 2.615(2) Å. The Ce-Si distances (for the Si1, Si2, Si4 and Si5 participating in the Ce←H-Si structure) in **2** are 3.15 ± 0.01 Å, which is 0.05 Å shorter than the average Ce-Si distance in **1** (3.20 ± 0.01 Å). Interestingly, the average $C_{central}$-Si distance (1.835 ± 0.003 Å) associated with the bridging Ce←H-Si interactions is shorter than those associated with nonbridging $SiHMe_2$ groups (1.855 ± 0.001 Å) for both **1** and **2**. Although the β-SiH in either compound do not react to eliminate silene, the perturbation of distances over

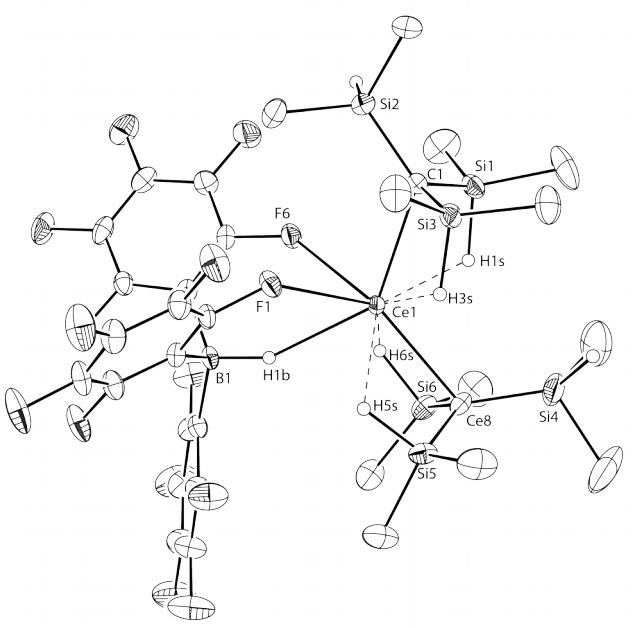


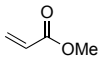
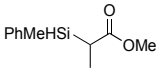
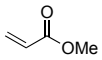
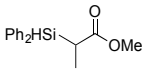
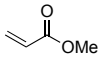
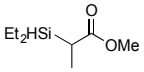
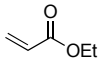
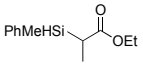
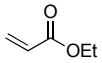
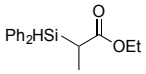
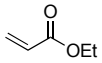
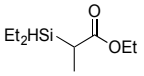
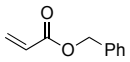
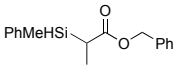
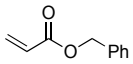
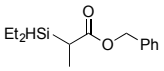
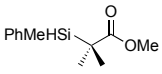
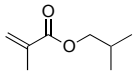
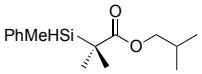
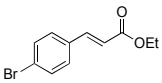
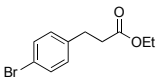
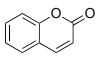
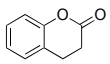
Figure 2: ORTEP diagram of Ce{C(SiHMe2)3}2HB(C6F5)3 (2) plotted at 35% probability. The only H atoms included in the image are bonded to Si or B and were objectively located.

the whole ligand suggests there are electronic consequences resulting from the agostic-like structure.

Compound **2** catalyzes the hydrosilylation of α,β-unsaturated esters with secondary silanes to give α-silyl esters (Table 1). This catalyst also mediates the addition of tertiary silanes to acrylates and methacrylates affording isomeric products, silyl ketene acetals as products. These results contrast to the catalytic action of $To^{M}MgHB(C_6F_5)_3$, which provides silyl ketene acetals for additions of both secondary and tertiary silanes to methacrylates, but polymerizes acrylates rather than catalyzing their hydrosilylation.[11] Neither divalent zwitterionic $YbC(SiHMe_2)_3HB(C_6F_5)_3$,[12a] nor trivalent neutral **1** provide either hydrosilylation product under related conditions. To identify which species is thermodynamically favored, the relative energies (ΔG) of six rotational isomers of the silyl ketene acetal Me(H)C=C(OSiHPh2)OMe and twelve rotational isomers of the α-silyl ester Me(Ph2HSi)HCCO2Me were compared by computation, with the latter found to be more stable by 9.5 to 12.2 kcal/mol.

The α-silyl ester products were unambiguously characterized by NMR and infrared spectroscopy. For example, the ^{1}H NMR spectrum of methyl α-diphenylsilylpropionate contained a doublet resonance at 4.94 ppm assigned to an SiH ($^3J_{HH}$ = 3.0 Hz, $^1J_{SiH}$ = 205 Hz) that was coupled to a quartet of doublets at 2.73 ppm ($^3J_{HH}$ = 7.2 Hz), assigned to an α-methine, that also coupled to a doublet at 1.35 ppm for a methyl group. These signals correlated with the ^{29}Si NMR signal at –9.33 ppm in a ^{1}H-^{29}Si HMBC experiment. The ^{1}H NMR spin system and 2D Hetcor

Table 1. 2 Catalyzed hydrosilylation of acylates and methacrylates.

Silane	Acrylate	Product[a]	Yield (isolated)
$PhMeSiH_2$			**84 (82)**
Ph_2SiH_2			**81 (80);** **72[b] (72)[c]**
Et_2SiH_2			**82 (81)**
$PhMeSiH_2$			**88 (85)**
Ph_2SiH_2			**77 (74)**
Et_2SiH_2			**82 (79)**
$PhMeSiH_2$			**83 (81)**
Et_2SiH_2			**78 (77)**
$PhMeSiH_2$			**89 (88)[d]**
$PhMeSiH_2$			**82 (81)**
Ph_2SiH_2			**85 (82)**
Et_2SiH_2			**84 (81)**

[a] Conditions: 1 mol% 2, $CHCl_3$, r.t., 10 min.; [b] benzene-d_6; [c] toluene; [d] 0 °C, 1 h.

experiment establishes the presence of a Si–C bond. Moreover, a correlation in a ^{1}H-^{13}C HMBC experiment was observed between a carbonyl resonance at 175.93 ppm and

the ^{1}H NMR signal of the α-methyl. Finally, a band in the infrared spectrum at 1725 cm^{-1} was consistent with the ν_{CO} of an ester.

Although the transformation occurs efficiently in chloroform, other solvents including benzene, toluene, and methylene chloride also afford α-silyl esters. In addition, the catalyst is extremely active, giving full conversion of methyl acrylate and $PhMeSiH_2$ with 0.05 mol % **2** within 5 min. During these reactions, the pale yellow reaction mixture turns colorless upon catalyst deactivation, and the timing of this change along with NMR yield for incomplete conversions was used with the catalyst turnover number of 2200 to estimate the turnover frequency of 37 s^{-1} (133,200 h^{-1}).

Because $B(C_6F_5)_3$ catalyzes the addition of tertiary silanes to esters[18] to α,β-unsaturated esters to give 1,2-addition and α-silyl esters, respectively,[9] and small amounts of $B(C_6F_5)_3$ could be present in the reaction via dissociation of **2**, disambiguation of **2** from $B(C_6F_5)_3$ required study of the latter's catalytic chemistry with secondary silanes. In contrast to the reactions of tertiary silanes, $PhMeSiH_2$ and methyl acrylate react in the presence of 1 mol % $B(C_6F_5)_3$ to give a complex mixture of unidentified species. The proposed two step pathway for $B(C_6F_5)_3$-catalyzed formation of α-silyl esters involves 1,4-addition giving silyl ketene acetals followed by rearrangement to the product. This pathway was tested for **2**-catalyzed hydrosilylation by treatment of the proposed silyl ketene acetal intermediate $Me_2C{=}C(OSiPhMeH)OMe$, synthesized by $To^MMgHB(C_6F_5)_3$-catalyzed hydrosilylation of benzyl methacrylate with phenylmethylsilane,[11] with either **2** or $B(C_6F_5)_3$. However, the α-silyl ester product $Me_2(PhMeHSi)CCO_2CH_2Ph$ is not detected in either reaction mixture after even 1 d.

Moreover, Ph_2SiH_2 and methylmethacrylate, or trans-4-ethyl bromocinnamate and $PhMe_2SiH_2$, react in the presence of $B(C_6F_3)_3$ to give mixtures involving C-O cleavage, whereas **2** provides the selective hydrogenation product. These results indicate that the catalytic hydrosilylation chemistry of **2** is distinct from that of $B(C_6F_5)_3$ in terms of the identity of the active species, the nature of accessible reaction partners, and its mode of action. The catalyst and its new homoleptic tris(alkyl) cerium precursor contain two Ce←H-Si groups per ligand, which are characterized by low energy SiH in IR spectra, fluxional processes frozen at low temperature in NMR studies, and distorted structures revealed by X-ray crystallography. Remarkably, although Ce and Si centers in catalyst and reductant are oxophilic and form strong O–E bonds, the observed Si-C bond formation is not impeded. Furthermore, eliminated tris(dimethylsilyl) ligands are not observed as side products during catalysis, suggesting that other ancillary ligands may be accessible for controlling enantioselectivity in these addition reactions.

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Keywords: hydrosilylation • cerium alkyl • α-silyl esters • earth abundant • catalysis

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[13] $C_{21}H_{63}CeSi_9$: M_r 708.64; P-1; a = 11.504(1), b = 11.542(1), c = 16.704(2), α = 100.352(2), β = 98.519(2), γ = 114.706(2), V = 1919.3(3) Å^3; Z = 2, ρ_{calcd} = 1.226, μ = 1.477, λ = 0.7173 Å; 173 K; Reflect. measured: 30348, independent: 9901; R_{int} 0.0365, R 0.0303, wR 0.0661. CCDC 1507399.

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[16] $C_{32}H_{43}BCeF_{15}Si_6$, M_r 1032.13; P-1; a = 11.477(2), b = 13.408(2), c = 15.194(2), α = 82.826(2), β = 76.552(2), γ = 75.376(2), V = 2194.9(6) $Å^3$; Z = 2, ρ_{calcd} = 1.563, μ = 1.288, λ = 0.7173 Å; 173 K; Reflect. measured: 29404, independent: 8949; R_{int} 0.0322, R 0.0286, wR 0.0661. CCDC 1507398.

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CHAPTER 6. GENERAL CONCLUSIONS

1 Directed Acyclic Graph task management

As computing systems become more heterogeneous thanks to different types of processors (CPU, GPU, MIC), network architectures, issues of load balancing and inter-process communications become correspondingly more complex. Global syncs cause delays by forcing parallel processes to stand idle while other processes work through a backlog of tasks. In a cyclic process, the cost of regular inefficiencies scales with the number of cycles.

Some of these delays can be eliminated by eliminating unnecessary dependencies. This was accomplished using the PaRSEC task engine. PaRSEC provides a framework for making dependencies between tasks more fine grained so that task execution can be based on actual data dependencies.

First, this was demonstrated by implementing a cyclic eigenvalue and eigenvector solver based on the Jacobi method[1]. During the diagonalizer process, all global syncs were removed. The resulting solver works well but requires further optimization before it is likely to be competitive with other currently available parallel eigensolvers.

Once the diagonalizer was implemented, a functional implementation of the iterative Hartree-Fock SCF method followed. This code is able to correctly determine the energies of the provided test systems. Although providing a solid demonstration that cyclic algorithms can be expressed with the PaRSEC DAG engine, this specific algorithm is unlikely to outperform other SCF accelerators. However, it may provide some improvements when used in conjunction with those methods. For instance, the DIIS process actually requires a global sync during each SCF iteration, but using the task based approach for every other part of the process may remove some delays between invocations of the DIIS process. Further testing is needed.

Both implementated cyclic processes would benefit from implementation with a task manager that is designed to handle processes that can ”decide” whether they’re done or not.

2 Zirconium Catalysis

Two interlocking catalytic cycles were identified for the zirconium catalyzed cycloamination of 4-pentenamine. Because of the complex interconnectedness of the cycles, which one will be preferred at a given time will be dependent on the concentration of the 4-pentenamine. With scarce substrate, an oelefin insertion mechanism with slightly lower energy than the competing 2π+2π cycloaddition reaction is more likely to occur. This is because the dissociation of a coordinated substrate molecule is less thermodynamically favored than the competing cycloaddition reaction. When there is abundant substrate, the extra amine molecules are more likely to get in the way of forward reactions than to help them.

Additionally, cyclizations with an equatorial orientation have lower barrier heights than those with an axial orientation. Both the olefin insertion and 2π+2π cyclizations have lower barrier heights than most of the studied hydrogen transfers. That the hydrogen transfers are the rate limiting step in both cycles is consistent with the observation that deuteration of the amine impacts the stereoselectivity of the reaction[2].

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APPENDIX. CHAPTER 3. SUPPLEMENTAL INFORMATION FOR ZIRCONIUM CATALYZED CYCLOAMINATION OF 4-PENTENAMINE, A MODEL SYSTEM

Below are the MP2, B3LYP and M06-L electronic energies. Also included are the zero-point energies, enthalpy and entropy corrections, and imaginary frequencies (if any) from the B3LYP Hessian calculation on the located minima and transition state for each reaction.

The geometries were minimized using B3LYP theory with the 6-311G(d, p) basis set for light atoms and the Stuttgart 1997 RSC with ECP basis set for Zr. A Hessian calculation using the same theory was run on the located geometries to verify that there were no imaginary frequencies for minima and only one for transition states. Where relevant, another Hessian calculation was run with the amine hydrogens replaced by deuterium. For geometries with a coordinated amine the potential energy surface can be quite flat so eliminating imaginary frequencies associated with translation of the amine relative to the rest of the system can be very time consuming without yielding any significant energetic differences. Additional imaginary frequencies were verified to be associated with these kinds of motions. Once verified, single point energies were computed for each geometry using the same basis set and MP2, B3LYP and M06-L theories.

As in the main body of this paper, cyclization reactions are labeled with a “C” (C1 and C1-S are olefin insertions, C2 and C2-S are 2π+2π cycloadditions, C3 and C3-S are concerted). Hydrogen transfer reactions are labeled with an “H.” Substrate association reactions are labeled with an “A” and product dissociations are labeled with a “D.” Reactions with a coordinated spectator amine have a “-S” suffix while those with a formed but not yet dissociated product have a “-P” suffix. Axial reactions involve an amine opposite the coordinated cyclopentadienyl ring. Equatorial reactions only involve ligands opposite the oxazoline rings.

```
Axial Reaction C1

Reactant geometry

Zr        0.22323829        -0.52079223        0.73895093
```

C	0.90963607	1.78356490	1.30460696
C	0.19147585	1.30851185	2.44852676
H	-0.80003292	1.62383877	2.73795644
C	2.15065615	1.07782993	1.32115836
H	2.93594200	1.17865429	0.58477586
C	2.15454207	0.14560623	2.38098042
H	2.94806110	-0.54433285	2.63034716
C	0.93045678	0.28790938	3.08878586
H	0.63831548	-0.26175594	3.97194876
B	0.28822407	2.62578971	0.04403812
C	0.55876177	4.21579332	0.02190191
C	0.81841218	1.80014514	-1.28728811
C	-1.29178453	2.17788754	-0.02318519
N	-1.67428232	0.96614332	0.23346798
N	0.73415356	0.50538023	-1.34253793
O	1.35198060	2.38433590	-2.37002311
O	-2.24758184	3.00754979	-0.47549462
C	-3.11595368	0.85068791	-0.05997236
C	-3.48491309	2.25045006	-0.59051498
C	1.33078127	0.03194357	-2.60311536
C	1.61260859	1.34477768	-3.35963024
N	-1.20035592	-1.98966865	1.22642274
H	-3.29039038	0.05753326	-0.78950663
C	-2.52915764	-2.15053210	1.80189230
H	-2.46431137	-2.26759402	2.89568595
H	-3.10535501	-1.23717158	1.63570592
C	-3.32821773	-3.35250601	1.26674775
C	-3.88630107	-3.24401024	-0.16452837
H	-4.56720119	-4.09465286	-0.30792845
H	-4.50741636	-2.34559156	-0.25696179
C	-2.87935732	-3.28185604	-1.28119719
H	-2.08230488	-4.01529942	-1.17212264
C	-2.92784407	-2.55108046	-2.39241247

H	-3.70803818	-1.81331911	-2.55699591
C	1.23905698	4.84942235	1.07224163
H	1.59106045	4.25314384	1.90813920
C	0.12777450	5.03523562	-1.03583522
H	-0.40376031	4.59218619	-1.87123957
C	0.36133568	6.40776832	-1.04517410
H	0.01418535	7.00974925	-1.87916229
C	1.47863361	6.22399881	1.07458327
H	2.00870775	6.67899789	1.90540106
C	1.03983126	7.01038671	0.01347045
H	1.22371334	8.07966571	0.00917166
H	0.63950725	-0.62160586	-3.13950082
H	2.23805967	-0.53965870	-2.39002618
H	0.93592779	1.51408498	-4.19929772
H	2.64239595	1.45683484	-3.69677993
H	-3.67069547	0.60082887	0.84736805
H	-3.78154653	2.25791173	-1.64073613
H	-4.24521765	2.76051328	0.00133478
H	-2.70644380	-4.25425643	1.34642886
H	-4.17670695	-3.51494889	1.94219303
H	-0.69511805	-2.86624054	1.34562212
H	-2.19566776	-2.66886961	-3.18329806
N	1.60933116	-2.01804379	0.23716669
H	2.57638014	-1.94123972	0.53251105
C	1.45024846	-3.17961327	-0.63109222
H	0.40451821	-3.23660803	-0.95458408
H	2.04831668	-3.07678331	-1.55158845
C	1.83655912	-4.50397737	0.04739644
H	1.22460871	-4.63655831	0.94700550
H	2.87629353	-4.44214344	0.38996549
C	1.68138431	-5.72423135	-0.87803273
H	2.30575643	-5.59591648	-1.76911696
H	0.64085259	-5.76918690	-1.22810826

C	2.02921774	-7.02072939	-0.20279051
H	1.42801877	-7.27618677	0.66922643
C	3.00167249	-7.84706259	-0.57634904
H	3.62821814	-7.63495872	-1.43786965
H	3.20650564	-8.76600934	-0.03872994

MP2 Electronic Energy(Ha): 1489.151680321631

B3LYP Electronic Energy(Ha): 1493.008227566263

M06-L Electronic Energy(Ha): 1492.814175906775

Zero point energy correction(kcal/mol): 376.804

Enthalpy correction(kcal/mol): 400.437

Entropy correction(cal/mol): 226.679

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.668

Deuterated enthalpy correction(kcal/mol): 396.531

Deuterated entropy correction(cal/mol): 228.068

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.71390050	-0.72342835	0.36555661
C	0.25824208	1.28653038	1.36225479
C	-0.95037116	1.13690370	2.11933802
H	-1.83444871	1.74747751	2.01426414
C	1.13081926	0.26779793	1.84008270
H	2.13128935	0.08152023	1.47711952
C	0.47059261	-0.48720158	2.84202947
H	0.87281091	-1.33809587	3.37521045
C	-0.81454431	0.05931159	3.01773954
H	-1.57569307	-0.30854637	3.69045166
B	0.48769697	2.27818999	0.09255726
C	1.24448771	3.66798305	0.41845262
C	1.20387895	1.36254173	-1.06753034
C	-1.00713333	2.38098937	-0.58119819
N	-1.79253047	1.34972115	-0.64614277

N	0.86410239	0.12558226	-1.25290222
O	2.05927848	1.86607525	-1.97754114
O	-1.46006602	3.50003956	-1.17549884
C	-2.97966637	1.72060226	-1.44290186
C	-2.81083205	3.23893767	-1.64341449
C	1.45449081	-0.33812226	-2.52383936
C	2.45958346	0.77485970	-2.85335557
N	-2.45743677	-1.86590514	1.12124648
H	-2.98230415	1.17891541	-2.39452947
C	-3.84149750	-1.57357324	1.44627628
H	-4.07474752	-1.84652304	2.48353361
H	-4.01715805	-0.49504284	1.35947057
C	-4.75195906	-2.32538422	0.46186591
C	-4.15458829	-2.10355367	-0.93079693
H	-4.63627086	-2.75690912	-1.66817043
H	-4.33058435	-1.07423266	-1.25925224
C	-2.67503907	-2.40155420	-0.95820969
H	-2.41698123	-3.42616898	-0.70959801
C	-1.74894367	-1.68915415	-1.72735691
H	-2.09178039	-0.83839792	-2.30440975
C	1.64830342	3.97452272	1.72694825
H	1.41496096	3.27922463	2.52676700
C	1.57498577	4.60310722	-0.57774581
H	1.28943382	4.40981058	-1.60592389
C	2.27803808	5.76975029	-0.28692673
H	2.52508695	6.46453173	-1.08365669
C	2.35045850	5.14094441	2.03091212
H	2.64998839	5.33968360	3.05527054
C	2.67262562	6.04383620	1.02197719
H	3.22650773	6.94845399	1.25045496
H	0.66754298	-0.42764019	-3.28109736
H	1.92915426	-1.31186660	-2.41505904
H	2.42059684	1.13391566	-3.88078706

H	3.48809774	0.50617130	-2.59994707
H	-3.90347615	1.47132243	-0.91578386
H	-2.87745809	3.56610642	-2.68082068
H	-3.49441501	3.83290187	-1.03309697
H	-4.74236345	-3.39545451	0.70264147
H	-5.79258167	-1.99068748	0.51659128
H	-2.18495619	-2.77362044	1.48208932
H	-0.90207268	-2.22793070	-2.13617890
N	0.49789476	-2.44943988	0.43864570
H	0.88446414	-2.54322423	1.37200389
C	1.38454328	-3.17567160	-0.45899850
H	0.91197110	-3.29326620	-1.44096629
H	2.30761189	-2.59551756	-0.63207024
C	1.80631001	-4.55485677	0.07204275
H	0.97385329	-5.26150714	-0.01607478
H	2.02811158	-4.46927430	1.14233633
C	3.05987748	-5.10351987	-0.63563930
H	3.88134877	-4.38962445	-0.50790189
H	2.86590021	-5.17008757	-1.71452418
C	3.48479469	-6.44806190	-0.11711461
H	2.81187717	-7.27738113	-0.33065767
C	4.58599042	-6.67838852	0.59225632
H	5.28337150	-5.88082711	0.83288942
H	4.83225409	-7.66810954	0.95986509

MP2 Electronic Energy(Ha): 1489.133335414874

B3LYP Electronic Energy(Ha): 1492.973996761142

M06-L Electronic Energy(Ha): 1492.791839232954

Zero point energy correction(kcal/mol): 377.145

Enthalpy correction(kcal/mol): 399.706

Entropy correction(cal/mol): 214.865

Imaginary Frequencies: -258.06

Deuterated zero point energy correction(kcal/mol): 372.930

Deuterated enthalpy correction(kcal/mol): 395.714

Deuterated entropy correction(cal/mol): 216.164

Deuterated imaginary Frequencies: -257.74

Product geometry

Zr	-0.05589524	-0.66083724	0.26099133
C	0.52809205	1.48572276	1.33894666
C	-0.50598490	0.95981814	2.17223560
H	-1.52274938	1.32011519	2.21064061
C	1.68458243	0.69685379	1.63146868
H	2.65414528	0.81425349	1.16851394
C	1.35474319	-0.29697110	2.57473527
H	2.02036367	-1.04874160	2.97585288
C	-0.01268064	-0.14605593	2.90282089
H	-0.56516301	-0.74320665	3.61523768
B	0.35832943	2.55082842	0.11246273
C	0.75047524	4.08662709	0.42432205
C	1.17118768	1.85714604	-1.14378274
C	-1.17946041	2.31377675	-0.41481798
N	-1.72323912	1.13800706	-0.43875559
N	1.14313819	0.57227967	-1.32048187
O	1.81674044	2.54816058	-2.09616570
O	-1.91662533	3.31188563	-0.94189237
C	-3.02684273	1.24415863	-1.12253643
C	-3.21118721	2.76181883	-1.30476970
C	1.83085993	0.22906044	-2.57499132
C	2.35344751	1.59638889	-3.06285286
N	-1.88773469	-2.07933114	0.85220845
H	-2.99408905	0.70997605	-2.07649200
C	-3.24115373	-1.75332308	1.36956311
H	-3.27785369	-1.90185384	2.45017370
H	-3.45571666	-0.70066156	1.17265554
C	-4.19271593	-2.65918285	0.57736287
C	-3.56344380	-2.64930505	-0.82314279

H	-3.85901486	-3.50398166	-1.43474542
H	-3.86361130	-1.74570628	-1.36079965
C	-2.03472714	-2.62771299	-0.59067915
H	-1.65743764	-3.65350173	-0.55777274
C	-1.17128576	-1.76163428	-1.50024810
H	-1.77830675	-1.09521242	-2.11717727
C	1.16387708	4.48267470	1.70505520
H	1.22308383	3.73863210	2.49310317
C	0.69295724	5.09084069	-0.55799261
H	0.37919470	4.83440583	-1.56391187
C	1.02865040	6.41309598	-0.27873152
H	0.97280282	7.16202017	-1.06272159
C	1.50210654	5.80458781	1.99714778
H	1.81771430	6.07285536	3.00061824
C	1.43592790	6.77746267	1.00407421
H	1.69837313	7.80694723	1.22469109
H	1.12768597	-0.23130987	-3.27383963
H	2.63340579	-0.48706088	-2.38575660
H	1.98973383	1.88504387	-4.04903943
H	3.44075928	1.68163849	-3.03987689
H	-3.82542365	0.80112823	-0.52274973
H	-3.43441509	3.06743655	-2.32675206
H	-3.95603615	3.18908257	-0.62975022
H	-4.18691184	-3.67016825	0.99891150
H	-5.22429453	-2.29964594	0.59105582
H	-1.48391521	-2.80642888	1.43402446
H	-0.55295093	-2.35735862	-2.17389493
N	1.24890172	-2.32001936	0.29654351
H	1.91520347	-2.29116571	1.06084119
C	1.56236751	-3.48482203	-0.52234756
H	0.87868695	-3.52506194	-1.37307312
H	2.57486498	-3.39579152	-0.94863233
C	1.48433903	-4.81423498	0.24663601

H 0.47064614 -4.93548707 0.64763448

H 2.15593242 -4.77498966 1.11255465

C 1.84990514 -6.03321066 -0.61971085

H 2.86864943 -5.91962246 -1.00610909

H 1.18374400 -6.05460406 -1.49308135

C 1.73453823 -7.33614252 0.11959784

H 0.74109616 -7.58145389 0.49430935

C 2.73478077 -8.18014605 0.35498431

H 3.74236828 -7.97904150 0.00278457

H 2.58508035 -9.10280471 0.90438804

MP2 Electronic Energy(Ha): 1489.171004223724

B3LYP Electronic Energy(Ha): 1493.004934036188

M06-L Electronic Energy(Ha): 1492.820817868319

Zero point energy correction(kcal/mol): 379.146

Enthalpy correction(kcal/mol): 401.660

Entropy correction(cal/mol): 216.165

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.772

Deuterated enthalpy correction(kcal/mol): 397.480

Deuterated entropy correction(cal/mol): 217.274

Deuterated imaginary Frequencies: -0.00

Axial Reaction C2

Reactant geometry

Zr -1.01870635 -1.17354660 -0.02282478

C -1.64463223 1.20782415 0.24786101

C -2.50429474 0.74436212 -0.79551931

H -2.41783415 1.00812236 -1.84053675

C -2.13858369 0.58476890 1.43598195

H -1.71909934 0.70424247 2.42526257

C -3.20402314 -0.29389168 1.11805632

H -3.77523382 -0.89239179 1.81337162

C	-3.43262815	-0.19469574	-0.28017832
H	-4.20838666	-0.70451530	-0.83366456
B	-0.11709287	1.78852246	0.03991640
C	0.08040558	3.38803675	0.12328076
C	0.82456700	0.92768144	1.11466919
C	0.41154518	1.11074923	-1.39050467
N	0.17283808	-0.13156295	-1.71323940
N	0.65746785	-0.34854699	1.32796128
O	1.84925699	1.47509254	1.77280822
O	1.16618870	1.78086085	-2.26474807
C	0.83877312	-0.44874760	-2.99016897
C	1.47342863	0.89922246	-3.38807576
C	1.66848960	-0.83127103	2.28706008
C	2.51148525	0.43203281	2.55440757
N	-1.01941258	-3.04324642	-0.12120356
H	1.57879300	-1.23943254	-2.84434380
H	1.17847529	-1.20687591	3.18875568
C	-1.25254967	-4.46009550	-0.10455720
H	-2.22242364	-4.67188668	0.37111676
H	-1.33260912	-4.85138395	-1.13238923
C	-0.18167022	-5.28326747	0.64237104
C	1.15094241	-5.50106148	-0.10574326
H	1.74077327	-6.25410304	0.42877399
H	0.91709341	-5.93202834	-1.08958022
C	1.99651592	-4.27498800	-0.30936150
H	1.52256351	-3.46410523	-0.85442606
C	3.24794164	-4.13186692	0.12376786
H	3.75268699	-4.91686508	0.68013998
H	3.81995568	-3.23069418	-0.07202176
C	-1.01477809	4.23117586	0.36214077
H	-1.99843355	3.79115356	0.49057862
C	1.33222630	4.00754117	-0.03536786
H	2.21075187	3.39902105	-0.22119227

C	1.48298784	5.38958700	0.03960842
H	2.46501703	5.83415005	-0.08773323
C	-0.87602583	5.61726403	0.43939215
H	-1.74668034	6.23791382	0.62573038
C	0.37598815	6.20310614	0.27799428
H	0.49016093	7.28037206	0.33707780
H	0.00890206	-4.81306258	1.61303766
H	-0.60552258	-6.27423656	0.84680749
H	2.55740817	0.86671241	-3.49356008
H	1.03507185	1.34430921	-4.28152531
H	0.11005314	-0.80302891	-3.72227225
H	3.53876949	0.35945306	2.19604842
H	2.51262357	0.75396218	3.59522942
H	2.24435829	-1.65048297	1.85292773

MP2 Electronic Energy(Ha): 1237.820556820536

B3LYP Electronic Energy(Ha): 1241.008396994402

M06-L Electronic Energy(Ha): 1240.849711291559

Zero point energy correction(kcal/mol): 279.086

Enthalpy correction(kcal/mol): 297.342

Entropy correction(cal/mol): 192.455

Imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.39246359	1.45130375	-0.02265023
C	-1.45735505	-0.72959220	-0.34477059
C	-2.31945147	-0.13421086	0.63242133
H	-2.35378232	-0.39700031	1.68042519
C	-1.77034752	-0.05546206	-1.56129329
H	-1.31183011	-0.24447322	-2.52129601
C	-2.79406801	0.90663342	-1.33382048
H	-3.22404953	1.56671341	-2.07392842
C	-3.14320911	0.84275846	0.02379270
H	-3.86487599	1.46904546	0.52767629

B	-0.13008998	-1.63349079	-0.03958431
C	-0.31296963	-3.24052561	-0.09703068
C	1.00575017	-1.06502384	-1.10279945
C	0.40978854	-1.08321236	1.42993530
N	0.32059119	0.16655385	1.79248814
N	1.09628590	0.18777710	-1.44305909
O	1.89749633	-1.87955556	-1.68960707
O	0.96579362	-1.89190771	2.34152479
C	0.81563376	0.31513034	3.17210661
C	1.35458870	-1.09185278	3.49583089
C	2.17250999	0.34402028	-2.43747578
C	2.72022076	-1.08891707	-2.59232305
N	-0.98151782	3.24078573	0.20551045
H	1.58742842	1.08600403	3.23331761
H	1.76485281	0.74004084	-3.37171242
C	-1.24509550	4.63661866	0.17212682
H	-2.24406508	4.84982803	-0.23713217
H	-1.23573131	5.06246448	1.19030617
C	-0.17505118	5.33495939	-0.68630998
C	1.23770844	4.81007650	-0.31416198
H	1.80109441	4.55337923	-1.21557289
H	1.80811803	5.60263382	0.18563809
C	1.25076827	3.62335093	0.62360659
H	0.91321778	3.83009458	1.63394128
C	2.00564373	2.49322829	0.41097097
H	2.56642803	2.38993607	-0.50969918
H	2.30347241	1.85287354	1.23032827
C	-1.55765413	-3.80931092	-0.40365423
H	-2.40074750	-3.15390364	-0.59638969
C	0.74707149	-4.13178092	0.14373646
H	1.72995807	-3.74053254	0.38356862
C	0.57604255	-5.51213321	0.08034015
H	1.41785713	-6.17077993	0.27037790

C	-1.74124713	-5.19106218	-0.46989960
H	-2.71930029	-5.59524293	-0.71137014
C	-0.67296859	-6.04975031	-0.22825669
H	-0.80942062	-7.12493706	-0.27973602
H	-0.37669059	5.09917688	-1.73517235
H	-0.23166594	6.42350558	-0.58452796
H	2.44210532	-1.13397418	3.57483232
H	0.90931994	-1.54657421	4.37984826
H	-0.00627447	0.61287729	3.82926442
H	3.75898374	-1.19877111	-2.27890744
H	2.60035283	-1.49900578	-3.59525828
H	2.93254935	1.04416346	-2.08324118

MP2 Electronic Energy(Ha): 1237.805469092657

B3LYP Electronic Energy(Ha): 1240.980432174257

M06-L Electronic Energy(Ha): 1240.834049561463

Zero point energy correction(kcal/mol): 278.824

Enthalpy correction(kcal/mol): 295.790

Entropy correction(cal/mol): 176.547

Imaginary Frequencies: -100.66 -12.77

Product geometry

Zr	-0.13839756	-1.40867942	0.22809233
C	-1.33856519	0.70720348	0.54576141
C	-2.24397273	0.01747065	-0.32155452
H	-2.41276885	0.25541410	-1.36210696
C	-1.43603837	0.02689156	1.80088452
H	-0.89841791	0.28874344	2.70016596
C	-2.29571255	-1.09283734	1.67117953
H	-2.56259350	-1.79210481	2.45159555
C	-2.80556854	-1.08633238	0.34668519
H	-3.49602857	-1.80426940	-0.07091180
B	-0.15776600	1.73994520	0.06947329
C	-0.51260433	3.31383980	0.06057339

C	1.15618047	1.31936396	0.98051023
C	0.33106720	1.13058735	-1.39677519
N	0.36872515	-0.15355603	-1.62174666
N	1.38720678	0.08557028	1.31291484
O	2.11062325	2.19560106	1.33141129
O	0.79233955	1.88638399	-2.39617666
C	0.94597145	-0.41159519	-2.95270941
C	1.17932151	1.01136764	-3.50044624
C	2.70578004	-0.00274762	1.96403554
C	3.12206321	1.47531987	2.09760023
N	-0.59182078	-3.32994392	-0.37112320
H	1.86974692	-0.98724330	-2.85692830
H	2.62732467	-0.50439763	2.93096938
C	-1.55581492	-4.41302251	-0.50336872
H	-2.44369527	-4.21683595	0.10366663
H	-1.89569839	-4.50435182	-1.54485291
C	-0.80933846	-5.71621108	-0.06903183
C	0.60967140	-5.24617264	0.31785387
H	0.67033034	-5.04902719	1.39361259
H	1.38537331	-5.97433597	0.06699243
C	0.77346325	-3.91628033	-0.43870106
H	1.02431142	-4.14233529	-1.48973334
C	1.69529080	-2.83013528	0.12855305
H	2.06038083	-3.10490954	1.12768076
H	2.56904899	-2.61979653	-0.49426862
C	-1.77794774	3.76702305	0.46202471
H	-2.52072655	3.04242798	0.78026839
C	0.41201709	4.29361953	-0.34110519
H	1.40478302	3.99301721	-0.65755810
C	0.09160949	5.64869812	-0.34265400
H	0.83043444	6.37839647	-0.65882956
C	-2.11000872	5.12211429	0.46497419
H	-3.09937676	5.43563194	0.78273221

C	-1.17451153	6.07025710	0.06136298
H	-1.42682229	7.12544679	0.06136238
H	-1.31646291	-6.21690515	0.75863274
H	-0.77105279	-6.42629723	-0.89914608
H	2.21903181	1.22880906	-3.74326517
H	0.54718275	1.26215351	-4.35253474
H	0.24953385	-0.98949815	-3.56375441
H	4.09482496	1.70890027	1.66619067
H	3.08232525	1.84588711	3.12329048
H	3.38714624	-0.58597387	1.33956211

MP2 Electronic Energy(Ha): 1237.841050815979

B3LYP Electronic Energy(Ha): 1241.015894905244

M06-L Electronic Energy(Ha): 1240.867971815012

Zero point energy correction(kcal/mol): 279.802

Enthalpy correction(kcal/mol): 297.312

Entropy correction(cal/mol): 186.248

Imaginary Frequencies: -0.00

Axial Reaction C3

Reactant geometry

Zr	-0.29130644	0.68025196	-0.34360985
C	0.49066496	-1.43607607	-1.33548183
C	-0.47144022	-0.92354384	-2.26278479
H	-1.46363448	-1.32208327	-2.41504791
C	1.62971191	-0.58418757	-1.46673706
H	2.54392807	-0.67157238	-0.89607309
C	1.34147286	0.45943232	-2.37296388
H	2.00024523	1.26523388	-2.66009895
C	0.02755541	0.24857936	-2.87245925
H	-0.48103420	0.86032647	-3.60337168
B	0.20380864	-2.50307048	-0.12760589
C	0.62268495	-4.03780543	-0.39406230

C	0.89650822	-1.80004756	1.20053306
C	-1.36596064	-2.25504588	0.29705420
N	-1.89430632	-1.07006727	0.30383427
N	0.71337267	-0.54033230	1.45677344
O	1.64824680	-2.46347073	2.09099729
O	-2.12566852	-3.23072359	0.82641625
C	-3.18316230	-1.13816530	1.02069561
C	-3.41877617	-2.65083654	1.15938078
C	1.44550550	-0.18182309	2.68356937
C	2.00504409	-1.53784663	3.16016440
N	0.86684697	2.34611288	0.16664014
N	-1.99327967	1.90742628	-0.48385092
C	-3.36920210	1.78598576	-0.94775125
H	-3.59540706	0.72622942	-1.09274833
H	-3.09043967	-0.63649685	1.99000836
H	2.22796963	0.54421163	2.45218294
C	2.14347854	2.98468484	-0.13506587
H	2.76283622	2.27984709	-0.69762243
H	1.99865346	3.85603785	-0.79025241
C	2.92204710	3.43712525	1.10843240
C	-4.42918960	2.38956916	-0.00722265
C	-4.47911949	3.93075257	0.02860862
H	-5.37359212	4.22079287	0.59627390
H	-3.48905164	2.25145809	-1.93981549
H	-1.72749519	2.88833572	-0.50188163
C	-3.29485705	4.60827448	0.66174737
H	-3.04800653	4.28087448	1.67086179
H	-4.62157732	4.31675615	-0.98737617
C	-2.57091608	5.57739339	0.10498276
H	-1.74851224	6.04870100	0.63154252
H	0.34404786	2.95021760	0.80321800
H	-2.77986274	5.93888534	-0.89758212
C	0.45431486	-5.04160655	0.57568647

H	0.02777496	-4.78571157	1.53957463
C	1.17667118	-4.43412318	-1.62039784
H	1.32536784	-3.69033966	-2.39682029
C	0.81697531	-6.36430683	0.33574697
H	0.67241266	-7.11320662	1.10820931
C	1.54371919	-5.75640907	-1.87273875
H	1.96944761	-6.02518396	-2.83438767
C	1.36504475	-6.72898266	-0.89339913
H	1.64882794	-7.75881785	-1.08342059
C	4.26481868	4.12253780	0.78489336
H	4.88922123	3.45185224	0.18386375
H	4.80121272	4.28403478	1.72878882
C	4.12204939	5.44472152	0.08274675
H	3.51572775	6.18819523	0.60027093
C	4.67377680	5.76743815	-1.08353780
H	5.28570218	5.06169269	-1.63756929
H	4.53813218	6.74795963	-1.52588365
H	-5.41604849	2.03350443	-0.32851314
H	-4.26595354	2.00271649	1.00534648
H	2.29731797	4.12451024	1.69439548
H	3.10837361	2.56861567	1.74868709
H	-3.68640264	-2.97873221	2.16301466
H	-4.14861374	-3.03723498	0.44426606
H	-3.97856845	-0.64202742	0.46582282
H	1.54150119	-1.90209857	4.07841271
H	3.08898852	-1.55964733	3.27034088
H	0.77414360	0.27488433	3.41488186

MP2 Electronic Energy(Ha): 1489.151316049260

B3LYP Electronic Energy(Ha): 1493.008981780676

M06-L Electronic Energy(Ha): 1492.812021563407

Zero point energy correction(kcal/mol): 376.803

Enthalpy correction(kcal/mol): 400.470

Entropy correction(cal/mol): 229.846

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.280

Deuterated enthalpy correction(kcal/mol): 396.288

Deuterated entropy correction(cal/mol): 233.352

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.20095590	0.70122963	-0.18718376
C	1.63618867	-1.24082511	0.03638839
C	2.18166680	-0.58992751	-1.11228563
H	2.08166611	-0.92830772	-2.13275568
C	2.02896408	-0.42285848	1.14371613
H	1.79595023	-0.61396758	2.18063881
C	2.73466582	0.70936807	0.67863868
H	3.13983319	1.50485477	1.28614928
C	2.82599390	0.60682796	-0.72875012
H	3.31229655	1.30900571	-1.38971044
B	0.46586065	-2.38970085	0.03152378
C	1.00419531	-3.90891877	0.15604983
C	-0.56690109	-1.90079878	1.23126749
C	-0.39963725	-2.05968465	-1.34569806
N	-0.54480444	-0.85011043	-1.80932932
N	-0.77766581	-0.64264589	1.49463838
O	-1.26228129	-2.75898464	1.99222890
O	-1.01307748	-3.01322946	-2.06381461
C	-1.27287147	-0.90609835	-3.08987571
C	-1.74105738	-2.37031224	-3.15109588
C	-1.68508000	-0.53054438	2.65098073
C	-2.11217027	-1.98974225	2.89454617
N	0.41462644	2.67901270	-0.35837772
N	-2.09879223	1.30623790	-0.40510411
C	-3.21228440	0.31691539	-0.45482336
H	-2.90111294	-0.63661845	-0.02638542

H	-2.10076625	-0.19622386	-3.11037802
H	-1.14352255	-0.10340809	3.50032209
C	1.40002220	3.75157805	-0.39783741
H	2.35847845	3.37676041	-0.77348527
H	1.06500627	4.52039558	-1.10651886
C	1.62221011	4.41169784	0.97321376
C	-4.42168894	0.91536521	0.29957444
C	-4.19885603	2.42217372	0.24043520
H	-4.78502232	2.96684950	0.98445037
H	-3.49098273	0.12268391	-1.49372062
H	-2.05386343	1.75815786	-1.31847595
C	-2.70758436	2.67532000	0.47247162
H	-2.43205230	2.40944625	1.49677772
H	-4.47469191	2.82155921	-0.74258390
C	-2.09687309	3.90661076	0.02341914
H	-1.72854824	4.56066511	0.80973301
H	-0.58114835	3.19292557	-0.31725969
H	-2.64112231	4.44263819	-0.75532809
C	1.22074303	-4.51667674	1.40407983
H	0.94003644	-3.99335386	2.31143488
C	1.39065444	-4.64995057	-0.97333374
H	1.24598790	-4.23271496	-1.96398668
C	1.78021643	-5.78756312	1.52163559
H	1.92771746	-6.22260081	2.50501475
C	1.95119497	-5.92140938	-0.86868839
H	2.23347935	-6.46178889	-1.76665831
C	2.14814794	-6.49930779	0.38283046
H	2.58176421	-7.48980075	0.46931900
C	2.59357227	5.60785107	0.93950717
H	3.55203969	5.30535460	0.50147480
H	2.80486343	5.90260954	1.97586583
C	2.05535619	6.80413953	0.20428076
H	1.08800587	7.16842142	0.54935779

C	2.65600607	7.43448885	-0.80098481
H	3.61846072	7.10747607	-1.18368071
H	2.20973977	8.30058492	-1.27686458
H	-5.36781014	0.59408312	-0.14304660
H	-4.42945869	0.58005474	1.34204864
H	0.65345714	4.73735447	1.36537834
H	2.00170409	3.65696451	1.67050098
H	-2.80713346	-2.49253151	-2.95069720
H	-1.48391564	-2.88543290	-4.07530262
H	-0.59199767	-0.64760740	-3.90671772
H	-3.14930351	-2.19119380	2.62126454
H	-1.92918691	-2.34577302	3.90749709
H	-2.52582822	0.12573968	2.42798154

MP2 Electronic Energy(Ha): 1489.088912961907

B3LYP Electronic Energy(Ha): 1492.926886030672

M06-L Electronic Energy(Ha): 1492.743086320292

Zero point energy correction(kcal/mol): 376.139

Enthalpy correction(kcal/mol): 398.565

Entropy correction(cal/mol): 220.323

Imaginary Frequencies: -497.86

Deuterated zero point energy correction(kcal/mol): 371.651

Deuterated enthalpy correction(kcal/mol): 394.354

Deuterated entropy correction(cal/mol): 223.303

Deuterated imaginary Frequencies: -486.56

Product geometry

Zr	-0.01746288	1.13717892	0.07705913
C	0.42653696	-1.13092332	1.17673734
C	1.53916642	-0.26605674	1.44597202
H	2.53888216	-0.39840529	1.05470455
C	-0.66120175	-0.58752768	1.91068077
H	-1.66309902	-0.99407232	1.91616538
C	-0.24208802	0.59225089	2.58904603

H	-0.84110472	1.20014408	3.25394941
C	1.13612052	0.78240943	2.31192504
H	1.76423041	1.56834134	2.70462727
B	0.41037794	-2.33758042	0.07689045
C	1.61819893	-3.42046005	0.28464191
C	-1.05782954	-3.06143552	0.07820202
C	0.49376840	-1.59965541	-1.39164948
N	0.41295889	-0.30554695	-1.60123055
N	-2.15690185	-2.56109462	-0.36201174
O	-1.13787356	-4.31192575	0.62369077
O	0.63530207	-2.31748929	-2.51083384
C	0.60150776	-0.02887749	-3.04339615
C	0.56922437	-1.43292906	-3.66379585
C	-3.22914197	-3.55034615	-0.13798457
C	-2.51581102	-4.74268324	0.53551305
N	0.73249584	2.75859562	-0.46915732
N	-2.33260194	1.71586150	-0.22032406
C	-3.10523283	0.70274735	-1.03539323
H	-2.70592792	-0.29978274	-0.86114054
H	-0.19012484	0.61738859	-3.42563863
H	-4.01474742	-3.12305592	0.49462649
C	1.44963703	3.97700391	-0.71119832
H	2.01953894	3.90414815	-1.65221422
H	0.74877141	4.81374552	-0.85222796
C	2.43027048	4.34111605	0.41585779
C	-4.58326068	0.80151237	-0.57641688
C	-4.62846468	2.02614556	0.35080310
H	-5.39395936	1.94721547	1.12537614
H	-2.97727168	0.94421034	-2.09214542
H	-2.23704833	2.56130576	-0.78148444
C	-3.21310919	2.08912134	0.93887468
H	-3.10019161	1.29625645	1.68415620
H	-4.82559821	2.94245456	-0.21768778

C	-2.81535076	3.42665118	1.54602113
H	-3.47433955	3.66733545	2.38344544
H	-1.78776946	3.41458719	1.91479217
H	-2.90142991	4.23217100	0.80949374
C	2.31586519	-3.49978042	1.50066161
H	2.07086610	-2.80800814	2.29885837
C	1.97365702	-4.36188273	-0.69796329
H	1.45766212	-4.35845344	-1.65051411
C	3.31251753	-4.44971465	1.72551096
H	3.82413005	-4.47717756	2.68270298
C	2.97056309	-5.31209294	-0.48678281
H	3.21460482	-6.02018040	-1.27292654
C	3.64981761	-5.36042158	0.72879691
H	4.42657568	-6.09915970	0.89682586
C	3.21782796	5.64133416	0.16103636
H	3.75562993	5.57155986	-0.79134860
H	3.98173265	5.73705347	0.94360388
C	2.36661264	6.88052037	0.17096126
H	1.79103373	7.04609541	1.08194397
C	2.27178144	7.76795562	-0.81546722
H	2.82470310	7.64751465	-1.74250581
H	1.64376278	8.64812679	-0.73246722
H	-5.26950460	0.89130031	-1.41992410
H	-4.85742563	-0.10289172	-0.02908449
H	1.87124439	4.42447461	1.35541718
H	3.13319592	3.51177925	0.54470421
H	-0.36043853	-1.65210792	-4.19232805
H	1.41817955	-1.65943526	-4.30727927
H	1.55488148	0.48321167	-3.19416781
H	-2.54789516	-5.66215420	-0.05275208
H	-2.87227820	-4.95496225	1.54572155
H	-3.69342753	-3.82310346	-1.09104966

MP2 Electronic Energy(Ha): 1489.159037850055

B3LYP Electronic Energy(Ha): 1493.002351865337

M06-L Electronic Energy(Ha): 1492.803674655920

Zero point energy correction(kcal/mol): 378.518

Enthalpy correction(kcal/mol): 401.977

Entropy correction(cal/mol): 240.504

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.690

Deuterated enthalpy correction(kcal/mol): 397.397

Deuterated entropy correction(cal/mol): 243.743

Deuterated imaginary Frequencies: -0.00

Axial Reaction C4

Reactant geometry

Zr	0.10918428	-0.24927929	0.61894987
C	-0.19389401	2.13330379	1.30145773
C	-1.48989834	1.57914162	1.54980074
H	-2.37084739	1.75605641	0.95029275
C	0.63573187	1.64131510	2.35261220
H	1.68909290	1.85095721	2.46936264
C	-0.11365013	0.78495604	3.18546559
H	0.24172139	0.27256143	4.06654673
C	-1.43846876	0.75405549	2.69057328
H	-2.26927282	0.22296880	3.13664857
B	0.27776482	2.96536998	-0.02098734
C	0.27426636	4.57691387	0.09470543
C	1.72144594	2.28927110	-0.41402440
C	-0.65522451	2.35100819	-1.22625248
N	-0.94958732	1.09184516	-1.27035699
N	1.91880404	1.02232341	-0.23654509
O	2.72933608	2.94907736	-1.01269209
O	-1.11184561	3.09593826	-2.25255079
C	-1.72671012	0.82738358	-2.49469882

C	-1.86984519	2.22399418	-3.13538832
C	3.22526731	0.64597161	-0.79642218
C	3.81776973	2.00315459	-1.22728321
N	1.42138111	-1.55907742	1.60654415
H	-1.19791441	0.12274655	-3.14418585
C	2.18709881	-1.69550076	2.83776098
H	3.13884096	-1.14276089	2.76737339
H	1.63307847	-1.22966699	3.65580535
C	2.53776308	-3.13657221	3.24324386
C	1.36888002	-4.03584944	3.68972922
H	1.80323194	-4.87791613	4.24641884
H	0.73142166	-3.50044576	4.40228734
C	0.52777112	-4.63142273	2.59514669
H	1.07796478	-5.00906905	1.73392378
C	-0.79204372	-4.80828306	2.63372768
C	-0.15325803	5.22128827	1.26513242
H	-0.48278608	4.62016254	2.10668252
C	0.69201130	5.40351877	-0.96306138
H	1.03271006	4.95208867	-1.88862236
C	0.68363306	6.79216230	-0.85943556
H	1.01384093	7.39882280	-1.69709777
C	-0.16677609	6.61189028	1.38079062
H	-0.50455013	7.07453341	2.30304518
C	0.25255667	7.40493023	0.31658468
H	0.24486506	8.48677430	0.40064086
H	3.08593338	-0.04520585	-1.63193776
H	3.83340035	0.14053339	-0.04265420
H	4.10082454	2.05363997	-2.27875818
H	4.65978901	2.32417917	-0.61154203
H	-2.69347589	0.38092777	-2.24821066
H	-1.43759923	2.29999324	-4.13390549
H	-2.89831265	2.58767445	-3.16112965
H	3.07934809	-3.62521393	2.42190282

H	3.25059886	-3.07471549	4.07377806
H	1.84470048	-2.15608378	0.89852394
H	-1.31860138	-5.32474537	1.83853809
N	0.34581821	-1.51965298	-1.08917168
H	0.29149583	-1.03056883	-1.97645854
C	0.60896218	-2.92723189	-1.32817870
H	0.71107293	-3.44201526	-0.36429755
H	-0.24137973	-3.42226209	-1.83408046
C	1.86924191	-3.20753145	-2.16655252
H	2.74210698	-2.79211939	-1.64945274
H	1.79064643	-2.67000124	-3.11934267
C	2.09022019	-4.70422730	-2.45192060
H	1.21874616	-5.11351348	-2.97489647
H	2.15968988	-5.23786671	-1.49377810
C	3.33043486	-4.97473093	-3.25562006
H	4.26901615	-4.66521646	-2.79674420
C	3.36035414	-5.53497550	-4.46135355
H	2.45127085	-5.85927299	-4.95963928
H	4.29141111	-5.69325575	-4.99391366
N	-1.76169873	-1.82127179	0.99324060
C	-2.86511643	-1.85733787	0.00764110
H	-3.34918540	-0.87799488	0.01582788
H	-2.40398550	-1.97723730	-0.97500667
C	-3.89694807	-2.96094678	0.25581182
H	-3.38957684	-3.93196597	0.27073714
H	-4.34536603	-2.82893175	1.24878262
C	-5.01284977	-2.99902583	-0.80741019
H	-5.63532955	-3.88132792	-0.61389494
H	-4.57297453	-3.13982577	-1.80082575
C	-5.89079417	-1.77774675	-0.80943326
H	-6.38104220	-1.54752870	0.13628062
C	-6.11412808	-0.98843847	-1.85663048
H	-5.65446315	-1.18117154	-2.82168583

H	-6.77300120	-0.13001860	-1.79215723
H	-1.38801533	-4.46933496	3.47634022
H	-1.28203080	-2.72050149	1.02058819
H	-2.13906809	-1.68846191	1.92768848

MP2 Electronic Energy(Ha): 1740.467158231413

B3LYP Electronic Energy(Ha): 1744.981065187540

M06-L Electronic Energy(Ha): 1744.750886656348

Zero point energy correction(kcal/mol): 474.915

Enthalpy correction(kcal/mol): 504.231

Entropy correction(cal/mol): 271.180

Imaginary Frequencies: -0.00

Transition State geometry

Zr	0.64369903	-0.47579197	0.71432125
C	-0.22925142	2.02387409	0.96879709
C	-1.43782566	2.04271813	1.72902168
H	-2.42897354	2.14488121	1.30010963
C	0.82353699	1.90560036	1.94113564
H	1.87575171	2.06350986	1.74221886
C	0.24985835	1.85440480	3.23523881
H	0.79079636	1.77858635	4.16980995
C	-1.14896371	1.95134483	3.10130041
H	-1.86880894	1.94855704	3.91052584
B	-0.17683237	2.45547998	-0.60101778
C	-0.51622203	4.00319348	-0.94097538
C	1.27840186	2.00180070	-1.17382754
C	-1.09079104	1.31703275	-1.35409482
N	-0.99905013	0.06327286	-1.02394869
N	1.79755752	0.86138429	-0.84078986
O	1.96762352	2.69547518	-2.09297086
O	-1.87596893	1.57401211	-2.41691345
C	-1.71406465	-0.73673365	-2.04081983
C	-2.50662106	0.32652315	-2.81495316

C	2.96158041	0.59963286	-1.70932813
C	3.20347238	1.97076160	-2.35532930
N	2.83441821	-0.93336922	1.06977293
H	-0.99100998	-1.26038625	-2.67462937
C	3.94973932	-0.06601518	1.42978994
H	4.78716337	-0.15552799	0.72554855
H	3.62189407	0.97616703	1.39374267
C	4.43541711	-0.39989963	2.85516421
C	3.19372826	-0.68414841	3.69880442
H	3.47123356	-1.13098721	4.66126916
H	2.64856625	0.23702143	3.91936897
C	2.27840109	-1.65204267	2.99687803
H	2.73836506	-2.60428722	2.74672680
C	0.89576518	-1.63681057	3.13180281
C	-0.60338792	4.96668856	0.07523426
H	-0.50929967	4.64912394	1.10827104
C	-0.65029313	4.46857588	-2.26128453
H	-0.59010765	3.76413402	-3.08401033
C	-0.85221855	5.81573156	-2.55248437
H	-0.94590785	6.13771885	-3.58531521
C	-0.80304739	6.31923532	-0.20412708
H	-0.85837995	7.03589670	0.60952528
C	-0.92598535	6.75141536	-1.52180882
H	-1.07574775	7.80294602	-1.74458932
H	2.70042243	-0.16949085	-2.44465315
H	3.81597050	0.24340362	-1.13968585
H	3.35700554	1.94594623	-3.43319619
H	4.01811502	2.52602358	-1.88391246
H	-2.36705834	-1.48316161	-1.58459297
H	-2.43775028	0.24293874	-3.89890314
H	-3.55791064	0.37456367	-2.52069951
H	5.07286959	-1.29189639	2.82951710
H	5.03474488	0.41262863	3.27696303

H	3.16953273	-1.82608787	0.72847993
H	0.38046547	-2.58742376	3.03526852
N	0.54777400	-2.32151665	-0.26982511
H	-0.38676658	-2.45578767	-0.64964139
C	1.32826823	-3.50571037	-0.60409745
H	2.39456468	-3.29387233	-0.46403101
H	1.09186492	-4.34204621	0.07383703
C	1.09251997	-3.97351823	-2.04939580
H	1.45356160	-3.20424277	-2.74146663
H	0.01138130	-4.05631365	-2.21557869
C	1.73343087	-5.33298700	-2.38358482
H	1.39858886	-6.08174475	-1.65746726
H	2.82346622	-5.25506080	-2.27909369
C	1.39209684	-5.79766087	-3.77248918
H	1.79532162	-5.20012943	-4.58923282
C	0.62100681	-6.84239469	-4.06046359
H	0.19371008	-7.46501554	-3.27946697
H	0.38787205	-7.11591761	-5.08338527
N	-1.55938967	-1.01563470	1.78125066
C	-2.76708104	-1.70231345	1.27947206
H	-3.24464130	-1.06214851	0.53649759
H	-2.45848561	-2.62218642	0.77109707
C	-3.74208993	-2.04388811	2.41411335
H	-3.19109426	-2.58346090	3.19399132
H	-4.09516130	-1.11437009	2.87625749
C	-4.94645100	-2.90377078	1.99151873
H	-5.49784249	-3.17261510	2.90153620
H	-4.59692283	-3.84484862	1.55218713
C	-5.88965195	-2.21913184	1.04228549
H	-6.27456454	-1.25473144	1.37278015
C	-6.29083839	-2.70722132	-0.12806348
H	-5.94048924	-3.66909731	-0.49131300
H	-6.99502634	-2.17408242	-0.75642074

H 0.44319639 -0.88256443 3.76554467

H -1.24074886 -1.51438728 2.60419162

H -1.80456863 -0.07646980 2.11153523

MP2 Electronic Energy(Ha): 1740.403960163998

B3LYP Electronic Energy(Ha): 1744.910324516896

M06-L Electronic Energy(Ha): 1744.686179357604

Zero point energy correction(kcal/mol): 474.681

Enthalpy correction(kcal/mol): 502.568

Entropy correction(cal/mol): 255.585

Imaginary Frequencies: -335.88 -21.17

Product geometry

Zr 0.72218958 0.51494496 0.04387555

C 1.55592696 -1.78185681 -0.49224544

C 2.12814714 -1.02108539 -1.55513765

H 1.79712824 -1.03770049 -2.58359084

C 2.29854678 -1.42276172 0.67095932

H 2.14006750 -1.82585605 1.65964812

C 3.27275492 -0.45368253 0.33302103

H 3.99003748 -0.00114971 0.99945685

C 3.16783300 -0.21142469 -1.05146563

H 3.77555480 0.48236472 -1.61578561

B 0.18910092 -2.66338401 -0.55643981

C 0.34918522 -4.21752189 -0.97003613

C -0.53320018 -2.40376460 0.89430013

C -0.79289389 -1.77247836 -1.52550709

N -0.75186292 -0.47899322 -1.48099385

N -0.53123020 -1.24822175 1.48546969

O -1.23620910 -3.37588672 1.51164581

O -1.72157495 -2.28709918 -2.34892576

C -1.77640472 0.08061426 -2.37567205

C -2.41102602 -1.17921920 -3.00063086

C -1.42412745 -1.34374671 2.66230468

C	-1.67669354	-2.85253244	2.79139294
N	1.42712712	1.49689745	2.37857801
H	-2.48972927	0.67721412	-1.80340443
C	1.62177134	0.57030346	3.52669243
H	1.07073136	0.93669279	4.40271541
H	1.25073136	-0.42207050	3.27984660
C	3.13871583	0.59523537	3.80743977
C	3.63818160	1.91512768	3.16964609
H	4.18785466	2.54234592	3.87413185
H	4.30264654	1.71792434	2.32559250
C	2.36769127	2.62659929	2.67904358
H	1.94495356	3.18248025	3.53043960
C	2.57180037	3.59670600	1.52723646
C	1.61589529	-4.78635027	-1.17053065
H	2.49715100	-4.16414842	-1.05074410
C	-0.75726824	-5.06759045	-1.14203071
H	-1.75813585	-4.67431423	-1.00050135
C	-0.60887458	-6.40696264	-1.49316084
H	-1.48667565	-7.03345670	-1.61834199
C	1.77751275	-6.12733395	-1.52101435
H	2.77441265	-6.53156229	-1.66742844
C	0.66318300	-6.94511689	-1.68429930
H	0.78219659	-7.98838164	-1.95800038
H	-2.34818964	-0.79182996	2.47175859
H	-0.96031494	-0.92002624	3.55527531
H	-2.72213034	-3.12519485	2.93037897
H	-1.07261614	-3.32409873	3.57111071
H	-1.31216456	0.73203127	-3.12006025
H	-3.47678012	-1.28523985	-2.79609058
H	-2.23934363	-1.26940377	-4.07398332
H	3.33315112	0.55471748	4.88061187
H	3.63175668	-0.26826289	3.35944292
H	0.48176537	1.87532356	2.37562031

H	1.63600050	4.08737056	1.25103499
N	-0.90678365	1.80364512	0.60414316
H	-1.07944305	2.47396305	-0.13824905
C	-1.98533652	1.91939055	1.57231881
H	-1.74717147	1.32094545	2.45968072
H	-2.07654461	2.95751644	1.93694138
C	-3.37090218	1.48951740	1.05662072
H	-3.31962140	0.44518124	0.72859362
H	-3.61758971	2.08227135	0.16798483
C	-4.48749102	1.66533494	2.10183580
H	-4.53641709	2.71353002	2.41694616
H	-4.22740832	1.08315904	2.99726375
C	-5.83577951	1.22601414	1.60554476
H	-5.91854802	0.17624975	1.32535010
C	-6.90102435	2.01102117	1.47285799
H	-6.86711223	3.06375706	1.73819219
H	-7.84535599	1.63250840	1.09808353
N	1.21027481	2.05658520	-1.30594717
C	0.63734516	3.33915409	-1.70616182
H	-0.18147221	3.20719196	-2.43029974
H	0.19494674	3.82767314	-0.83034424
C	1.67231124	4.29240300	-2.31727223
H	2.48339864	4.44477282	-1.59804455
H	2.12294815	3.81561763	-3.19809322
C	1.09286281	5.66121088	-2.72482081
H	1.92624642	6.30485971	-3.03424959
H	0.63309830	6.14446997	-1.85538897
C	0.09751241	5.59230439	-3.84994925
H	0.45613978	5.12283352	-4.76601433
C	-1.14748140	6.05945828	-3.81463571
H	-1.55018971	6.53702123	-2.92616920
H	-1.80724600	5.98828705	-4.67209496
H	3.28485431	4.37156171	1.82357810

H 2.95257956 3.08262948 0.64384865

H 1.93431635 1.81005228 -1.96984471

MP2 Electronic Energy(Ha): 1740.488060189588

B3LYP Electronic Energy(Ha): 1744.985856514812

M06-L Electronic Energy(Ha): 1744.766770341267

Zero point energy correction(kcal/mol): 477.012

Enthalpy correction(kcal/mol): 505.470

Entropy correction(cal/mol): 261.688

Imaginary Frequencies: -0.00

Axial Reaction H1

Reactant geometry

Zr -0.39326573 -0.49002124 -0.20099370

C -0.45104779 1.52397069 1.30194766

C -1.76812123 0.95616871 1.34128279

H -2.64923000 1.38037398 0.88165869

C 0.36256259 0.63050254 2.04886011

H 1.42713016 0.74430794 2.20690129

C -0.40669796 -0.48595519 2.46917528

H -0.06340147 -1.31600396 3.07290055

C -1.74029400 -0.27489676 2.03668855

H -2.58538300 -0.91689890 2.23718495

B 0.07614558 2.66494059 0.24622000

C 0.19736580 4.17536964 0.80412866

C 1.47788212 2.06079692 -0.40504102

C -0.90259842 2.47767202 -1.06945767

N -1.18843893 1.29204183 -1.50637102

N 1.61623348 0.82327920 -0.77705619

O 2.52767513 2.85959262 -0.66880930

O -1.42243091 3.49074916 -1.77941786

C -2.05741382 1.39502265 -2.68876637

C -2.17764073 2.92073693 -2.89188906

C	2.92472055	0.66560817	-1.43814303
C	3.56680354	2.06047867	-1.29560439
N	1.41937607	-2.05602239	0.28599157
N	-1.30933920	-1.81942480	-1.16312943
C	-2.08958580	-2.79881447	-1.85834369
H	-3.00088616	-2.34092614	-2.28128590
H	-1.60329202	0.88698387	-3.54234436
H	3.52199844	-0.11271240	-0.95346090
H	1.01251498	-2.64877718	1.00573066
C	1.91110134	-2.90341212	-0.82994966
H	1.03720791	-3.41556187	-1.23558582
H	2.27160160	-2.23435348	-1.61422254
H	2.19643537	-1.56909721	0.72872252
C	-2.52163218	-4.00641728	-1.00207495
H	-1.52996124	-3.19223789	-2.72386216
C	3.01410643	-3.89821190	-0.45253081
C	2.56990482	-4.99665278	0.53100851
H	2.22266945	-4.53444206	1.46507216
H	1.71602896	-5.53962250	0.11213997
C	3.67469101	-5.96264268	0.85796760
H	4.55533879	-5.53329343	1.33424187
C	3.65163407	-7.26667780	0.60159613
H	2.79514094	-7.73880807	0.12963031
H	4.48448890	-7.91124459	0.85824206
C	0.56630839	5.25445178	-0.01790840
H	0.77702281	5.07783957	-1.06740788
C	-0.06688705	4.47167607	2.14952666
H	-0.35972730	3.66753777	2.81704469
C	0.03212968	5.76886603	2.65404742
H	-0.18101389	5.95927746	3.70128640
C	0.66771738	6.55329943	0.47332727
H	0.95399845	7.36236661	-0.19154566
C	0.40100063	6.81723273	1.81628766

H	0.47842065	7.82830450	2.20238689
C	-3.49317834	-3.64587700	0.13277005
H	-4.39093084	-3.19526214	-0.31342672
H	-3.03854135	-2.88133930	0.76708237
C	-3.89651504	-4.83214049	0.96112858
H	-4.39119035	-5.64151148	0.42383282
C	-3.68793851	-4.96887244	2.26804842
H	-4.00028643	-5.85663153	2.80695233
H	-3.20190616	-4.19027608	2.84909977
H	3.37016466	-4.37329888	-1.37283913
H	3.87364033	-3.35559318	-0.03721365
H	-1.62786852	-4.47691285	-0.57544396
H	-2.98891575	-4.75256589	-1.65853829
H	3.82287291	2.52880527	-2.24616007
H	4.43975716	2.07510180	-0.64108809
H	2.78708412	0.37210031	-2.48348899
H	-1.72104091	3.27781672	-3.81606684
H	-3.19815734	3.29790050	-2.82522850
H	-3.01892127	0.91525780	-2.49097382

MP2 Electronic Energy(Ha): 1489.143888562985

B3LYP Electronic Energy(Ha): 1492.993383580229

M06-L Electronic Energy(Ha): 1492.795501430708

Zero point energy correction(kcal/mol): 377.470

Enthalpy correction(kcal/mol): 401.190

Entropy correction(cal/mol): 229.337

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.682

Deuterated enthalpy correction(kcal/mol): 396.687

Deuterated entropy correction(cal/mol): 232.130

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.14710685	0.46940565	0.15942901

C	0.75266998	-1.71508169	1.16369765
C	1.98854663	-1.02151292	0.94634882
H	2.71968142	-1.26495401	0.18897569
C	0.13782291	-1.04658461	2.26053662
H	-0.83123619	-1.28761581	2.67448834
C	0.91663675	0.07021587	2.64181594
H	0.69279619	0.76704018	3.43722606
C	2.08153976	0.08130498	1.82667690
H	2.90412634	0.77753502	1.89873099
B	0.00213254	-2.72572303	0.10835211
C	0.13411032	-4.30812164	0.38737683
C	-1.55226801	-2.15557252	0.02596759
C	0.52707833	-2.22230516	-1.37269258
N	0.63093774	-0.95467016	-1.63154135
N	-1.82785236	-0.88517613	-0.02970205
O	-2.60865092	-2.97474932	-0.05992355
O	0.80331116	-3.03775796	-2.39726253
C	1.02218258	-0.76515863	-3.03804780
C	1.19675687	-2.21477895	-3.53893118
C	-3.28486549	-0.71300224	-0.18829284
C	-3.81235887	-2.16182783	-0.17618734
N	-1.15092976	2.26671460	0.95880283
N	0.64768581	2.07527574	-0.84723737
C	1.26368958	3.03530532	-1.72825242
H	1.87481935	2.51810886	-2.48495061
H	0.24312649	-0.22033605	-3.57699596
H	-3.69077787	-0.11411204	0.62824863
H	-0.26103103	2.53961568	-0.01314429
C	-2.56058509	2.58789764	0.75281291
H	-2.82559526	2.30776551	-0.27465261
H	-3.21248639	1.99385446	1.41151262
H	-0.85374146	2.58866520	1.87679761
C	2.15388387	4.07954060	-1.02707453

H	0.49081708	3.58228312	-2.29007374
C	-2.90689773	4.07152091	0.96404112
C	-2.22078842	5.02549052	-0.02787391
H	-1.13759487	4.86742863	0.03058672
H	-2.52228638	4.77129655	-1.05047163
C	-2.52514855	6.47060315	0.24530231
H	-2.22124038	6.84008196	1.22447567
C	-3.12930255	7.30616389	-0.59466126
H	-3.45136140	6.98586712	-1.58134273
H	-3.31986709	8.34047721	-0.33120196
C	-0.43136470	-5.27035422	-0.46715516
H	-0.97858392	-4.94799028	-1.34673335
C	0.83102111	-4.78960949	1.50536467
H	1.28489792	-4.07983534	2.18968568
C	0.95981805	-6.15469338	1.76344158
H	1.50689509	-6.49004926	2.63882844
C	-0.30891123	-6.63514295	-0.22053047
H	-0.75763443	-7.35043046	-0.90263753
C	0.38913557	-7.08474964	0.89961483
H	0.48671859	-8.14755017	1.09448711
C	3.40322365	3.48401123	-0.35825701
H	3.98093199	2.94562967	-1.12298742
H	3.09918356	2.74446803	0.38640081
C	4.27929451	4.52455873	0.27950599
H	4.68182399	5.28306785	-0.39172233
C	4.57865507	4.59318600	1.57365006
H	5.21264026	5.37723745	1.97251054
H	4.20062247	3.86282539	2.28331831
H	-3.99376622	4.19521862	0.88897591
H	-2.63647182	4.35421159	1.99013209
H	1.56136105	4.61390757	-0.27627421
H	2.46074592	4.82489809	-1.77205971
H	-4.32313910	-2.45556703	-1.09341059

H -4.44843320 -2.38958578 0.67975824

H -3.50534775 -0.19353212 -1.12476415

H 0.54740535 -2.47783288 -4.37367848

H 2.22713033 -2.47122489 -3.78727136

H 1.94231327 -0.18124616 -3.10363750

MP2 Electronic Energy(Ha): 1489.107470177655

B3LYP Electronic Energy(Ha): 1492.961045151109

M06-L Electronic Energy(Ha): 1492.759559808025

Zero point energy correction(kcal/mol): 373.636

Enthalpy correction(kcal/mol): 397.221

Entropy correction(cal/mol): 231.217

Imaginary Frequencies: -1636.29

Deuterated zero point energy correction(kcal/mol): 370.028

Deuterated enthalpy correction(kcal/mol): 393.845

Deuterated entropy correction(cal/mol): 233.367

Deuterated imaginary Frequencies: -1175.24

Product geometry

Zr 0.23794408 -0.53399353 0.03211842

C -0.38260563 1.49064894 1.30357735

C -1.53091718 0.63763884 1.35868122

H -2.45150757 0.79579173 0.81640539

C 0.58200483 0.87730263 2.15987011

H 1.58080572 1.24921234 2.34222589

C 0.07644941 -0.34638269 2.64776634

H 0.58614685 -1.04051629 3.30086226

C -1.24582172 -0.49892187 2.14916297

H -1.91717351 -1.31716813 2.36483308

B -0.08969856 2.66860998 0.20349545

C -0.36058115 4.18906675 0.66701433

C 1.45144374 2.34823960 -0.30969060

C -0.87732845 2.18916509 -1.15661987

N -0.94792375 0.93957327 -1.50010427

N	1.80778839	1.14232556	-0.63691187
O	2.41397801	3.27626762	-0.40975565
O	-1.33125452	3.06555135	-2.06820296
C	-1.43262261	0.86191067	-2.89270102
C	-1.88703282	2.30305477	-3.17770278
C	3.24367559	1.13618175	-0.96780127
C	3.59950442	2.63517015	-0.96713310
N	1.89239113	-1.74241126	0.50620476
N	-0.66393665	-2.08658630	-1.05499410
C	-1.91867960	-2.35545590	-1.74964786
H	-2.58904290	-1.50138594	-1.60592808
H	-0.61657489	0.53944323	-3.54794749
H	3.79405347	0.56897175	-0.21215293
H	-0.14629847	-2.95697442	-0.95575578
C	2.78181181	-2.51104987	-0.36017432
H	2.33653505	-2.57002725	-1.36130001
H	3.75053822	-2.00263266	-0.48996372
H	2.27159596	-1.72125655	1.44735029
C	-2.64296236	-3.62952301	-1.28523404
H	-1.75602362	-2.44279616	-2.83588560
C	3.06926411	-3.93643492	0.14491059
C	1.83059590	-4.84615382	0.19010466
H	1.05080065	-4.33120239	0.76377940
H	1.44340266	-4.98789807	-0.82568015
C	2.10722601	-6.18502255	0.81146805
H	2.45262860	-6.16297897	1.84481722
C	1.97443531	-7.36129941	0.20532068
H	1.63478455	-7.43526287	-0.82370616
H	2.19444749	-8.29290709	0.71434467
C	-0.09619586	5.28656096	-0.17067337
H	0.30567404	5.11517662	-1.16363587
C	-0.88105144	4.47731921	1.93728975
H	-1.09752994	3.65904200	2.61678061

C	-1.12797028	5.78550255	2.35498016
H	-1.53150542	5.96963973	3.34565451
C	-0.33792780	6.59634286	0.23499912
H	-0.12164442	7.41977091	-0.43847250
C	-0.85672642	6.85253356	1.50361660
H	-1.04611664	7.87201118	1.82288870
C	-3.09359734	-3.60258813	0.18528692
H	-3.72341848	-2.71506687	0.33773471
H	-2.22173143	-3.48552519	0.83368028
C	-3.86422148	-4.83024170	0.58141099
H	-4.79972142	-4.99735698	0.04791370
C	-3.48549571	-5.71193177	1.50207422
H	-4.08388395	-6.58540869	1.73583519
H	-2.55947443	-5.59134205	2.05662703
H	3.83220970	-4.39383820	-0.49571845
H	3.51012921	-3.86993805	1.14834365
H	-1.98948203	-4.49630597	-1.44411174
H	-3.51652803	-3.78378977	-1.93134891
H	3.75328865	3.04315508	-1.96802424
H	4.44778875	2.89628187	-0.33574257
H	3.42029729	0.66375933	-1.93645355
H	-1.49916090	2.72618583	-4.10340058
H	-2.97219484	2.42335075	-3.15013983
H	-2.24344579	0.14182090	-2.99355019

MP2 Electronic Energy(Ha): 1489.156024774353

B3LYP Electronic Energy(Ha): 1493.012099300995

M06-L Electronic Energy(Ha): 1492.816952580175

Zero point energy correction(kcal/mol): 376.796

Enthalpy correction(kcal/mol): 400.447

Entropy correction(cal/mol): 228.863

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.240

Deuterated enthalpy correction(kcal/mol): 396.237

Deuterated entropy correction(cal/mol): 232.250

Deuterated imaginary Frequencies: -0.00

Axial Reaction H2

Reactant geometry

Zr	-0.34276932	0.70278942	0.03299735
C	0.68772789	-1.21983612	1.19019208
C	1.75495780	-0.27662953	1.12366338
H	2.61794014	-0.35825636	0.47762304
C	-0.21040950	-0.70068441	2.17765946
H	-1.13862744	-1.16094013	2.48262795
C	0.26755127	0.53566081	2.65632854
H	-0.20914853	1.16691662	3.39180844
C	1.48951954	0.80559315	1.99806586
H	2.12167990	1.66432475	2.17200865
B	0.37799544	-2.44266989	0.15220075
C	0.91587043	-3.90705993	0.56956013
C	-1.24830714	-2.32469089	-0.08893671
C	0.87102921	-1.90993299	-1.32776858
N	0.79370159	-0.66233306	-1.67727548
N	-1.81363993	-1.16230032	-0.18719489
O	-2.06230566	-3.37896383	-0.25532212
O	1.21036076	-2.76339545	-2.31258702
C	1.02300374	-0.56417397	-3.13155322
C	1.49344227	-1.98122581	-3.50584460
C	-3.24690723	-1.34166781	-0.47440970
C	-3.41499430	-2.87508310	-0.46018045
N	1.29755907	2.23434670	-0.98035528
N	-1.66400548	2.16153641	0.67415566
C	-2.40905534	2.84576240	1.71092705
H	-1.97908351	3.84275110	1.90612424
H	0.09200947	-0.27725655	-3.62934620

H	-3.85269739	-0.84438147	0.28656111
C	1.99466993	3.39941888	-0.37289629
H	2.56886181	3.03188027	0.48011657
H	2.71052717	3.82467057	-1.08470034
C	1.01331815	4.47350033	0.08568914
C	-3.85783909	3.01094618	1.15019669
C	-3.74478264	2.65015967	-0.35363959
H	-4.26110415	3.36224290	-1.00291780
H	-2.37960122	2.29419360	2.65364215
C	-2.22530388	2.60898922	-0.62400495
H	-1.89353274	3.64632187	-0.81695016
H	-4.17013346	1.66125114	-0.54504692
C	-1.65819038	1.64755323	-1.68094652
H	-1.22816606	2.17646528	-2.54048321
H	0.76865092	2.54122694	-1.79458172
H	-2.43295273	0.98566766	-2.07756279
C	0.66162980	-5.05198505	-0.20585767
H	0.08226037	-4.95967804	-1.11776110
C	1.66927350	-4.09317667	1.73831053
H	1.88540218	-3.23579554	2.36781575
C	1.13300358	-6.30928709	0.16301632
H	0.91647385	-7.17163931	-0.45988478
C	2.14738644	-5.34791026	2.11780508
H	2.72675100	-5.45262478	3.02985276
C	1.88078988	-6.46364796	1.32969351
H	2.24911038	-7.44218114	1.61976297
C	1.70995766	5.67283952	0.75701123
H	2.29587885	5.32986600	1.61696238
H	0.92964911	6.33208526	1.15585472
C	2.58750703	6.46673891	-0.17159689
H	2.09072642	6.88042332	-1.04917028
C	3.88569491	6.69928555	0.00019229
H	4.42365498	6.31275984	0.86087604

H 4.45650464 7.29197154 -0.70571214

H 2.56709018 -2.04229540 -3.69657305

H 1.77407626 0.19434699 -3.37023185

H 0.95272295 -2.42974774 -4.33849992

H -3.78539862 -3.28920310 -1.39818493

H -4.03099051 -3.23967094 0.36295068

H -3.49728896 -0.89928150 -1.44111543

H -4.55526805 2.34726301 1.66646940

H -4.21763881 4.03209741 1.29849070

H 0.43395569 4.82775239 -0.77600301

H 0.29564305 4.02587027 0.77746731

H 1.98984970 1.57576465 -1.32928089

MP2 Electronic Energy(Ha): 1489.174788912467

B3LYP Electronic Energy(Ha): 1493.000966047560

M06-L Electronic Energy(Ha): 1492.819542723897

Zero point energy correction(kcal/mol): 378.911

Enthalpy correction(kcal/mol): 401.628

Entropy correction(cal/mol): 220.152

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.480

Deuterated enthalpy correction(kcal/mol): 397.375

Deuterated entropy correction(cal/mol): 221.263

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr 0.20075980 -0.71683126 0.08206413

C -0.63274762 1.27212712 1.24223272

C -1.74551411 0.37917746 1.27107422

H -2.64218954 0.48168999 0.67755483

C 0.32187991 0.71087244 2.15108801

H 1.29493625 1.12506224 2.37132312

C -0.16928200 -0.50882980 2.66479142

H 0.33695679 -1.16506137 3.35711998

C	-1.45689965	-0.71935811	2.11301761
H	-2.10323106	-1.56200720	2.31181684
B	-0.35551109	2.45602923	0.14509603
C	-0.79347775	3.95068169	0.56174563
C	1.23432300	2.25745152	-0.23363526
C	-1.00469167	1.89839890	-1.26378943
N	-0.92908866	0.64919310	-1.60175449
N	1.72091456	1.06902169	-0.41165467
O	2.09950320	3.26814679	-0.40553257
O	-1.52717859	2.71709060	-2.19391463
C	-1.40784600	0.49684891	-2.98892590
C	-1.93076252	1.90520992	-3.33315676
C	3.15545594	1.17492795	-0.73057970
C	3.38181823	2.69941829	-0.80176525
N	-1.21494615	-2.24101906	-0.85971243
N	1.70479528	-2.03220555	0.62472807
C	2.62416716	-2.46285818	1.66282123
H	2.30380432	-3.43017150	2.08235873
H	-0.58390077	0.17805938	-3.63408301
H	3.74952813	0.69495449	0.05120447
C	-1.87174424	-3.43137478	-0.30183961
H	-2.55014361	-3.14839172	0.51864600
H	-2.49952327	-3.89953805	-1.06889291
C	-0.88699947	-4.47271428	0.22843248
C	4.00545632	-2.63504030	0.95866841
C	3.67980914	-2.64352128	-0.55846211
H	4.14458535	-3.47975230	-1.08673737
H	2.65774645	-1.74791234	2.48759517
C	2.13733549	-2.71007993	-0.61594595
H	1.84888265	-3.77320242	-0.54868552
H	4.02446573	-1.72247964	-1.03495570
C	1.37095091	-2.07454037	-1.77996290
H	1.29739994	-2.74583222	-2.64235369

H	-0.05869555	-2.25886076	-1.47300027
H	1.87427919	-1.17080098	-2.14633925
C	-0.56750886	5.05703651	-0.27576915
H	-0.08167266	4.90899788	-1.23422838
C	-1.42616580	4.20737553	1.78707364
H	-1.61851101	3.38179849	2.46518626
C	-0.95092448	6.34487428	0.08716708
H	-0.76028494	7.17599242	-0.58460667
C	-1.81576732	5.49389643	2.16188872
H	-2.30320509	5.65340064	3.11846907
C	-1.57934499	6.56976434	1.31187612
H	-1.87939690	7.57248377	1.59768309
C	-1.58537059	-5.67442379	0.89362659
H	-2.21723378	-5.32746230	1.71891382
H	-0.81188352	-6.31181341	1.34014312
C	-2.40525738	-6.50509182	-0.05448782
H	-1.86703702	-6.90784182	-0.91273302
C	-3.69964483	-6.78200339	0.07817514
H	-4.27898426	-6.40487432	0.91595602
H	-4.22620432	-7.39962697	-0.64064101
H	-3.01833555	1.95715149	-3.40782132
H	-2.19229830	-0.26148717	-3.05744378
H	-1.48600431	2.33936089	-4.22820784
H	3.60492246	3.05924977	-1.80713027
H	4.13724295	3.06949917	-0.10928205
H	3.38023467	0.67302363	-1.67397173
H	4.67765028	-1.81218645	1.21358527
H	4.49516373	-3.55733139	1.27961761
H	-0.25744015	-4.82840536	-0.59492677
H	-0.21521994	-4.00057494	0.95164960
H	-1.86704294	-1.74818718	-1.45865084

MP2 Electronic Energy(Ha): 1489.146398439322

B3LYP Electronic Energy(Ha): 1492.970853162876

M06-L Electronic Energy(Ha): 1492.789799206470

Zero point energy correction(kcal/mol): 375.361

Enthalpy correction(kcal/mol): 397.915

Entropy correction(cal/mol): 221.585

Imaginary Frequencies: -1504.58

Deuterated zero point energy correction(kcal/mol): 371.964

Deuterated enthalpy correction(kcal/mol): 394.672

Deuterated entropy correction(cal/mol): 222.450

Deuterated imaginary Frequencies: -1097.43

Product geometry

Zr	0.04571067	0.71794579	-0.13333499
C	-0.53159148	-1.37160133	-1.30853385
C	-1.67499235	-0.53359089	-1.48914596
H	-2.62622121	-0.66100346	-0.99339589
C	0.48931347	-0.79874190	-2.12969552
H	1.49804750	-1.17513798	-2.22615957
C	0.00600753	0.38746831	-2.72723739
H	0.54545042	1.04049315	-3.39631986
C	-1.34450940	0.55511695	-2.32484742
H	-2.00165522	1.36026596	-2.62050190
B	-0.33022459	-2.49144520	-0.12794944
C	-0.62513359	-4.02677179	-0.52241483
C	1.18378929	-2.18445945	0.44691083
C	-1.19491419	-1.91359337	1.14914422
N	-1.20148373	-0.65150217	1.44656257
N	1.56366185	-0.96976760	0.69807711
O	2.09616574	-3.13750500	0.68913842
O	-1.84819678	-2.71243595	2.00833889
C	-1.92303162	-0.45887360	2.71789853
C	-2.43805053	-1.87535005	3.04391584
C	2.96504815	-0.98824011	1.15486791
C	3.28111730	-2.49482780	1.24410802

N	-1.31124369	2.14852156	0.63543935
N	1.70214034	2.00489485	-0.41224840
C	2.56629372	2.20376932	-1.58273846
H	2.27380793	3.12370481	-2.11656216
H	-1.24474189	-0.06863868	3.48218252
H	3.59866957	-0.46231248	0.43668091
C	-1.90174601	3.39871516	0.14549192
H	-2.58685455	3.20871128	-0.69973393
H	-2.52080142	3.84940220	0.93158790
C	-0.87050142	4.43275745	-0.30866261
C	4.00690342	2.36618088	-1.04175113
C	3.80574433	2.81314066	0.42299232
H	4.30109811	3.76072730	0.65022316
H	2.48341273	1.37987854	-2.28946237
C	2.27023478	2.92824697	0.59448977
H	1.98207417	3.95562047	0.31359922
H	4.20167508	2.06747569	1.11847986
C	1.81049656	2.69491829	2.03143981
H	2.29323451	3.41630419	2.69753922
H	0.72981668	2.80835636	2.12910197
H	2.09130104	1.69291029	2.37440027
C	-0.44916512	-5.08039014	0.39121265
H	-0.10178717	-4.86320836	1.39591374
C	-1.07574999	-4.37351681	-1.80460107
H	-1.22295750	-3.59066199	-2.54188167
C	-0.70853329	-6.40406949	0.04623219
H	-0.56111823	-7.19258881	0.77756883
C	-1.33954747	-5.69616290	-2.16213316
H	-1.68724484	-5.92623214	-3.16430874
C	-1.15667927	-6.71883042	-1.23608189
H	-1.35968741	-7.74924955	-1.50836604
C	-1.50667383	5.69713492	-0.91831349
H	-2.13513718	5.42406095	-1.77363806

H	-0.69997830	6.32792754	-1.31342668
C	-2.31213316	6.50675642	0.06014187
H	-1.77712619	6.83330198	0.95208699
C	-3.58967738	6.84870806	-0.08114594
H	-4.16547859	6.54706694	-0.95128368
H	-4.10595492	7.44520718	0.66280260
H	-3.52224846	-1.97156538	2.96982142
H	-2.73985200	0.25901097	2.60373736
H	-2.10717126	-2.25625762	4.00994890
H	3.40163810	-2.85375618	2.26766679
H	4.13895453	-2.80728521	0.64921026
H	3.06621683	-0.48423747	2.11851198
H	4.54602969	1.41672479	-1.09157637
H	4.57665241	3.09017526	-1.62912985
H	-0.24525217	4.71301217	0.54575303
H	-0.20090326	3.97748375	-1.04479628
H	-2.00239740	1.69484911	1.22298085

MP2 Electronic Energy(Ha): 1489.183690959185

B3LYP Electronic Energy(Ha): 1493.018767691602

M06-L Electronic Energy(Ha): 1492.836334755089

Zero point energy correction(kcal/mol): 378.207

Enthalpy correction(kcal/mol): 401.283

Entropy correction(cal/mol): 223.367

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.111

Deuterated enthalpy correction(kcal/mol): 397.384

Deuterated entropy correction(cal/mol): 224.690

Deuterated imaginary Frequencies: -0.00

Axial Reaction H3

Reactant geometry

Zr	0.54270384	0.80597287	-0.30413109

C	-0.10033904	-1.31587423	-1.40178857
C	-1.03164822	-0.35819600	-1.91266532
H	-2.07463840	-0.29712748	-1.63810744
C	1.14696520	-0.99508986	-2.02197283
H	2.08061774	-1.51310411	-1.85289772
C	1.00076852	0.16929063	-2.80683155
H	1.76772351	0.65740875	-3.38973453
C	-0.36195978	0.56804168	-2.73903122
H	-0.80202443	1.41124016	-3.25069266
B	-0.33343980	-2.30506658	-0.11807104
C	-0.78264428	-3.82169937	-0.43190555
C	1.05719307	-2.14409127	0.75928745
C	-1.33028086	-1.46093232	0.88342234
N	-1.21993198	-0.17464615	1.02019401
N	1.57016471	-0.97305635	0.98092590
O	1.71810267	-3.17670811	1.30323172
O	-2.19358032	-2.05552334	1.72300402
C	-2.03337059	0.25169551	2.17552194
C	-2.85468130	-1.00888677	2.49328167
C	2.78743733	-1.12344522	1.79754578
C	2.87238229	-2.64819761	2.02040752
N	-0.49389724	2.58749397	0.06833698
N	2.41028777	1.80612949	-0.24618798
C	3.63717486	1.49631611	-1.00020661
H	3.40781283	1.08381553	-1.98313387
H	-1.37588153	0.54261315	3.00165132
H	3.65412509	-0.72474723	1.26566814
C	-1.88136942	3.03509673	0.06726970
H	-2.53055699	2.16282726	-0.06486481
H	-2.15731014	3.48050670	1.03497820
C	-2.19547905	4.04847246	-1.04315322
C	4.41533648	2.81387019	-1.07423698
C	4.16211219	3.38902134	0.31991138

H	4.30240650	4.47051530	0.38509505
H	4.25437443	0.74472490	-0.47822747
C	2.70534920	2.97454242	0.63303153
H	2.04683323	3.80849661	0.34199404
H	4.84288867	2.92407193	1.04228674
C	2.47994367	2.71489015	2.12686414
H	2.72201206	3.60925218	2.71109920
H	1.43753259	2.45987992	2.33533888
H	3.11789881	1.89789284	2.47513277
C	-0.98760166	-4.25949920	-1.74870683
H	-0.83650247	-3.56143757	-2.56606424
C	-0.99059490	-4.76757332	0.58705908
H	-0.84620290	-4.47692493	1.62218955
C	-1.37911272	-5.56663514	-2.04025485
H	-1.52809617	-5.86903922	-3.07206465
C	-1.38107320	-6.07472614	0.30869240
H	-1.53245261	-6.77856995	1.12117693
C	-1.57785969	-6.48146793	-1.01040851
H	-1.88209172	-7.49935649	-1.23076663
C	-3.67045054	4.49461912	-1.08496109
H	-4.32006945	3.62229072	-1.21999053
H	-3.80987343	5.12545049	-1.97232038
C	-4.11024752	5.26902571	0.12664427
H	-3.51928971	6.15544592	0.35759688
C	-5.14412321	4.96787563	0.90753922
H	-5.76506470	4.09721100	0.71736434
H	-5.41294353	5.58239282	1.75944968
H	-3.88787681	-0.94679763	2.14464851
H	-2.65622941	1.11053618	1.92906519
H	-2.84290382	-1.30599751	3.54101349
H	2.77712979	-2.94584751	3.06524034
H	3.76487823	-3.10801967	1.59502698
H	2.68876299	-0.56955319	2.73431503

H 5.47521594 2.67390254 -1.30180876

H 3.98311135 3.46088384 -1.84427743

H -1.55383942 4.93021429 -0.91414799

H -1.92309907 3.60814343 -2.00756561

H 0.11916552 3.40096938 0.04703215

MP2 Electronic Energy(Ha): 1489.185493546703

B3LYP Electronic Energy(Ha): 1493.024257439461

M06-L Electronic Energy(Ha): 1492.837589787317

Zero point energy correction(kcal/mol): 378.064

Enthalpy correction(kcal/mol): 401.053

Entropy correction(cal/mol): 222.716

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.624

Deuterated enthalpy correction(kcal/mol): 396.943

Deuterated entropy correction(cal/mol): 226.314

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr 0.16184850 0.59605064 -0.36360889

C 0.11202104 -1.63683564 -1.43371835

C -0.79844575 -0.81680023 -2.17861298

H -1.87565692 -0.89744436 -2.15934441

C 1.41004088 -1.17451692 -1.79297518

H 2.33940453 -1.55053084 -1.38857584

C 1.30245914 -0.05823972 -2.65252840

H 2.12060042 0.51221196 -3.06693634

C -0.07861574 0.16374969 -2.90200486

H -0.49585135 0.91418052 -3.55797188

B -0.25276157 -2.56681915 -0.13279565

C -0.34547372 -4.15920667 -0.36754133

C 0.80780700 -2.09415049 1.05087570

C -1.60796558 -1.85742986 0.48902373

N -1.67730231 -0.56553174 0.56982374

N	1.16118397	-0.85164099	1.23191669
O	1.23625804	-2.94651235	1.99087058
O	-2.66328691	-2.52128167	0.97884294
C	-2.95303256	-0.17640292	1.19168667
C	-3.62146260	-1.53847748	1.47975362
C	1.86083464	-0.74286243	2.52917272
C	2.09573003	-2.21236506	2.91068495
N	-0.67392519	2.31526959	0.07494467
N	1.86854635	2.22312483	-0.13088316
C	2.33368191	3.02665604	-1.27233336
H	1.47937106	3.33663654	-1.88201595
H	-2.77358564	0.40908918	2.09614108
H	2.78998423	-0.18360516	2.43410993
C	-1.60137671	3.38995118	0.31702336
H	-2.51307196	3.00150235	0.79845474
H	-1.17958317	4.11775203	1.02568899
C	-2.02249464	4.13619938	-0.96040423
C	3.09523858	4.23420204	-0.65620594
C	3.30469952	3.84738063	0.83026098
H	2.63596948	4.42544359	1.47236752
H	3.00505839	2.45948814	-1.93214450
C	2.91365507	2.35033572	0.89376549
H	2.48408958	2.10715921	1.87195977
H	4.32675665	4.02839914	1.17324362
C	4.12696308	1.43751533	0.64228452
H	4.84963885	1.51006580	1.46191427
H	3.81908550	0.39402896	0.54106881
H	4.64757312	1.71506725	-0.27862929
C	-0.05783496	-4.72322858	-1.61922501
H	0.22927759	-4.07111738	-2.43797737
C	-0.71691583	-5.04860448	0.65579463
H	-0.95197144	-4.66060727	1.64106474
C	-0.13250687	-6.09818696	-1.84416592

H	0.09730382	-6.49849469	-2.82651123
C	-0.79563607	-6.42229362	0.44308108
H	-1.08734439	-7.07950555	1.25628646
C	-0.50222762	-6.95495529	-0.81158363
H	-0.56302538	-8.02490280	-0.98066734
C	-3.07654655	5.23428555	-0.71633991
H	-3.96825698	4.79675803	-0.25265394
H	-3.39336685	5.62669709	-1.69131696
C	-2.58360732	6.37888700	0.12477883
H	-1.69982829	6.89321588	-0.25274597
C	-3.13438171	6.80143849	1.25942959
H	-4.01486948	6.32124429	1.67651579
H	-2.72989147	7.64258089	1.81131584
H	-4.55940599	-1.69184410	0.94594882
H	-3.53615359	0.44279949	0.50585031
H	-3.77303068	-1.73907777	2.54078827
H	1.79797146	-2.47083762	3.92563379
H	3.12182801	-2.54228337	2.73589601
H	1.22084761	-0.22001600	3.24774496
H	4.04332083	4.40513963	-1.17166471
H	2.51366379	5.15432657	-0.74239097
H	-1.13277876	4.57373790	-1.42855076
H	-2.42059418	3.40642718	-1.67324302
H	0.59546064	2.60591764	0.13149835

MP2 Electronic Energy(Ha): 1489.138778975435

B3LYP Electronic Energy(Ha): 1492.974161651659

M06-L Electronic Energy(Ha): 1492.781903175515

Zero point energy correction(kcal/mol): 375.197

Enthalpy correction(kcal/mol): 398.123

Entropy correction(cal/mol): 229.107

Imaginary Frequencies: -1580.08

Deuterated zero point energy correction(kcal/mol): 371.581

Deuterated enthalpy correction(kcal/mol): 394.744

Deuterated entropy correction(cal/mol): 231.983

Deuterated imaginary Frequencies: -1135.44

Product geometry

Zr	0.03121611	0.72189171	-0.09819019
C	-0.14493596	-1.41641414	-1.39022027
C	-1.15673228	-0.53923330	-1.90697787
H	-2.22005382	-0.63982081	-1.74359750
C	1.08406681	-0.89899997	-1.87845245
H	2.06078860	-1.30857865	-1.66262386
C	0.84796762	0.29452689	-2.60552460
H	1.59273918	0.89958567	-3.10308113
C	-0.55199470	0.51409886	-2.63302953
H	-1.06305674	1.31845545	-3.14151401
B	-0.31886770	-2.48027615	-0.15678722
C	-0.45655392	-4.04016061	-0.55139373
C	0.90331605	-2.14776151	0.91488182
C	-1.56448702	-1.85955028	0.72727004
N	-1.59710672	-0.59052301	0.98294029
N	1.29915204	-0.94587052	1.21772621
O	1.45314178	-3.13382223	1.64724710
O	-2.57582436	-2.57584024	1.24272423
C	-2.80609332	-0.27392114	1.75785361
C	-3.41965335	-1.66674241	2.01378405
C	2.21179697	-1.02913358	2.37518643
C	2.42016551	-2.54350716	2.55570291
N	-0.84906872	2.31882251	0.36744597
N	2.07111019	2.17988920	0.13511720
C	2.18667699	3.21919366	-0.93737157
H	1.27667433	3.81612307	-0.93598595
H	-2.54710859	0.25191592	2.67910565
H	3.15104835	-0.51004970	2.17852163
C	-1.62731453	3.50326225	0.56462684

H	-2.25358414	3.40910100	1.46918144
H	-0.97965530	4.37620056	0.75453762
C	-2.55105465	3.83515603	-0.62077614
C	3.47667232	4.02918234	-0.64340906
C	4.14845698	3.29380175	0.54106908
H	3.94380117	3.81823909	1.47877706
H	2.24955564	2.71935784	-1.90283876
C	3.47555431	1.90507809	0.57015945
H	3.43768297	1.51163958	1.58757423
H	5.23333182	3.22644419	0.43769133
C	4.15887772	0.88485081	-0.33766957
H	5.17835463	0.69911516	0.01022828
H	3.61427544	-0.05986648	-0.33822042
H	4.22175277	1.23859238	-1.37009625
C	-0.31921799	-4.46234867	-1.88217719
H	-0.12268812	-3.72184464	-2.65093432
C	-0.71866020	-5.03920094	0.40236482
H	-0.83770934	-4.76300283	1.44456958
C	-0.43184109	-5.80432325	-2.24751937
H	-0.31987370	-6.09247318	-3.28813934
C	-0.83467531	-6.38129238	0.05013243
H	-1.03948670	-7.12519757	0.81388421
C	-0.69020099	-6.77154994	-1.28069285
H	-0.78061081	-7.81647330	-1.55880820
C	-3.39861338	5.10713103	-0.41993501
H	-3.98042959	5.02615763	0.50552972
H	-4.12550103	5.16807032	-1.24045020
C	-2.59575150	6.37801527	-0.40101704
H	-1.98575118	6.55915290	-1.28636360
C	-2.58054286	7.27634505	0.58009082
H	-3.17044158	7.14187586	1.48207619
H	-1.98349330	8.17949374	0.51745838
H	-4.44191147	-1.77782654	1.65308919

H -3.46097471 0.37981982 1.17613453

H -3.36949231 -1.97972951 3.05817791

H 2.20681139 -2.90961385 3.55969922

H 3.41293704 -2.88153412 2.25176449

H 1.74650893 -0.56188492 3.24975806

H 4.12589972 4.04810354 -1.52087386

H 3.25179556 5.06646807 -0.38984150

H -1.94003754 3.93498682 -1.52575163

H -3.21394692 2.98047055 -0.79112946

H 1.59902715 2.64629510 0.90992015

MP2 Electronic Energy(Ha): 1489.169813384013

B3LYP Electronic Energy(Ha): 1493.003448931228

M06-L Electronic Energy(Ha): 1492.815611431537

Zero point energy correction(kcal/mol): 379.064

Enthalpy correction(kcal/mol): 402.172

Entropy correction(cal/mol): 226.028

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.408

Deuterated enthalpy correction(kcal/mol): 397.775

Deuterated entropy correction(cal/mol): 228.731

Deuterated imaginary Frequencies: -0.00

Axial Reaction H4

Reactant geometry

Zr -0.86358874 -0.52796663 0.33151480

C -1.29847170 1.90901630 0.18814594

C -2.05094364 1.36836019 -0.89554184

H -1.79901471 1.45229771 -1.94245565

C -2.00344641 1.51640229 1.36962374

H -1.70626387 1.76386608 2.37819566

C -3.11597622 0.72497530 1.02216009

H -3.81743432 0.26607577 1.70266513

C	-3.14372180	0.62600059	-0.38773481
H	-3.88785434	0.10121585	-0.96581651
B	0.19134954	2.57970877	0.14396836
C	0.25740967	4.19192181	0.07855519
C	0.95444763	1.91078931	1.44071475
C	0.93326508	1.80335003	-1.09473104
N	0.80314890	0.52614256	-1.25655660
N	0.82054965	0.65421776	1.73346039
O	1.74208465	2.61733657	2.27166519
O	1.71271519	2.43150118	-1.99656551
C	1.59161551	0.11376445	-2.43148712
C	2.15467610	1.44533265	-2.96972176
C	1.55778856	0.37293182	2.98011534
C	2.27762669	1.70500587	3.27050814
N	-1.31388064	-1.74154946	2.05446826
H	2.38747505	-0.58051613	-2.14116104
H	0.85944352	0.08741200	3.77085554
C	-1.75111809	-1.29983394	3.38182939
H	-0.98597892	-1.50131800	4.15046059
H	-1.92762638	-0.22409044	3.40310318
C	-3.03229491	-2.11409836	3.71467309
C	-3.01342828	-3.28360021	2.70065856
H	-3.18041533	-4.25521429	3.17399990
H	-3.79147501	-3.14801728	1.94635930
C	-1.62221126	-3.18236521	2.02311155
H	-1.68036463	-3.51332560	0.98312352
C	-0.58821945	-4.06357863	2.75524536
H	-0.88087981	-5.11799084	2.71609729
H	0.40455080	-3.98340415	2.30183761
C	-0.90991322	4.96892786	0.04996390
H	-1.87452754	4.47190261	0.07353519
C	1.47840902	4.88746139	0.04495727
H	2.40985606	4.33082027	0.06422877

C	1.53307769	6.27744416	-0.01330039
H	2.49468104	6.78077926	-0.03798799
C	-0.86858181	6.36259490	-0.00865128
H	-1.79357368	6.93039475	-0.02950681
C	0.35558208	7.02394727	-0.04035607
H	0.39400695	8.10737345	-0.08581991
H	3.24360343	1.48144576	-3.01458515
H	1.74648244	1.72982073	-3.94109141
H	0.95727758	-0.39986973	-3.15632877
H	3.35917423	1.65508096	3.12897841
H	2.06313271	2.12179006	4.25432207
H	2.26045791	-0.45535899	2.84887901
H	-3.02563085	-2.46344312	4.75046238
H	-3.92916584	-1.50329567	3.58988099
N	-1.43911011	-1.92562566	-1.13998962
H	-0.81720316	-2.73036138	-1.13262698
C	-2.57793835	-2.24941550	-1.99809964
H	-3.05577304	-1.32277556	-2.32333663
H	-3.34186837	-2.80954047	-1.43525762
C	-2.21822719	-3.07937284	-3.24094488
H	-1.65207878	-3.96519962	-2.92503939
H	-3.14498179	-3.45918364	-3.68888710
C	-1.41524089	-2.32028054	-4.31555357
H	-0.54707742	-1.84422068	-3.85160274
H	-1.03202011	-3.04805807	-5.04249911
C	-2.23143536	-1.29353817	-5.05017970
H	-3.10486012	-1.67876207	-5.57638704
C	-1.97892427	0.01135774	-5.10435168
H	-1.12656567	0.44735898	-4.59231748
H	-2.61272992	0.69294235	-5.66033612
N	1.21404271	-1.93372241	0.39834811
C	1.58332406	-3.13229441	-0.38057171
H	1.17608500	-2.15825699	1.39003583

H	1.90340116	-1.19657443	0.28258270
H	0.79752320	-3.87676190	-0.22933094
H	1.56475520	-2.86178013	-1.43971532
C	2.93621271	-3.76020101	-0.01892462
H	2.93835397	-4.02409460	1.04585780
H	3.03263278	-4.70313623	-0.56781476
C	4.15607893	-2.87657888	-0.33642860
H	4.07176409	-1.92684492	0.20884838
H	4.16310033	-2.62940387	-1.40390865
C	5.45760185	-3.52980385	0.03748306
H	5.58004746	-3.77226508	1.09233666
C	6.43466481	-3.83259342	-0.81129782
H	6.35702073	-3.61101877	-1.87164900
H	7.34930594	-4.30965537	-0.47860587
H	-0.49374383	-3.78583259	3.80886395

MP2 Electronic Energy(Ha): 1740.503287120593

B3LYP Electronic Energy(Ha): 1744.993399615611

M06-L Electronic Energy(Ha): 1744.776558395654

Zero point energy correction(kcal/mol): 476.709

Enthalpy correction(kcal/mol): 505.223

Entropy correction(cal/mol): 261.329

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.887

Deuterated enthalpy correction(kcal/mol): 496.898

Deuterated entropy correction(cal/mol): 265.653

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.49266833	-0.44458115	0.57910874
C	-0.48987900	1.95421121	1.11244439
C	-1.87190865	1.65897505	0.90062103
H	-2.45675405	1.96166606	0.04465456
C	-0.15815857	1.33438619	2.35562127

H	0.81631389	1.35120754	2.81930049
C	-1.28062054	0.64281754	2.86000011
H	-1.32404745	0.07013248	3.77472664
C	-2.34919172	0.85212312	1.95893850
H	-3.35152345	0.47202820	2.07604255
B	0.56657601	2.58907947	0.04205980
C	0.74773323	4.19262850	0.06890056
C	1.94506948	1.71703211	0.26804277
C	0.11643404	1.94867243	-1.40328368
N	-0.29309456	0.72079817	-1.47998364
N	1.92160685	0.44000712	0.49016636
O	3.16840666	2.26495911	0.13401800
O	0.25146529	2.58216749	-2.58033225
C	-0.42465035	0.34286714	-2.89673392
C	-0.21915673	1.68308319	-3.62698450
C	3.31159051	-0.06153942	0.44701983
C	4.14872573	1.22800647	0.41142437
N	0.33411805	-2.11294922	2.02347759
H	0.33774684	-0.39840994	-3.15612780
H	3.53645711	-0.68528857	1.31238401
C	1.50467362	-1.84232369	2.89796277
H	2.38074963	-2.41505808	2.55534173
H	1.78593854	-0.78729140	2.88240310
C	1.10903033	-2.30468267	4.30589733
C	0.18526773	-3.48400952	4.00808416
H	0.77838299	-4.37197172	3.75908156
H	-0.47605397	-3.74789212	4.83712302
C	-0.59727205	-3.01850988	2.76491084
H	-1.47080845	-2.44368783	3.10633350
C	-1.11459149	-4.19003209	1.93059916
H	-1.75576889	-4.83269696	2.54222366
H	-1.70491143	-3.84056748	1.08297201
C	0.04289550	4.98740022	0.98527652

H	-0.63523880	4.51028278	1.68573112
C	1.61089962	4.86398127	-0.81477028
H	2.17813379	4.29336551	-1.54202110
C	1.76215868	6.24781496	-0.78576477
H	2.43794503	6.73231291	-1.48364668
C	0.18650374	6.37484906	1.02415031
H	-0.37588014	6.95647628	1.74787031
C	1.04863058	7.01208239	0.13670271
H	1.16437501	8.09061071	0.16174220
H	0.53659457	1.65763766	-4.41114145
H	-1.14433237	2.10080466	-4.02898206
H	-1.40194414	-0.09994658	-3.09381143
H	4.90280461	1.25584250	-0.37427337
H	4.61646931	1.46055884	1.37086962
H	3.46486235	-0.67177272	-0.45102794
H	1.97278065	-2.56790925	4.92158625
H	0.55966116	-1.51241536	4.82443081
N	-2.18370930	-1.49606535	-0.05174643
H	-1.88601375	-2.25890066	-0.65597208
C	-3.63034078	-1.60128116	0.12963619
H	-4.02783288	-0.62826386	0.42463780
H	-3.86174303	-2.29419522	0.95414820
C	-4.38831658	-2.08868322	-1.11506501
H	-3.93204650	-3.02235266	-1.46733771
H	-5.41269375	-2.34677620	-0.81936441
C	-4.44079445	-1.07955858	-2.27868814
H	-3.42817094	-0.74640973	-2.52196733
H	-4.82877071	-1.59672441	-3.16572826
C	-5.31385307	0.11150933	-1.99723625
H	-6.35178946	-0.11424488	-1.75254813
C	-4.92676833	1.38382556	-2.02796262
H	-3.90347995	1.66044315	-2.26312846
H	-5.61564553	2.19553611	-1.82316596

N	0.71101377	-2.19390092	-0.47272913
C	0.31814416	-3.24620946	-1.41099373
H	0.68515121	-2.45943703	0.78752919
H	1.60381696	-1.80475095	-0.75675544
H	-0.57256765	-3.74476347	-1.01526003
H	0.02673741	-2.82514536	-2.38633114
C	1.38423918	-4.32916053	-1.64757992
H	1.66606878	-4.76762164	-0.68339466
H	0.93917847	-5.13414412	-2.24378948
C	2.64496996	-3.82405110	-2.37199637
H	3.10855205	-3.02695354	-1.77552739
H	2.36423006	-3.37927943	-3.33374128
C	3.66362193	-4.90617957	-2.59507464
H	4.04691018	-5.38653520	-1.69550348
C	4.10611146	-5.31484547	-3.78043866
H	3.75138904	-4.86838836	-4.70486996
H	4.83930341	-6.10814009	-3.87203264
H	-0.28438520	-4.79655959	1.55592742

MP2 Electronic Energy(Ha): 1740.488964527036

B3LYP Electronic Energy(Ha): 1744.976569373462

M06-L Electronic Energy(Ha): 1744.756043989785

Zero point energy correction(kcal/mol): 474.075

Enthalpy correction(kcal/mol): 501.859

Entropy correction(cal/mol): 253.551

Imaginary Frequencies: -1361.90

Deuterated zero point energy correction(kcal/mol): 466.072

Deuterated enthalpy correction(kcal/mol): 494.312

Deuterated entropy correction(cal/mol): 257.680

Deuterated imaginary Frequencies: -975.78

Product geometry

Zr	-0.45108759	-0.52240457	0.40150918
C	-0.57550149	1.87048903	1.06449522

C	-1.94021591	1.55225029	0.78840362
H	-2.49695934	1.86778981	-0.08110666
C	-0.28159608	1.22765130	2.30512301
H	0.66675501	1.27590176	2.81857574
C	-1.41051141	0.50777703	2.74765331
H	-1.48973176	-0.06935594	3.65743680
C	-2.44303206	0.71211187	1.80461806
H	-3.44317988	0.31405036	1.87236723
B	0.49801358	2.59275075	0.07329744
C	0.62543446	4.19907292	0.18608940
C	1.89625527	1.75718465	0.31749630
C	0.11159683	2.01631568	-1.41366219
N	-0.32700732	0.80481150	-1.55411149
N	1.89959089	0.47612804	0.51295537
O	3.10903952	2.33976941	0.24353519
O	0.33599300	2.68093355	-2.56071028
C	-0.38246035	0.47320753	-2.98733299
C	-0.10073739	1.82925636	-3.66037184
C	3.29874865	0.00925262	0.55203787
C	4.11178925	1.31733425	0.49483221
N	0.26366302	-2.19814455	2.14991192
H	0.37236559	-0.28347775	-3.22034154
H	3.49464401	-0.56497514	1.46015178
C	1.33613369	-1.81810671	3.13151725
H	2.25070509	-2.37351850	2.90228975
H	1.56178065	-0.75572953	3.05823487
C	0.80038807	-2.21634173	4.51265110
C	-0.07536410	-3.43216269	4.20177056
H	0.54752542	-4.32393353	4.06512691
H	-0.80667784	-3.65344329	4.98224576
C	-0.74569999	-3.05510356	2.87082364
H	-1.61444743	-2.42381573	3.07917948
C	-1.19491672	-4.24663124	2.03554253

H	-1.92991131	-4.83650415	2.58949529
H	-1.65474572	-3.91560811	1.10382657
C	-0.14835590	4.92437637	1.10458231
H	-0.84162702	4.39052734	1.74683773
C	1.50506237	4.94115810	-0.62160884
H	2.12456166	4.42577591	-1.34739851
C	1.60696599	6.32615188	-0.51858471
H	2.29728057	6.86636474	-1.15911866
C	-0.05481173	6.31211201	1.21705824
H	-0.67041581	6.83866924	1.93978227
C	0.82530546	7.02035017	0.40408937
H	0.90234452	8.09955622	0.48652275
H	0.69567295	1.80759993	-4.40353500
H	-0.99117360	2.28578772	-4.09737615
H	-1.35780531	0.06440801	-3.25597399
H	4.84196023	1.35555659	-0.31354875
H	4.60608887	1.56069630	1.43748687
H	3.50609698	-0.64791797	-0.29833919
H	1.60508072	-2.42751485	5.21956566
H	0.19513318	-1.40842454	4.93327570
N	-2.09817972	-1.65716493	-0.21848288
H	-1.76736684	-2.37924713	-0.85392103
C	-3.54022587	-1.82706796	-0.05342563
H	-3.98203476	-0.87957379	0.25973423
H	-3.75492205	-2.54894284	0.75163440
C	-4.26117571	-2.31697156	-1.31923705
H	-3.76920847	-3.22977692	-1.67830587
H	-5.28285675	-2.61057888	-1.04788459
C	-4.31969661	-1.28959644	-2.46662331
H	-3.31266411	-0.91987646	-2.67785009
H	-4.66846276	-1.80346122	-3.37167618
C	-5.23922859	-0.13383514	-2.18615997
H	-6.27634917	-0.39804726	-1.97895803

C	-4.89272791	1.15040481	-2.17602956
H	-3.87187017	1.46425772	-2.37104024
H	-5.61351079	1.93472297	-1.97402176
N	0.75747282	-1.94152930	-0.73849135
C	0.50334364	-3.11027608	-1.56754385
H	0.69536355	-2.73556095	1.39799164
H	1.58013939	-1.46249813	-1.09059235
H	-0.36538336	-3.64908877	-1.17039242
H	0.23769983	-2.84380327	-2.60855464
C	1.65943226	-4.12735035	-1.63266261
H	1.90482086	-4.45378692	-0.61448910
H	1.31824460	-5.01526368	-2.17892865
C	2.92929521	-3.59098506	-2.31558362
H	3.28675729	-2.71429028	-1.75984130
H	2.68628504	-3.24946881	-3.32856151
C	4.03593283	-4.60521930	-2.37709827
H	4.38431797	-4.98269046	-1.41601494
C	4.59485847	-5.07216681	-3.48976731
H	4.27971569	-4.72944522	-4.47106995
H	5.38739235	-5.81152616	-3.46269919
H	-0.34873792	-4.90027188	1.79930048

MP2 Electronic Energy(Ha): 1740.502579775213

B3LYP Electronic Energy(Ha): 1744.996046801934

M06-L Electronic Energy(Ha): 1744.776626634551

Zero point energy correction(kcal/mol): 476.819

Enthalpy correction(kcal/mol): 505.226

Entropy correction(cal/mol): 262.954

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.897

Deuterated enthalpy correction(kcal/mol): 496.813

Deuterated entropy correction(cal/mol): 267.811

Deuterated imaginary Frequencies: -0.00

Axial Reaction H5

Reactant geometry

Zr	0.94688253	-1.11718836	-0.15368491
C	1.86151470	1.17430168	-0.24310437
C	2.65783246	0.52565525	0.75466977
H	2.59893595	0.70701241	1.81878415
C	2.28878022	0.60808503	-1.48187945
H	1.88748314	0.85211394	-2.45476387
C	3.25591140	-0.39332154	-1.24579759
H	3.73914728	-1.00505970	-1.99322836
C	3.49324800	-0.43690449	0.14985142
H	4.18858566	-1.09008970	0.65602653
B	0.50630168	2.06503898	0.00154698
C	0.68044961	3.67075953	0.02575765
C	-0.52252895	1.50895923	-1.16132162
C	-0.12227806	1.43486269	1.38842541
N	-0.11758550	0.15785892	1.62493473
N	-0.59469943	0.24982260	-1.46268392
O	-1.28987985	2.32412049	-1.90949740
O	-0.63913546	2.19587238	2.36894647
C	-0.62598528	-0.08162288	2.98757976
C	-1.10561083	1.31524607	3.42868620
C	-1.43746418	0.09577586	-2.66072490
C	-2.06952526	1.48990131	-2.81404135
N	-1.27024613	-2.25202927	0.31652043
N	1.55260867	-2.97248745	0.57875811
C	2.53544263	-3.68448186	1.39195398
H	2.13656631	-3.93893587	2.38379623
H	-1.43325851	-0.81888036	2.99047626
H	-0.80935065	-0.18160046	-3.51324813
C	-2.61367316	-1.64163396	0.35979440
H	-2.55119435	-0.73019084	0.95793576

H	-2.86866476	-1.32506336	-0.65108391
C	-3.70526693	-2.56527420	0.90953119
C	2.90704949	-4.96881534	0.60463392
C	2.48568092	-4.64287526	-0.83361023
H	2.29669875	-5.52965883	-1.44461959
H	3.42119153	-3.05941208	1.56808678
C	1.22256230	-3.78587728	-0.64620727
H	0.38359754	-4.47617381	-0.43348314
H	3.25326061	-4.04287428	-1.33320734
C	0.86525121	-2.79441486	-1.76976062
H	-0.07775319	-3.02686344	-2.27486589
H	-1.03419890	-2.66721790	1.21590090
H	1.64967122	-2.75716405	-2.52839206
C	-0.41029306	4.53857568	0.20631330
H	-1.40627946	4.12528490	0.32966968
C	1.93997020	4.26677483	-0.13198455
H	2.80814810	3.63155672	-0.27601522
C	-0.25452973	5.92190379	0.22956953
H	-1.11996747	6.56201068	0.37060327
C	2.10930595	5.65176260	-0.11057459
H	3.10000728	6.07726480	-0.23636120
C	1.01061027	6.48657019	0.07099732
H	1.13609265	7.56417987	0.08820650
C	-5.10220798	-1.91234681	0.92770268
H	-5.06958313	-0.98013621	1.50251073
H	-5.78546242	-2.58426368	1.46118924
C	-5.66031243	-1.64332625	-0.44303743
H	-5.76443821	-2.51550681	-1.08816271
C	-6.03577236	-0.45376401	-0.90520547
H	-5.95788938	0.44328895	-0.29800496
H	-6.44781893	-0.33478637	-1.90092568
H	-0.67129459	1.65980705	4.36648923
H	0.17724665	-0.46971765	3.62164500

H	-2.19265953	1.40419333	3.48067023
H	-3.11056711	1.52556245	-2.48427189
H	-1.99071185	1.91505839	-3.81365506
H	-2.18290863	-0.69111764	-2.53426955
H	3.96540533	-5.22346779	0.69889156
H	2.33149677	-5.82156872	0.97870229
H	-3.74101348	-3.48453364	0.31154170
H	-3.44267754	-2.87140940	1.92932564
H	-1.27004008	-3.02824791	-0.33983229

MP2 Electronic Energy(Ha): 1489.161733159814

B3LYP Electronic Energy(Ha): 1492.988849188805

M06-L Electronic Energy(Ha): 1492.807669838283

Zero point energy correction(kcal/mol): 378.344

Enthalpy correction(kcal/mol): 401.218

Entropy correction(cal/mol): 224.905

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.931

Deuterated enthalpy correction(kcal/mol): 396.980

Deuterated entropy correction(cal/mol): 226.041

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.88061907	-0.86263729	-0.22862301
C	1.55440868	1.48191360	0.16135443
C	2.05895615	0.79922497	1.31327498
H	1.64804394	0.86033391	2.31027399
C	2.42567082	1.11501776	-0.90515299
H	2.32440128	1.43275047	-1.93239556
C	3.39433655	0.20340207	-0.43784913
H	4.17238116	-0.25735195	-1.02790492
C	3.17415506	0.01574263	0.94594152
H	3.77445278	-0.59146328	1.60659387
B	0.12747919	2.25983153	0.01883109

C	0.17406369	3.87313397	0.10930438
C	-0.51393657	1.66218803	-1.37211818
C	-0.81863448	1.53116257	1.15054178
N	-0.80185164	0.24904280	1.34555626
N	-0.24940513	0.45761341	-1.78385148
O	-1.43494217	2.31701417	-2.09542642
O	-1.64429668	2.23476698	1.94677376
C	-1.74988581	-0.07019524	2.43427159
C	-2.24374627	1.31400081	2.89828332
C	-1.11337225	0.13233412	-2.93125571
C	-1.79960024	1.47807999	-3.23108531
N	-0.74333777	-2.25369449	-0.48798229
N	1.73172561	-2.92967409	0.74360214
C	2.70110248	-3.37374818	1.78482302
H	2.17543222	-3.88034064	2.59757223
H	-2.56446354	-0.69075601	2.05959458
H	-0.51730039	-0.23184583	-3.77028287
C	-2.10197888	-2.44468816	0.00490668
H	-2.09612290	-2.49501133	1.10152002
H	-2.76532045	-1.60107751	-0.24820021
C	-2.74061544	-3.74005048	-0.51284500
C	3.70695542	-4.28632606	1.06111483
C	3.69901048	-3.73687800	-0.37042644
H	4.08877790	-4.44143093	-1.10767803
H	3.20466763	-2.50591804	2.21255154
C	2.22606043	-3.41156771	-0.64227676
H	1.69721612	-4.34790280	-0.84937627
H	4.29866839	-2.82359452	-0.43271710
C	1.91690445	-2.35017643	-1.70351370
H	1.24351105	-2.74117143	-2.47205437
H	0.81996353	-3.34959196	0.89327604
H	2.82352586	-2.00854477	-2.20450562
C	-0.98076180	4.66579358	-0.01100579

H	-1.94056669	4.18787820	-0.17441721
C	1.38388010	4.55142769	0.31923182
H	2.29986051	3.97752769	0.41748037
C	-0.93125121	6.05483846	0.07407012
H	-1.84366115	6.63511456	-0.02257723
C	1.44589555	5.94270575	0.40697363
H	2.40095308	6.43194790	0.57130160
C	0.28589050	6.70184189	0.28451132
H	0.32751420	7.78399057	0.35218362
C	-4.09260439	-4.08779303	0.13893000
H	-3.95845732	-4.22059652	1.21852430
H	-4.42052608	-5.05874287	-0.25485359
C	-5.17797762	-3.07809366	-0.11045000
H	-5.37965365	-2.85070507	-1.15720664
C	-5.90027550	-2.47206996	0.82816860
H	-5.73929383	-2.67069096	1.88395446
H	-6.68267514	-1.76427763	0.57845821
H	-1.89462228	1.59259260	3.89437256
H	-1.24536664	-0.62340632	3.23141365
H	-3.32581139	1.43634649	2.84891746
H	-2.88712400	1.42953944	-3.27370061
H	-1.42224522	1.96429351	-4.13252747
H	-1.81591596	-0.65448934	-2.64563008
H	4.69301260	-4.26869928	1.53039045
H	3.35469319	-5.32279462	1.06765568
H	-2.86622157	-3.67064291	-1.60183002
H	-2.04298982	-4.56689367	-0.33564296
H	-0.62280219	-2.79262979	-1.34015822

MP2 Electronic Energy(Ha): 1489.149723832961

B3LYP Electronic Energy(Ha): 1492.983155232311

M06-L Electronic Energy(Ha): 1492.798195732721

Zero point energy correction(kcal/mol): 378.488

Enthalpy correction(kcal/mol): 400.254

Entropy correction(cal/mol): 213.189

Imaginary Frequencies: -30.41 -12.04

Product geometry

Zr	0.64521637	-1.11332881	0.22825441
C	1.70705545	1.16233441	0.27672242
C	2.06903483	0.56151644	1.52580847
H	1.68152735	0.84083046	2.49482080
C	2.49338819	0.49382512	-0.70553919
H	2.45172088	0.68012069	-1.76922047
C	3.24626791	-0.52805082	-0.09842379
H	3.91513803	-1.20996742	-0.60328892
C	2.98523126	-0.48359394	1.29887867
H	3.43695913	-1.10739694	2.05700437
B	0.44500608	2.16586026	0.00398773
C	0.77102974	3.73868347	-0.14806971
C	-0.33135237	1.48862340	-1.27240544
C	-0.58255847	1.76981822	1.21958575
N	-0.80251958	0.52882049	1.50853090
N	-0.41606407	0.20055554	-1.40454295
O	-0.97955937	2.20275613	-2.20610691
O	-1.17620694	2.67392179	2.02224101
C	-1.58471232	0.47249992	2.75851917
C	-2.00931541	1.93738800	2.96230010
C	-1.20642908	-0.11715748	-2.60577914
C	-1.65376359	1.27215990	-3.10159877
N	-1.02548375	-2.33515937	0.74406600
N	1.62852587	-3.34046328	0.58099143
C	2.96901316	-3.84170085	0.99114308
H	2.95244515	-4.13741400	2.04210176
H	-2.43545083	-0.20136777	2.66979138
H	-0.58614513	-0.64469721	-3.33376522
C	-2.46609147	-2.10282100	0.78360382

H	-2.87811481	-2.29957808	1.78868606
H	-2.65985961	-1.04939997	0.57161884
C	-3.24931981	-2.97073355	-0.21360127
C	3.28334389	-4.98481079	0.01873508
C	2.72715125	-4.43584389	-1.30061095
H	2.54249288	-5.20670626	-2.05128231
H	3.70526680	-3.04585726	0.88017587
C	1.42301088	-3.70813162	-0.91440496
H	0.59357349	-4.42097696	-0.93534994
H	3.43158059	-3.71892901	-1.73359444
C	1.05069083	-2.44138220	-1.66752608
H	0.16283500	-2.59058168	-2.28320756
H	0.94324698	-3.84236810	1.13589920
H	1.86261394	-2.08675843	-2.30663739
C	-0.24201716	4.69302464	-0.34544680
H	-1.27639841	4.36910058	-0.39756635
C	2.08671700	4.22097649	-0.08858077
H	2.89940140	3.51800295	0.06532554
C	0.04059921	6.04996674	-0.47746962
H	-0.76773176	6.75878857	-0.62836288
C	2.38293708	5.57832401	-0.21958383
H	3.41394414	5.91429917	-0.16776130
C	1.35887023	6.50030036	-0.41535926
H	1.58283531	7.55706508	-0.51761525
C	-4.77641021	-2.76498107	-0.15513695
H	-5.13638884	-2.94480970	0.86416519
H	-5.25013424	-3.52336400	-0.79150545
C	-5.22469759	-1.40562110	-0.61520366
H	-4.93728306	-1.13499791	-1.63135709
C	-5.93487062	-0.53774062	0.10044868
H	-6.25016130	-0.76277305	1.11516092
H	-6.23455726	0.42341727	-0.30194651
H	-1.81869993	2.33067261	3.96018573

H -0.95110005 0.10347393 3.57327482

H -3.05271374 2.11906798 2.69341529

H -2.72742465 1.44326111 -3.00737669

H -1.33956993 1.50304948 -4.11942623

H -2.04866087 -0.76380570 -2.35126274

H 4.35011066 -5.21635540 -0.02228372

H 2.75371364 -5.89685611 0.31499977

H -2.88370233 -2.77321971 -1.22786547

H -3.03260908 -4.02735695 -0.01101042

H -0.88828061 -3.34269141 0.73652509

MP2 Electronic Energy(Ha): 1489.162323222508

B3LYP Electronic Energy(Ha): 1492.992348568224

M06-L Electronic Energy(Ha): 1492.812286107799

Zero point energy correction(kcal/mol): 379.308

Enthalpy correction(kcal/mol): 401.760

Entropy correction(cal/mol): 216.013

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.547

Deuterated enthalpy correction(kcal/mol): 397.305

Deuterated entropy correction(cal/mol): 218.801

Deuterated imaginary Frequencies: -0.00

Axial Reaction H6

Reactant geometry

Zr -0.40943075 -0.81605077 -0.02200815

C 0.69988373 1.05963433 -1.18070787

C 1.72499155 0.06252283 -1.17920533

H 2.61323383 0.08014857 -0.56365688

C -0.26673785 0.60316807 -2.12814063

H -1.18235451 1.11516132 -2.38226310

C 0.12556446 -0.65359196 -2.64148444

H -0.40627284 -1.24103930 -3.37728530

C	1.37264808	-0.98136949	-2.05971179
H	1.94681867	-1.87128172	-2.26647267
B	0.52245710	2.28981763	-0.12070441
C	1.21727095	3.69356860	-0.51504451
C	-1.09745050	2.36065640	0.15024497
C	0.99207183	1.64928494	1.32387623
N	0.69961693	0.42189732	1.62295519
N	-1.83695489	1.29776950	0.19282723
O	-1.71764859	3.51917627	0.45453821
O	1.60486728	2.34219674	2.29634142
C	1.11995573	0.13371290	3.00276925
C	1.79884235	1.45033796	3.43498076
C	-3.18512207	1.69047693	0.64698804
C	-3.12837314	3.22862422	0.64243786
N	0.53627460	-2.62501471	0.46747333
N	-2.34309529	-1.98459166	-0.81157652
C	-3.50144645	-1.49090203	-1.60033903
H	-3.38426199	-1.75877267	-2.65184000
H	0.25000512	-0.11687885	3.61526883
H	-3.95734714	1.30404221	-0.02229638
C	1.69531941	-3.45232500	0.15057421
H	2.41824319	-2.86315025	-0.41969399
H	2.21236668	-3.75196367	1.07169929
C	1.34569782	-4.71665425	-0.65158380
C	-4.73028588	-2.11421854	-0.92585494
C	-4.35471046	-2.04877233	0.56136144
H	-4.91151567	-2.75638859	1.17870313
H	-3.53710416	-0.40113349	-1.53792902
C	-2.83618234	-2.33100955	0.61716233
H	-2.67208603	-3.40603967	0.73322280
H	-4.55511426	-1.04781577	0.95316464
C	-1.98349942	-1.53817143	1.60226171
H	-1.59050855	-2.17068590	2.40381200

H	-1.99395322	-2.83336698	-1.24545863
H	-2.55240168	-0.73333488	2.07325556
C	1.17864479	4.81463729	0.33255958
H	0.66994998	4.74277550	1.28761184
C	1.89022967	3.85118019	-1.73583298
H	1.94523445	3.01011138	-2.41976689
C	1.77647158	6.02251882	-0.01759545
H	1.72691999	6.86724781	0.66256710
C	2.49239466	5.05670807	-2.09811326
H	3.00428481	5.14026301	-3.05179560
C	2.43798728	6.14985984	-1.23840585
H	2.90494660	7.08974327	-1.51400129
C	2.56194986	-5.60871343	-0.97211199
H	3.32403776	-5.02372732	-1.49955665
H	2.23719364	-6.39434633	-1.66641266
C	3.17358886	-6.26075549	0.23702530
H	2.49888906	-6.88076343	0.82757819
C	4.44101990	-6.14619675	0.62363234
H	5.15155972	-5.54008803	0.06932192
H	4.81647441	-6.65590897	1.50391458
H	2.87300333	1.35477077	3.59897238
H	1.80062675	-0.72025533	3.02123678
H	1.34134436	1.92076384	4.30543959
H	-3.44873623	3.69323664	1.57468635
H	-3.67509010	3.67668786	-0.19045124
H	-3.37602461	1.28240495	1.64389712
H	-5.65484984	-1.58267071	-1.16313627
H	-4.85091357	-3.15337124	-1.25057964
H	0.60026781	-5.29946609	-0.09546855
H	0.86463720	-4.41204438	-1.58773977
H	0.06045637	-3.03659470	1.26605590

MP2 Electronic Energy(Ha): 1489.172261739470

B3LYP Electronic Energy(Ha): 1493.004950508496

M06-L Electronic Energy(Ha): 1492.821317789157

Zero point energy correction(kcal/mol): 379.126

Enthalpy correction(kcal/mol): 401.630

Entropy correction(cal/mol): 217.851

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.761

Deuterated enthalpy correction(kcal/mol): 397.461

Deuterated entropy correction(cal/mol): 218.955

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.16227396	-0.75946732	0.29953465
C	-0.48477411	1.39560968	1.30580288
C	-1.57343719	0.52273090	1.64256010
H	-2.56048994	0.55532210	1.20411749
C	0.60400460	0.96658575	2.11254283
H	1.59558592	1.39445984	2.10325559
C	0.21716851	-0.17349236	2.86638761
H	0.83267428	-0.71458006	3.57204480
C	-1.14672667	-0.42967685	2.58767942
H	-1.73965884	-1.23533937	2.99484678
B	-0.43428635	2.42738481	0.03614132
C	-0.90775700	3.93228105	0.37411954
C	1.07794875	2.27856762	-0.59923445
C	-1.26139956	1.63566808	-1.14902483
N	-1.13380033	0.35192752	-1.28570667
N	1.70729862	1.14833613	-0.66410126
O	1.67671828	3.31939626	-1.22050982
O	-2.01515568	2.23243404	-2.08580380
C	-1.87257490	-0.09975253	-2.47413584
C	-2.49341491	1.20711676	-3.00832131
C	2.90750225	1.33896151	-1.50391740
C	2.96713452	2.86302243	-1.70366569

N	-0.76312313	-2.45101409	0.13839623
N	2.24558319	-1.87526146	0.77539704
C	3.53073568	-1.26442671	1.21951436
H	3.60152517	-1.29101113	2.30810939
H	-1.18836666	-0.56361032	-3.18872245
H	3.80379804	0.95051956	-1.01517984
C	-1.66790666	-3.55580450	0.26477849
H	-2.47485418	-3.30346815	0.97345424
H	-2.16785929	-3.76877598	-0.69253053
C	-0.99018547	-4.84654731	0.75779941
C	4.62426518	-2.06682841	0.50279961
C	3.97950165	-2.35518370	-0.86052712
H	4.43550198	-3.19754425	-1.38418598
H	3.54887623	-0.21787107	0.91168533
C	2.49381217	-2.62739198	-0.54618809
H	2.36750188	-3.69049747	-0.31980353
H	4.06646455	-1.48070621	-1.51143032
C	1.43224386	-2.20915568	-1.55587042
H	1.25465109	-2.99317000	-2.29856783
H	1.96247371	-2.56036543	1.46893127
H	1.72985563	-1.31476194	-2.11319034
C	-0.02228268	4.85151812	0.96139950
H	1.01451892	4.56847135	1.11420722
C	-2.23196157	4.36501517	0.19828685
H	-2.95530035	3.69980653	-0.26023623
C	-0.42789795	6.12565011	1.35084182
H	0.28782435	6.80682894	1.80044861
C	-2.65070568	5.63799395	0.58380257
H	-3.68329230	5.93557196	0.42972576
C	-1.74930494	6.52646398	1.16378392
H	-2.07075569	7.51784777	1.46491913
C	-1.96063024	-6.03054956	0.93456160
H	-2.76792815	-5.74885248	1.61990833

H	-1.41455215	-6.85192991	1.41647339
C	-2.54578060	-6.53584955	-0.35493653
H	-1.82236171	-6.84439300	-1.10986175
C	-3.84269793	-6.63872565	-0.63159011
H	-4.60182338	-6.34304916	0.08658853
H	-4.19374094	-7.02425302	-1.58231713
H	-3.58336348	1.21809652	-2.98070486
H	-2.61916158	-0.84541676	-2.19297957
H	-2.15555934	1.48130800	-4.00785496
H	3.07271712	3.17776210	-2.74155258
H	3.74095614	3.34468655	-1.10065651
H	2.78793237	0.79899933	-2.44929927
H	5.56666587	-1.51887865	0.43142051
H	4.82316404	-3.00047130	1.03980472
H	-0.19591583	-5.12447060	0.05403079
H	-0.50213349	-4.63594898	1.71585588
H	0.17141943	-2.45390735	-0.85572751

MP2 Electronic Energy(Ha): 1489.127561381088

B3LYP Electronic Energy(Ha): 1492.954328108460

M06-L Electronic Energy(Ha): 1492.769404829767

Zero point energy correction(kcal/mol): 375.605

Enthalpy correction(kcal/mol): 398.213

Entropy correction(cal/mol): 226.330

Imaginary Frequencies: -1615.35

Deuterated zero point energy correction(kcal/mol): 372.065

Deuterated enthalpy correction(kcal/mol): 394.800

Deuterated entropy correction(cal/mol): 226.986

Deuterated imaginary Frequencies: -1178.47

Product geometry

Zr	-0.01723712	0.69617456	-0.20619836
C	-0.26990848	-1.48683335	-1.41224186
C	-1.35084795	-0.65146003	-1.85407305

H	-2.39002905	-0.77269365	-1.58404206
C	0.89153259	-0.95362398	-2.02992848
H	1.89603225	-1.32862673	-1.88969825
C	0.55189076	0.21202838	-2.76611766
H	1.22371964	0.81913836	-3.35918041
C	-0.85032349	0.39158679	-2.66657223
H	-1.42997883	1.16819261	-3.14337549
B	-0.30268624	-2.51164196	-0.13237477
C	-0.45653246	-4.08482678	-0.46335399
C	1.01898524	-2.13068812	0.79366600
C	-1.46774226	-1.87973159	0.85085931
N	-1.50538720	-0.60381647	1.07170262
N	1.40676798	-0.91333622	1.03241161
O	1.68950655	-3.08844675	1.46236225
O	-2.40959173	-2.59895288	1.48141783
C	-2.64462590	-0.28762848	1.94657486
C	-3.19585363	-1.68388821	2.30408110
C	2.45316718	-0.94878765	2.07166102
C	2.75040573	-2.45114842	2.22265420
N	-0.86631591	2.31278067	0.23039633
N	2.09238013	1.98101201	-0.49721806
C	3.41196936	1.39782932	-0.85905411
H	3.31260999	0.76750747	-1.74172166
H	-2.31477240	0.27510853	2.82223903
H	3.33610744	-0.38182871	1.76912731
C	-1.60759360	3.51963531	0.42733757
H	-2.34968659	3.38855602	1.23456835
H	-0.94805146	4.33370177	0.77204419
C	-2.35555209	3.99744212	-0.82986580
C	4.33070009	2.60929135	-1.04378963
C	3.86751255	3.56980224	0.07026976
H	3.93639650	4.61630878	-0.23205587
H	3.75265748	0.76732303	-0.03538958

C	2.39955245	3.15962053	0.40128630
H	1.69296651	3.94425328	0.12906280
H	4.49344528	3.45114772	0.95874139
C	2.19974695	2.82849261	1.87633331
H	2.45396662	3.70035182	2.48591418
H	1.72595450	2.39139180	-1.35605505
H	2.84710158	2.00567370	2.19227708
C	-0.45553742	-4.54766739	-1.78762488
H	-0.35484114	-3.82967095	-2.59530433
C	-0.59721734	-5.05627674	0.54301116
H	-0.60783643	-4.74858937	1.58320023
C	-0.58349304	-5.90210969	-2.09773667
H	-0.57880833	-6.22195077	-3.13511450
C	-0.72697249	-6.41048191	0.24644614
H	-0.83519680	-7.13227237	1.05015980
C	-0.71967849	-6.84129064	-1.07970244
H	-0.82111292	-7.89579290	-1.31445917
C	-3.16767880	5.29166611	-0.62471985
H	-3.86787470	5.16470134	0.20897106
H	-3.77851273	5.45936925	-1.52145622
C	-2.32155164	6.51211040	-0.39089459
H	-1.59420458	6.73382213	-1.17235909
C	-2.39639114	7.32337691	0.66078214
H	-3.10358328	7.14542671	1.46563221
H	-1.75864711	8.19539533	0.75531915
H	-4.24552714	-1.82878573	2.04990381
H	-3.36716568	0.33073932	1.40762409
H	-3.03554345	-1.96108466	3.34751341
H	2.69935444	-2.81849959	3.24720456
H	3.70318026	-2.74904837	1.77943952
H	2.07345079	-0.50132013	2.99617772
H	5.39031134	2.35513379	-0.97361459
H	4.16436246	3.04956899	-2.03231014

H -1.62859282 4.14056447 -1.63866870

H -3.02633803 3.19638506 -1.15707158

H 1.15839272 2.56571277 2.06955132

MP2 Electronic Energy(Ha): 1489.173693214405

B3LYP Electronic Energy(Ha): 1493.005703204480

M06-L Electronic Energy(Ha): 1492.818492226350

Zero point energy correction(kcal/mol): 379.046

Enthalpy correction(kcal/mol): 402.000

Entropy correction(cal/mol): 223.912

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.709

Deuterated enthalpy correction(kcal/mol): 397.819

Deuterated entropy correction(cal/mol): 224.890

Deuterated imaginary Frequencies: -0.00

Axial Reaction H7

Reactant geometry

Zr 0.37716948 0.35884159 -0.40252356

C -0.26829523 -1.83515308 -1.38213109

C -1.27123826 -0.94540254 -1.87038194

H -2.29876574 -0.91935619 -1.53680422

C 0.90943896 -1.51818742 -2.12299898

H 1.87079763 -1.99653463 -2.00337942

C 0.64100760 -0.45792697 -3.01159324

H 1.34104575 -0.01542914 -3.70196516

C -0.71193417 -0.08795306 -2.84718289

H -1.23106261 0.68145728 -3.40196867

B -0.35898398 -2.81762165 -0.08430518

C -0.64281320 -4.38064980 -0.38467563

C 1.02852431 -2.51349396 0.73552522

C -1.46914931 -2.08929051 0.87830991

N -1.49945761 -0.80611227 1.04588998

N	1.55754878	-1.32798812	0.75896594
O	1.65624458	-3.43436290	1.48540370
O	-2.42867067	-2.79232962	1.51613654
C	-2.68154702	-0.47969900	1.86881721
C	-3.21097128	-1.85854304	2.30417445
C	2.70944931	-1.33334651	1.67994974
C	2.86140610	-2.82424654	2.02977466
N	-1.21723236	2.56515576	2.53536613
H	-2.41149894	0.14491382	2.71983000
H	3.59541329	-0.92099435	1.19330598
C	-0.80506936	3.96071707	2.84950116
H	-0.54711875	4.48488294	1.92582195
H	-1.64801017	4.49462084	3.29421731
C	0.42604040	3.88671022	3.79766565
C	0.60919989	2.37939709	4.06183559
H	1.65490649	2.09881751	4.20445587
H	0.06171871	2.08712496	4.96665570
C	-0.02900026	1.69700052	2.82517992
H	-0.39035982	0.70064769	3.09347116
C	0.87118874	1.60710112	1.59006541
H	1.04014010	2.63617106	1.23397896
H	1.86141777	1.26020246	1.91436747
C	-0.82950038	-4.84689564	-1.69436106
H	-0.77971529	-4.14095951	-2.51734512
C	-0.71874131	-5.33837142	0.64165568
H	-0.58113862	-5.02717680	1.67169709
C	-0.96543960	-6.68294445	0.37714511
H	-1.01693119	-7.39443306	1.19555539
C	-1.07815996	-6.19170286	-1.97228760
H	-1.21764077	-6.51467976	-2.99932029
C	-1.14693232	-7.11742652	-0.93539512
H	-1.33935471	-8.16452957	-1.14505617
H	-3.02746089	-2.07444154	3.35938072

H	-4.26458107	-2.02663458	2.08144508
H	-3.41402611	0.07703011	1.27279724
H	2.89037471	-3.03350716	3.09861202
H	3.71777699	-3.29706745	1.54480443
H	2.49045070	-0.71923984	2.55688387
H	1.30764208	4.30547401	3.30842287
H	0.26908702	4.45101330	4.71944685
H	-1.95473433	2.31375571	3.18692898
N	1.90973909	1.61303150	-1.09054425
H	2.23333613	2.16978689	-0.30525213
C	2.68962521	1.99894864	-2.26385374
H	2.10643587	1.81427548	-3.16811634
H	2.88018649	3.08049453	-2.24218950
C	4.03777418	1.26798584	-2.39900926
H	3.84840539	0.19183790	-2.46785162
H	4.50575862	1.57043876	-3.34531271
C	5.02266407	1.52405042	-1.24195855
H	4.56936171	1.20825112	-0.29719157
H	5.90383365	0.88794812	-1.39619282
C	5.47290499	2.95451309	-1.13590362
H	5.94173795	3.36982750	-2.02807266
C	5.34582601	3.72876104	-0.06127299
H	4.88767827	3.36092383	0.85235746
H	5.70171831	4.75308055	-0.05070598
N	-1.40254147	1.98019218	-0.40062856
C	-1.26550132	3.21747417	-1.20638286
H	-1.48721251	2.22589712	0.60365351
H	-2.25818081	1.49677074	-0.66010933
H	-0.33176296	3.69300083	-0.90291127
H	-1.13922392	2.92987430	-2.25380220
C	-2.42806849	4.20790661	-1.06743893
H	-2.54809560	4.47963225	-0.01223524
H	-2.15569512	5.12809144	-1.59570387

C	-3.76853279	3.69707780	-1.62714623
H	-4.05833094	2.77852908	-1.09885283
H	-3.64930949	3.42980581	-2.68304518
C	-4.87874546	4.70010531	-1.48228928
H	-5.11423950	5.00110585	-0.46213134
C	-5.56358764	5.23772309	-2.48682767
H	-5.36362217	4.96915922	-3.51993411
H	-6.35093170	5.96273958	-2.31489230

MP2 Electronic Energy(Ha): 1740.469943533054

B3LYP Electronic Energy(Ha): 1744.964429805197

M06-L Electronic Energy(Ha): 1744.742406738636

Zero point energy correction(kcal/mol): 478.023

Enthalpy correction(kcal/mol): 505.934

Entropy correction(cal/mol): 256.754

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.755

Deuterated enthalpy correction(kcal/mol): 497.148

Deuterated entropy correction(cal/mol): 260.738

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.49806350	0.15464283	-0.71891335
C	0.07593574	-2.13280335	-1.48443783
C	-0.74166653	-1.33758902	-2.34628560
H	-1.81845864	-1.26969641	-2.29914935
C	1.41795133	-1.88606493	-1.90807446
H	2.30421905	-2.31903651	-1.46739977
C	1.41665928	-0.93999436	-2.95688286
H	2.28182414	-0.56502185	-3.47977898
C	0.07256866	-0.59198072	-3.22565346
H	-0.26522905	0.11080956	-3.97352937
B	-0.40091503	-2.88500604	-0.11022056
C	-0.71722639	-4.46313093	-0.21959050

C	0.75467208	-2.47944236	0.98436188
C	-1.65141482	-1.95842810	0.41940237
N	-1.61064369	-0.66403106	0.35736409
N	1.27072384	-1.28882808	0.99965545
O	1.19951259	-3.31035455	1.93683914
O	-2.78096996	-2.48227383	0.92727422
C	-2.91786032	-0.13632339	0.79566450
C	-3.61777466	-1.37840436	1.37230072
C	2.25752232	-1.19944712	2.09190100
C	2.16155204	-2.58642673	2.75913662
N	-1.70290595	3.17457555	2.06441741
H	-2.80013309	0.65615545	1.53379499
H	3.25017548	-0.99322547	1.68417611
C	-2.42037983	3.46304922	3.30739530
H	-3.00203172	4.38416247	3.22003628
H	-3.11668490	2.65433775	3.59313603
C	-1.28745157	3.56368891	4.35570906
C	-0.09659894	2.80511605	3.71076457
H	0.70668006	3.49934710	3.45240991
H	0.32446737	2.03963258	4.36717597
C	-0.66683005	2.18719476	2.41290477
H	-1.12291300	1.21629051	2.68809261
C	0.33169033	1.95350896	1.28319130
H	0.85921360	2.90017981	1.09159048
H	1.09556435	1.26415743	1.66042043
C	-0.58789058	-5.14956939	-1.43573182
H	-0.26895127	-4.60488166	-2.31882014
C	-1.13403358	-5.21771234	0.89064837
H	-1.24954479	-4.73120439	1.85345783
C	-1.40582226	-6.57965687	0.79371150
H	-1.72582178	-7.13108173	1.67224490
C	-0.85777064	-6.51420753	-1.54545456
H	-0.74686171	-7.01194332	-2.50364006

C	-1.26844360	-7.23611320	-0.42877295
H	-1.47962211	-8.29735041	-0.50785266
H	-3.63104724	-1.39120528	2.46450651
H	-4.62568342	-1.54565881	0.99516339
H	-3.46013411	0.27800461	-0.06282223
H	1.76889323	-2.55578468	3.77628857
H	3.09531611	-3.14838758	2.74919348
H	2.00303851	-0.38884843	2.77838967
H	-1.02576712	4.60637647	4.54436419
H	-1.59399978	3.12824958	5.30901462
H	-2.31355621	2.85378763	1.32154548
N	2.25183367	1.27009391	-0.91253403
H	2.27049555	1.96564085	-0.16976611
C	3.46257534	1.44406712	-1.71084641
H	3.33382587	0.95244922	-2.67555210
H	3.61433405	2.51013982	-1.92758277
C	4.73936477	0.88802052	-1.05500308
H	4.60388439	-0.18429298	-0.87743300
H	5.56585471	0.98798683	-1.77057445
C	5.13557265	1.56839531	0.26988453
H	4.33143609	1.45401651	1.00385427
H	6.00622056	1.03830929	0.67713884
C	5.48162666	3.02414346	0.12177867
H	6.27872327	3.25041317	-0.58625311
C	4.90208736	4.02718626	0.77600681
H	4.10495630	3.85331647	1.49307306
H	5.20681832	5.05693470	0.62653588
N	-0.92213004	1.87443075	-1.16216662
C	-0.63599511	3.03849391	-2.00681652
H	-0.44910033	1.97054719	0.04777215
H	-1.89872194	1.60745891	-1.21487673
H	0.41494214	3.29753125	-1.85452567
H	-0.73411235	2.77819530	-3.07179485

C	-1.50226806	4.27077957	-1.70540407
H	-1.39220991	4.53219447	-0.64718680
H	-1.11699968	5.11611998	-2.28709563
C	-2.99337597	4.08523327	-2.03989381
H	-3.39388509	3.24823591	-1.45069973
H	-3.10676109	3.80941523	-3.09472617
C	-3.81490727	5.30896184	-1.74650857
H	-3.78811253	5.65900323	-0.71526096
C	-4.53783081	5.98221949	-2.63652291
H	-4.59072503	5.67351221	-3.67654758
H	-5.10369141	6.86478108	-2.36022702

MP2 Electronic Energy(Ha): 1740.431794771906

B3LYP Electronic Energy(Ha): 1744.929092688667

M06-L Electronic Energy(Ha): 1744.704327180939

Zero point energy correction(kcal/mol): 473.996

Enthalpy correction(kcal/mol): 501.892

Entropy correction(cal/mol): 257.767

Imaginary Frequencies: -1468.35

Deuterated zero point energy correction(kcal/mol): 465.879

Deuterated enthalpy correction(kcal/mol): 494.246

Deuterated entropy correction(cal/mol): 261.591

Deuterated imaginary Frequencies: -1069.67

Product geometry

Zr	-1.06896995	0.25441215	-0.82185824
C	-1.08809375	2.72375485	-0.98294630
C	-1.07684296	2.25664656	-2.33557396
H	-0.23341283	2.30677745	-3.00844914
C	-2.40161765	2.43883805	-0.49844924
H	-2.75591792	2.64438515	0.50213403
C	-3.13253343	1.74589987	-1.48540599
H	-4.14685066	1.38576980	-1.40386133
C	-2.30520030	1.62616034	-2.63534374

H	-2.58394693	1.17329430	-3.57619173
B	0.22237294	3.12532940	-0.08237108
C	0.51668049	4.69734912	0.12328660
C	0.03594648	2.25823153	1.30947620
C	1.45033948	2.25932207	-0.75806417
N	1.28006567	1.02869642	-1.12287605
N	-0.38538623	1.02895240	1.28167180
O	0.35886798	2.72064381	2.52383954
O	2.68787514	2.75418501	-0.93437471
C	2.54506443	0.51469059	-1.67799276
C	3.52188535	1.69232337	-1.47914741
C	-0.37002137	0.47108178	2.64501452
C	0.10584444	1.66479496	3.49847173
N	2.30907526	-3.29590419	0.94645716
H	2.86404498	-0.38556909	-1.14758668
H	-1.36499813	0.11910167	2.92318573
C	3.66836362	-2.79903716	0.72202783
H	3.99676740	-3.00817490	-0.29911036
H	3.75339629	-1.71057149	0.88981752
C	4.49660981	-3.55291765	1.78382027
C	3.46691578	-3.91976754	2.88703303
H	3.36937026	-5.00465534	2.97501167
H	3.74531533	-3.53494448	3.87029064
C	2.13006517	-3.31731321	2.40378660
H	2.05231001	-2.28867586	2.80667853
C	0.89141706	-4.09923449	2.82298114
H	0.94510357	-5.12244806	2.44263947
H	0.80446058	-4.13616947	3.91271329
C	-0.31367345	5.67211816	-0.44910496
H	-1.16797004	5.35652219	-1.03961817
C	1.60881678	5.16172019	0.87660987
H	2.28168239	4.44658503	1.33813831
C	1.85827672	6.52044359	1.04982298

H	2.71171381	6.84303850	1.63797239
C	-0.07397004	7.03659492	-0.28289822
H	-0.73851826	7.76202315	-0.74149952
C	1.01514566	7.46704248	0.46906329
H	1.20673278	8.52665910	0.60181203
H	4.31076259	1.48487557	-0.75434312
H	3.96908575	2.05898499	-2.40296501
H	2.41943569	0.25543796	-2.73440251
H	1.03605618	1.48164726	4.03622580
H	-0.64761890	2.03409253	4.19496466
H	0.31331800	-0.38106749	2.69957701
H	4.93624293	-4.45488520	1.35488020
H	5.31591215	-2.93836630	2.16170710
H	1.60501489	-2.73621478	0.47404929
N	-2.51942200	-1.01182744	-0.01290926
H	-2.13749819	-1.95309412	0.06702219
C	-3.90969758	-1.02535695	0.42836238
H	-4.32408464	-0.02358562	0.29862106
H	-4.50537831	-1.69567672	-0.20853436
C	-4.11952608	-1.43620601	1.89650875
H	-3.57157424	-0.74069833	2.54147936
H	-5.18354911	-1.31375746	2.13640696
C	-3.69463771	-2.87748886	2.24021386
H	-2.62623964	-3.01605783	2.04299572
H	-3.82587833	-3.02062853	3.32052642
C	-4.48530784	-3.93009914	1.51371715
H	-5.56575411	-3.88481948	1.64893958
C	-3.97588268	-4.88714111	0.74298458
H	-2.90615094	-4.97696094	0.57797622
H	-4.60656927	-5.62170223	0.25498438
N	-0.22995034	-1.38612348	-1.84989185
C	-0.82181323	-2.58018087	-2.45653832
H	-0.02128776	-3.63893873	2.43286727

H	0.70880335	-1.25676639	-2.21212768
H	-1.86230798	-2.64949035	-2.12833415
H	-0.85392068	-2.48547897	-3.55370787
C	-0.10568208	-3.89434195	-2.10108258
H	-0.06254017	-3.99303217	-1.01061871
H	-0.70358932	-4.73485547	-2.47262277
C	1.31656655	-4.01076264	-2.67739750
H	1.89808045	-3.13224785	-2.36785452
H	1.27321331	-3.99343233	-3.77262885
C	2.03625061	-5.24373735	-2.20820072
H	2.20037794	-5.29873612	-1.13312693
C	2.45885503	-6.23139210	-2.99250534
H	2.31234952	-6.20772504	-4.06876964
H	2.96705823	-7.10029950	-2.58913720

MP2 Electronic Energy(Ha): 1740.473167368485

B3LYP Electronic Energy(Ha): 1744.991060258857

M06-L Electronic Energy(Ha): 1744.753128539848

Zero point energy correction(kcal/mol): 475.765

Enthalpy correction(kcal/mol): 504.832

Entropy correction(cal/mol): 277.621

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.167

Deuterated enthalpy correction(kcal/mol): 496.706

Deuterated entropy correction(cal/mol): 281.221

Deuterated imaginary Frequencies: -0.00

Axial Reaction H8

Reactant geometry

Zr	-0.57881711	0.74899484	-0.51919559
C	-0.74770482	-1.72423785	-1.21275165
C	-2.06898281	-1.16108027	-1.21274248
H	-2.85342467	-1.41220787	-0.51289458

C	-0.07635313	-1.12124346	-2.30465137
H	0.94566747	-1.32512515	-2.59515325
C	-0.94804138	-0.19557476	-2.94528967
H	-0.72916173	0.38559406	-3.82902369
C	-2.19514871	-0.23932694	-2.27785981
H	-3.07939647	0.32525028	-2.53597821
B	-0.15902158	-2.71407345	-0.06100103
C	-0.84718958	-4.19262014	-0.03626181
C	1.47230371	-2.81096634	-0.21622773
C	-0.42126491	-1.89888580	1.33661832
N	-0.62794951	-0.61633402	1.39631505
N	2.34635098	-1.92066810	0.11156642
O	1.97021084	-3.93773081	-0.79851646
O	-0.45036135	-2.52698984	2.52610104
C	-0.92098928	-0.23641654	2.79226673
C	-0.65185288	-1.53631041	3.56940891
C	3.68286830	-2.41868178	-0.26840516
C	3.41219076	-3.83013497	-0.82738651
N	-1.78823122	2.00810200	0.15283044
N	0.63609422	2.43896862	-1.91872136
C	1.73549822	1.99129663	-2.84897837
H	1.83560491	0.90715553	-2.82143272
H	-0.28825388	0.59115470	3.12590303
H	4.13660262	-1.75530472	-1.01357329
C	-2.96300928	2.73012985	0.54472572
H	-3.22554734	3.49592555	-0.20732993
H	-3.83400387	2.06000618	0.59322521
C	-2.81202748	3.44059040	1.90213378
C	1.35983081	2.51771068	-4.24143906
C	0.56283661	3.78678272	-3.93025075
H	-0.08089010	4.10550695	-4.75262609
H	2.68426143	2.42768387	-2.52562461
H	1.06736716	2.97589460	-1.17132014

C	-0.24524612	3.40954753	-2.67971513
H	-1.13915699	2.85721011	-2.97963734
H	1.24151943	4.61604476	-3.69836959
C	-0.65692320	4.58792699	-1.80987025
H	-1.34091185	5.24069591	-2.35786496
H	-1.15651876	4.23480980	-0.90790196
H	0.21728965	5.18527282	-1.52549623
C	-0.52058841	-5.14378803	0.94699082
H	0.19162239	-4.88345056	1.72281367
C	-1.77513632	-4.59422928	-1.00818367
H	-2.05405477	-3.89922125	-1.79293028
C	-1.08830447	-6.41493222	0.96417466
H	-0.81032851	-7.12060016	1.74124026
C	-2.34965349	-5.86653185	-1.00376828
H	-3.06254945	-6.13899157	-1.77605716
C	-2.01020685	-6.78429140	-0.01466196
H	-2.45489952	-7.77411317	-0.00554471
C	-4.05041864	4.25523967	2.32463285
H	-4.29071558	4.99533099	1.55264283
H	-3.79569472	4.82159186	3.23026143
C	-5.26419716	3.41561475	2.61165683
H	-5.13070848	2.63982759	3.36581690
C	-6.45598157	3.54915206	2.03637624
H	-6.63870569	4.30451420	1.27765980
H	-7.29160591	2.91093849	2.30106759
H	2.24227479	2.69927674	-4.85784011
H	0.73433245	1.79398651	-4.76915340
H	-2.58307171	2.69070779	2.66840960
H	-1.94253160	4.10551156	1.85303018
H	0.25608059	-1.50027704	4.17546705
H	-1.48581353	-1.86609604	4.18839875
H	-1.95715423	0.10254157	2.86555400
H	3.82396617	-4.62939957	-0.20715401

H	3.74494567	-3.97186285	-1.85697974
H	4.34575374	-2.43306515	0.60206490
N	1.61705908	0.90780586	0.66703687
H	1.93558150	-0.07768098	0.55403292
H	1.27278661	0.96487880	1.62230904
C	2.77609915	1.81489004	0.54456845
C	3.82603666	1.62987927	1.64541812
H	3.23731209	1.64308445	-0.43127355
H	2.42056193	2.85226985	0.55833707
H	3.36102613	1.80256419	2.62327418
H	4.16728754	0.58893277	1.64097548
C	5.02959477	2.57601500	1.48656421
H	4.68811743	3.61701732	1.49842925
H	5.48376445	2.40384077	0.50123921
C	6.07223017	2.37690422	2.55093606
H	6.52341779	1.38641170	2.59234355
C	6.45986084	3.29904751	3.42641552
H	6.03804153	4.29987995	3.42323779
H	7.21486836	3.09045060	4.17572467

MP2 Electronic Energy(Ha): 1740.484465609720

B3LYP Electronic Energy(Ha): 1744.984480926708

M06-L Electronic Energy(Ha): 1744.751281168818

Zero point energy correction(kcal/mol): 477.807

Enthalpy correction(kcal/mol): 506.050

Entropy correction(cal/mol): 259.141

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 469.015

Deuterated enthalpy correction(kcal/mol): 497.580

Deuterated entropy correction(cal/mol): 261.102

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.29221075	0.22658619	-0.45291287

C	-0.84969578	-2.15521971	-0.79146725
C	-2.10712170	-1.54036156	-0.47860601
H	-2.64558378	-1.65032332	0.45129350
C	-0.53497453	-1.71415897	-2.10573443
H	0.35170570	-1.99157065	-2.65648507
C	-1.53789116	-0.82086074	-2.56178252
H	-1.57543646	-0.33756221	-3.52694558
C	-2.52075846	-0.72438150	-1.55161039
H	-3.41744659	-0.12399852	-1.59013061
B	0.15436257	-2.90105482	0.26102526
C	0.06566474	-4.51270949	0.32503203
C	1.65758628	-2.29795448	-0.04228639
C	-0.15113428	-2.12179867	1.67975147
N	-0.29857454	-0.83401541	1.69934451
N	1.86545227	-1.06843344	-0.39737117
O	2.76795663	-3.02020203	0.21892894
O	-0.27337257	-2.73515433	2.86845706
C	-0.64154891	-0.40962581	3.06835076
C	-0.47768269	-1.70814358	3.88207211
C	3.31223660	-0.79630734	-0.30789867
C	3.91910341	-2.19458645	-0.10433043
N	-1.41750840	1.76762353	0.07502409
N	0.83269490	1.47014319	-2.29190860
C	1.75398874	0.73326337	-3.23012713
H	1.81256185	-0.31596592	-2.95009268
H	0.02020148	0.38630174	3.41798686
H	3.68432859	-0.30772413	-1.21103552
C	-2.69075999	2.42967679	0.17129169
H	-2.66729478	3.40671511	-0.34599552
H	-3.47771441	1.85046338	-0.33442905
C	-3.14393579	2.69451414	1.61942964
C	1.18484042	0.95731910	-4.63482373
C	0.57031772	2.35570216	-4.53437488

H	-0.16962477	2.56213496	-5.31042382
H	2.75899451	1.16051955	-3.15750368
H	1.40974043	2.07561969	-1.71573617
C	-0.05250511	2.37637920	-3.13030385
H	-1.03727374	1.90739486	-3.16673782
H	1.35269958	3.12012254	-4.60857616
C	-0.19698369	3.76175603	-2.51740318
H	-0.87139828	4.36859165	-3.12700872
H	-0.61136643	3.69352256	-1.51068394
H	0.76879629	4.27743677	-2.47643358
C	0.82161997	-5.27270073	1.23469998
H	1.49077704	-4.76815814	1.92311819
C	-0.78051323	-5.22482760	-0.53811298
H	-1.38494556	-4.67668410	-1.25386384
C	0.73925443	-6.66197021	1.27989520
H	1.33764844	-7.21597692	1.99659442
C	-0.87109893	-6.61685911	-0.50299234
H	-1.53812440	-7.13270527	-1.18672417
C	-0.10974727	-7.34285470	0.40818088
H	-0.17656915	-8.42536628	0.44124460
C	-4.48871752	3.44210631	1.72552003
H	-4.43147376	4.39206986	1.18175376
H	-4.65695037	3.69779398	2.78020020
C	-5.66966470	2.65120333	1.23423962
H	-5.81233899	1.67877672	1.70588693
C	-6.53488731	3.04189067	0.30227705
H	-6.43601988	4.00080183	-0.19815954
H	-7.37326139	2.42098224	0.00648607
H	1.95419790	0.87424454	-5.40474238
H	0.41402462	0.21453342	-4.85643095
H	-3.21590951	1.73635813	2.14802957
H	-2.36973372	3.27567871	2.13212923
H	0.40092146	-1.70522608	4.53044504

H	-1.35532973	-1.98423663	4.46575791
H	-1.66246650	-0.01918048	3.08856972
H	4.62831947	-2.26457264	0.71974566
H	4.37660552	-2.59970821	-1.01028727
H	3.50707921	-0.12760998	0.53690712
N	0.95987223	1.85153233	0.86497416
H	1.06139813	1.44954854	1.79256748
H	-0.26768998	2.17343626	0.65527417
C	2.07315720	2.76478518	0.62904322
C	2.31094162	3.75746759	1.77607316
H	3.01655748	2.22376011	0.44160819
H	1.87442058	3.35011721	-0.27975796
H	1.39003499	4.32098146	1.95490297
H	2.51376927	3.19105768	2.69443865
C	3.47326474	4.72918421	1.50824298
H	3.26268748	5.31723962	0.60794217
H	4.37907402	4.14376584	1.29774655
C	3.74184655	5.65423801	2.66109606
H	4.01640208	5.17248853	3.59904639
C	3.65340359	6.98019015	2.62107553
H	3.37957309	7.50359938	1.70957210
H	3.85219237	7.59110503	3.49429288

MP2 Electronic Energy(Ha): 1740.465041757596

B3LYP Electronic Energy(Ha): 1744.955810622615

M06-L Electronic Energy(Ha): 1744.729385744270

Zero point energy correction(kcal/mol): 474.270

Enthalpy correction(kcal/mol): 502.166

Entropy correction(cal/mol): 254.585

Imaginary Frequencies: -1524.93

Deuterated zero point energy correction(kcal/mol): 466.562

Deuterated enthalpy correction(kcal/mol): 494.766

Deuterated entropy correction(cal/mol): 256.441

Deuterated imaginary Frequencies: -1093.94

Product geometry

Zr	-0.34690299	0.38495017	-0.38505128
C	-1.10676161	-1.89565756	0.29045111
C	-1.56804803	-1.09405112	1.37752230
H	-1.13013367	-1.06559484	2.36436247
C	-1.97914042	-1.59201996	-0.79928563
H	-1.92724501	-2.04263174	-1.77898523
C	-2.90844016	-0.60879009	-0.40374361
H	-3.69981978	-0.19201182	-1.00932263
C	-2.65167890	-0.29814156	0.95176670
H	-3.21323429	0.39650098	1.55702327
B	0.26147922	-2.78061915	0.22587146
C	0.14621352	-4.33111804	0.66427414
C	0.83346519	-2.52471879	-1.29465178
C	1.33731002	-1.88220226	1.07968911
N	1.29873729	-0.58938002	1.02091170
N	0.72832699	-1.37074969	-1.87390739
O	1.50834694	-3.46484679	-1.98514603
O	2.34670800	-2.39568024	1.80414641
C	2.43663466	-0.03175585	1.76866388
C	3.08803894	-1.28446670	2.38864606
C	1.45255617	-1.41884399	-3.15771749
C	1.86632631	-2.89898253	-3.27560494
N	-0.54867958	2.08555280	0.82103924
N	-1.46361372	1.46464542	-2.38935156
C	-1.73325306	0.59636564	-3.58812401
H	-1.59645371	-0.45384987	-3.33618896
H	3.10349848	0.50337934	1.08858333
H	0.81079234	-1.09761189	-3.98126509
C	-1.33081497	2.67901895	1.89781099
H	-1.57371954	3.72920188	1.66494435
H	-2.28676860	2.16224167	1.97651094

C	-0.62590886	2.64542260	3.26338343
C	-3.16947588	0.91512539	-4.02761037
C	-3.34802390	2.37307303	-3.59753123
H	-4.39387569	2.67455961	-3.50666457
H	-1.02319467	0.84686819	-4.38151771
H	-0.60845515	1.98425660	-2.57278784
C	-2.60747688	2.43678134	-2.25280244
H	-3.26461136	2.05149573	-1.46828654
H	-2.86796172	3.04522345	-4.31854953
C	-2.13631329	3.82876756	-1.85504395
H	-2.99384903	4.49897959	-1.75330781
H	-1.60837453	3.79792647	-0.90124682
H	-1.47022594	4.24926086	-2.61614154
C	1.26164325	-5.18640076	0.69391892
H	2.23655228	-4.79967810	0.41739552
C	-1.08549972	-4.89086451	1.03525927
H	-1.97201190	-4.26459185	1.02831754
C	1.15461089	-6.52247723	1.07152788
H	2.03810456	-7.15333780	1.08343878
C	-1.20547582	-6.22828654	1.41495474
H	-2.17592358	-6.62562795	1.69596934
C	-0.08335018	-7.05150235	1.43470331
H	-0.17006380	-8.09208778	1.72986285
C	-1.44625911	3.29000799	4.39866783
H	-1.69696437	4.32443837	4.13713614
H	-0.81319316	3.33945067	5.29382139
C	-2.70217043	2.53631363	4.73952833
H	-2.56137859	1.49574963	5.03146441
C	-3.93592874	3.03332222	4.71615700
H	-4.12790789	4.06406997	4.43240606
H	-4.79715364	2.43208822	4.98523987
H	-3.31539999	0.75490817	-5.09757636
H	-3.87968200	0.27347495	-3.49867709

H	-0.39694081	1.60370329	3.51506050
H	0.33626034	3.16500280	3.18162002
H	4.13957920	-1.41408513	2.13222631
H	2.97165637	-1.34414889	3.47211667
H	2.08704841	0.67875122	2.52082466
H	2.93443799	-3.05466181	-3.42732428
H	1.31127444	-3.44255208	-4.04287651
H	2.31578186	-0.74560569	-3.13666709
N	1.29134919	1.45231127	-1.31330257
H	2.01809464	0.83301554	-1.65688634
H	0.27668609	2.66316585	0.67638610
C	1.75503537	2.82781130	-1.41165696
C	3.00646095	3.15487360	-0.57550595
H	1.97632995	3.10599405	-2.45796988
H	0.94725600	3.50254352	-1.10059201
H	2.80272343	2.94587946	0.47982842
H	3.81652029	2.47717192	-0.87460856
C	3.47451811	4.61338728	-0.72934863
H	2.67365257	5.29396587	-0.41875598
H	3.65860986	4.81154677	-1.79418636
C	4.72146333	4.91632880	0.05144004
H	5.60307646	4.33758689	-0.22291209
C	4.81872640	5.80455117	1.03667536
H	3.96821282	6.40528183	1.34581899
H	5.74993772	5.96781658	1.56742327

MP2 Electronic Energy(Ha): 1740.500180667709

B3LYP Electronic Energy(Ha): 1744.998142183436

M06-L Electronic Energy(Ha): 1744.775734623454

Zero point energy correction(kcal/mol): 476.741

Enthalpy correction(kcal/mol): 505.291

Entropy correction(cal/mol): 265.375

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.262

Deuterated enthalpy correction(kcal/mol): 497.203

Deuterated entropy correction(cal/mol): 267.780

Deuterated imaginary Frequencies: -0.00

Axial Reaction C1

Reactant geometry

Zr	0.31239550	-0.54880293	0.40769290
C	1.11169257	1.69947167	1.08108897
C	0.65485190	1.07570607	2.28550213
H	-0.25059658	1.32859392	2.81736697
C	2.33098113	1.03203048	0.75205587
H	2.94115266	1.24051393	-0.11592142
C	2.56279175	-0.01535100	1.66710617
H	3.39317993	-0.70709827	1.65943066
C	1.51456810	0.00653642	2.62733264
H	1.41949875	-0.64798481	3.48210935
B	0.23541226	2.66736590	0.08704731
C	0.51583935	4.25284276	0.17243607
C	0.44686159	1.99627127	-1.40757357
C	-1.32327955	2.21165335	0.35427302
N	-1.64530839	0.96351981	0.47834959
N	0.39878860	0.70864259	-1.57393016
O	0.65120778	2.70599318	-2.52540043
O	-2.34314046	3.08497703	0.40810082
C	-3.10480848	0.86004354	0.65838701
C	-3.57326288	2.32912187	0.59647443
C	0.64106876	0.38607966	-2.99056686
C	0.69435336	1.77852322	-3.65075005
N	-1.19864519	-1.91572873	0.92675553
H	-3.54956595	0.24670448	-0.12935847
C	-1.17622054	-3.30338392	1.38812885
H	-0.14878940	-3.66925578	1.32477101

H	-1.45410225	-3.35417635	2.45326337
C	-2.08502740	-4.28079824	0.61950831
C	-3.59266976	-3.93019206	0.62507060
H	-4.18758305	-4.84864335	0.61806527
H	-3.83304436	-3.42302864	1.57083630
C	-4.02663187	-3.07086305	-0.53260159
C	1.45180670	4.77742811	1.07575059
H	1.99588337	4.09880633	1.72507362
C	-0.15990978	5.17625931	-0.64390754
H	-0.89488212	4.81964368	-1.35808211
C	0.08381197	6.54469022	-0.56431725
H	-0.45702581	7.22904807	-1.21045816
C	1.70462654	6.14672294	1.16512465
H	2.43621482	6.51608326	1.87684699
C	1.02032469	7.03760330	0.34356131
H	1.21271042	8.10339208	0.40839312
H	-0.16153565	-0.23767790	-3.39054752
H	1.57839534	-0.16742887	-3.09125564
H	-0.16797879	1.99140693	-4.28468727
H	1.60984027	1.97445416	-4.20780557
H	-3.34026700	0.39180832	1.61917856
H	-4.22860574	2.54416683	-0.24839540
H	-4.04312062	2.68093231	1.51526382
H	-1.74091369	-4.36943400	-0.41609297
H	-1.95371654	-5.26851159	1.07700190
H	-2.10955308	-1.51322738	1.12184364
N	1.53738312	-2.00794936	-0.47541858
H	2.54223079	-1.87359634	-0.41611934
C	1.25178165	-3.06706486	-1.44268369
H	0.21942149	-3.40248009	-1.30034806
H	1.30696090	-2.68656721	-2.47560680
C	2.20506992	-4.27030809	-1.35194666
H	3.23106823	-3.91705368	-1.52454363

H	1.97982274	-4.96086154	-2.17268606
C	2.14793313	-5.03419244	-0.01854095
H	1.14583082	-5.45310636	0.12183984
H	2.30981638	-4.31880279	0.79643535
C	3.16982115	-6.13145016	0.06816605
H	4.21037080	-5.81588841	-0.00659336
C	2.90305558	-7.42613992	0.21435438
H	1.88272166	-7.79057284	0.29119745
H	3.69148221	-8.16857651	0.26645668
H	-3.43978800	-2.17166386	-0.70360526
C	-5.03515421	-3.34974494	-1.35421201
H	-5.29750818	-2.69446274	-2.17754726
H	-5.63662402	-4.24629217	-1.23389532

MP2 Electronic Energy(Ha): 1489.152848551836

B3LYP Electronic Energy(Ha): 1493.009758220803

M06-L Electronic Energy(Ha): 1492.814843375796

Zero point energy correction(kcal/mol): 376.811

Enthalpy correction(kcal/mol): 400.554

Entropy correction(cal/mol): 230.316

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.656

Deuterated enthalpy correction(kcal/mol): 396.627

Deuterated entropy correction(cal/mol): 231.691

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.26546943	0.68891667	0.21776379
C	-0.74077720	-1.34522100	1.17487263
C	0.04614592	-0.86508860	2.26771333
H	0.97456624	-1.30133598	2.60595347
C	-1.84810930	-0.44628626	1.08547273
H	-2.64910403	-0.50953004	0.36320660
C	-1.71293313	0.56533414	2.06377619

H	-2.38813826	1.39303332	2.23158881
C	-0.53587318	0.30319238	2.79857518
H	-0.14412554	0.90585089	3.60527381
B	-0.32081584	-2.50865677	0.10810479
C	-0.85592711	-4.00072351	0.41601259
C	-0.75581466	-1.88735556	-1.34938651
C	1.31214872	-2.36659429	-0.00216985
N	1.90104639	-1.21143832	0.01457599
N	-0.58045801	-0.62986770	-1.60184903
O	-1.26123385	-2.61402031	-2.36098202
O	2.11803485	-3.42983661	-0.17806939
C	3.34505982	-1.41788334	-0.21147654
C	3.48967476	-2.95192085	-0.21631433
C	-1.02754098	-0.33912369	-2.97348975
C	-1.44948631	-1.72669631	-3.50185840
N	1.93806053	1.71768708	1.27574218
H	3.64881918	-0.97152727	-1.16340604
C	2.05172658	3.09479647	1.74938698
H	1.19286735	3.38840444	2.36890631
H	2.95052996	3.21131371	2.36830415
C	2.15388061	4.01761684	0.53188582
C	3.12869780	3.35502775	-0.45121540
H	3.14220964	3.89186462	-1.40439353
H	4.14096441	3.40101312	-0.03628119
C	2.76388657	1.90516903	-0.70391735
C	-1.60573585	-4.28048044	1.56801034
H	-1.83280824	-3.47406616	2.25812368
C	-0.59323592	-5.08160273	-0.44358690
H	-0.01861514	-4.91546424	-1.34857315
C	-1.05073869	-6.36779294	-0.16931012
H	-0.82875892	-7.17864715	-0.85618638
C	-2.06920964	-5.56522505	1.85400702
H	-2.64640772	-5.74342231	2.75595450

C	-1.79267095	-6.61646929	0.98480062
H	-2.15036111	-7.61760799	1.20178342
H	-0.21827603	0.10606428	-3.55768006
H	-1.85606240	0.37377646	-2.95493928
H	-0.82176067	-2.09495686	-4.31479445
H	-2.49623774	-1.78645431	-3.80036206
H	3.93527839	-0.94947384	0.58066834
H	3.96203289	-3.35212616	-1.11332638
H	4.00264823	-3.34109976	0.66519786
H	1.17083517	4.11815109	0.06894595
H	2.48942066	5.01992181	0.81400744
H	2.53274892	1.09689704	1.81303752
N	-0.97104744	2.31281490	-0.32558062
H	-1.84666834	2.28245841	0.18493143
C	-1.11954148	3.29929759	-1.39469297
H	-0.14380217	3.73037704	-1.64388832
H	-1.48168467	2.82606476	-2.32113307
C	-2.08874671	4.44162648	-1.05073795
H	-3.07619085	4.01273845	-0.83207633
H	-2.22094670	5.07232380	-1.93708853
C	-1.63977298	5.32001720	0.13039966
H	-0.68709518	5.80271568	-0.11296373
H	-1.45147719	4.67190182	0.99460529
C	-2.65261669	6.36516323	0.50124496
H	-3.62963195	5.99084775	0.80635586
C	-2.45017223	7.67935090	0.47565700
H	-1.49457119	8.10083979	0.17720554
H	-3.22728318	8.38188346	0.75496782
H	3.54470862	1.19468062	-0.46707502
C	1.79158188	1.49327863	-1.62203259
H	1.93152646	0.54274068	-2.12400883
H	1.24513693	2.24450886	-2.17948392

MP2 Electronic Energy(Ha): 1489.143229691771

B3LYP Electronic Energy(Ha): 1492.978668277293

M06-L Electronic Energy(Ha): 1492.801266791638

Zero point energy correction(kcal/mol): 377.136

Enthalpy correction(kcal/mol): 399.799

Entropy correction(cal/mol): 217.240

Imaginary Frequencies: -292.47

Deuterated zero point energy correction(kcal/mol): 372.399

Deuterated enthalpy correction(kcal/mol): 395.425

Deuterated entropy correction(cal/mol): 220.791

Deuterated imaginary Frequencies: -289.88

Product geometry

Zr	0.20102397	0.67277353	0.13843258
C	-0.70575015	-1.36752859	1.21324354
C	0.13374913	-0.79875277	2.21857582
H	1.09697823	-1.18380356	2.51844742
C	-1.86375206	-0.52931218	1.17204802
H	-2.70743744	-0.66336508	0.50986708
C	-1.71303409	0.53375390	2.08498344
H	-2.41795530	1.33388364	2.26396316
C	-0.46269964	0.37785944	2.72820344
H	-0.06123367	1.01972590	3.50040794
B	-0.30712067	-2.53690797	0.14521448
C	-0.82238106	-4.03131405	0.47754538
C	-0.78444467	-1.93388341	-1.31268311
C	1.31818391	-2.38018338	-0.04058481
N	1.90086805	-1.22373304	-0.02918498
N	-0.66092662	-0.67017990	-1.57539006
O	-1.22791509	-2.68717982	-2.33153388
O	2.11135923	-3.43432261	-0.31776494
C	3.32254045	-1.41249659	-0.37538254
C	3.47059552	-2.94421057	-0.46749471
C	-1.04147443	-0.41490871	-2.97341838

C	-1.47387108	-1.81037575	-3.47094285
N	2.10128782	1.79801561	1.05949881
H	3.54943443	-0.91119922	-1.32048710
C	2.02248649	3.12242657	1.74733270
H	1.06793401	3.23042193	2.26380459
H	2.82550532	3.20537225	2.48819890
C	2.21967813	4.14876615	0.62911242
C	3.23174670	3.46115813	-0.29621357
H	3.25277687	3.88205681	-1.30224610
H	4.23868025	3.55337404	0.12746131
C	2.78731598	1.98411261	-0.31616514
C	-1.53587115	-4.30607115	1.65376120
H	-1.74429470	-3.49566947	2.34508027
C	-0.58193101	-5.11751320	-0.38215783
H	-0.03464171	-4.95578660	-1.30429259
C	-1.02753590	-6.40298178	-0.08547530
H	-0.82386207	-7.21777035	-0.77340967
C	-1.98695178	-5.59003264	1.96214536
H	-2.53622558	-5.76367761	2.88228694
C	-1.73416418	-6.64619019	1.09168247
H	-2.08294455	-7.64672816	1.32545459
H	-0.19053192	-0.01046420	-3.52739994
H	-1.85068052	0.31729055	-3.01998005
H	-0.88515764	-2.18371935	-4.30921991
H	-2.53439575	-1.87817448	-3.71649258
H	3.97293695	-0.98453888	0.39301758
H	3.85293058	-3.29757286	-1.42538172
H	4.07052343	-3.37103917	0.33844625
H	1.27468115	4.31460007	0.10882975
H	2.56631918	5.10987788	1.01396612
H	2.62774057	1.14729409	1.63251736
N	-1.05216028	2.30836174	-0.31772333
H	-1.91099377	2.30133267	0.22201955

C	-1.20664335	3.28258192	-1.39779344
H	-0.22709327	3.68775726	-1.67165770
H	-1.59240623	2.80027428	-2.30950388
C	-2.15287521	4.44411098	-1.05659011
H	-3.14184144	4.03419728	-0.80994470
H	-2.29424267	5.06038478	-1.95167291
C	-1.66937782	5.33921667	0.09790694
H	-0.71780915	5.80809303	-0.17588429
H	-1.46896896	4.70435618	0.96941125
C	-2.66419498	6.40047209	0.47172812
H	-3.63546528	6.03997658	0.81001461
C	-2.45513278	7.71238747	0.40896822
H	-1.50559634	8.12088329	0.07517081
H	-3.22130468	8.42613344	0.69015100
H	3.65861963	1.32755288	-0.32698636
C	1.76719527	1.56234523	-1.37215212
H	2.19922692	0.87102839	-2.10008991
H	1.38596638	2.42539176	-1.92435394

MP2 Electronic Energy(Ha): 1489.171504724978

B3LYP Electronic Energy(Ha): 1493.002039881756

M06-L Electronic Energy(Ha): 1492.821012713729

Zero point energy correction(kcal/mol): 378.857

Enthalpy correction(kcal/mol): 401.478

Entropy correction(cal/mol): 218.692

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.950

Deuterated enthalpy correction(kcal/mol): 396.903

Deuterated entropy correction(cal/mol): 222.188

Deuterated imaginary Frequencies: -0.00

Axial Reaction C2

Reactant geometry

Zr	0.96949204	-1.20163706	0.08376824
C	1.66126124	1.17895330	0.11333022
C	2.25203900	0.63034326	1.29399164
H	1.92900444	0.83127398	2.30596387
C	2.41051809	0.61942837	-0.96713759
H	2.23140818	0.80894962	-2.01644772
C	3.36497184	-0.30362129	-0.47129531
H	4.07540063	-0.87219629	-1.05445372
C	3.26633002	-0.29596626	0.94543876
H	3.88794337	-0.85819175	1.62760836
B	0.13327256	1.78270321	0.00302789
C	-0.02466731	3.38895128	-0.01478942
C	-0.53794558	1.01680962	-1.31886887
C	-0.72301671	1.02679861	1.21861521
N	-0.55753155	-0.23232553	1.51614616
N	-0.35306856	-0.25085634	-1.56940947
O	-1.35914393	1.64128016	-2.16751553
O	-1.68301228	1.64416016	1.91262267
C	-1.50434738	-0.62375654	2.57588138
C	-2.27877957	0.68383435	2.83940936
C	-1.14618171	-0.64274355	-2.74866079
C	-1.77925250	0.69097918	-3.19351259
N	0.95176702	-3.07096280	0.14296556
H	-2.14095931	-1.43975756	2.22820121
H	-0.50192948	-1.07907936	-3.51480324
C	1.17943859	-4.48359019	0.23215924
H	2.21613581	-4.71843675	-0.05546432
H	1.07266257	-4.82593119	1.27474583
C	0.25058585	-5.34037574	-0.65007572
C	-1.20583495	-5.47864319	-0.16923334
H	-1.66937792	-6.27761040	-0.76546322
H	-1.22310707	-5.82841800	0.86949272
C	-2.07801972	-4.26177686	-0.30577577

C	-2.96821823	-3.84225510	0.59072934
C	1.10394190	4.21788388	0.06593060
H	2.08603524	3.76216175	0.14009488
C	-1.27293836	4.02848268	-0.10898087
H	-2.17638827	3.43165333	-0.17319738
C	-1.38880060	5.41587162	-0.12216043
H	-2.36917162	5.87598007	-0.19596126
C	1.00035392	5.60914653	0.05371614
H	1.89633543	6.21831195	0.11803068
C	-0.24904911	6.21486482	-0.04062883
H	-0.33598843	7.29625250	-0.05054142
H	0.26870634	-4.93820057	-1.66991909
H	0.67722007	-6.34936199	-0.70490029
H	-3.34217893	0.62256915	2.60720557
H	-2.15020122	1.07899099	3.84686315
H	-0.95989638	-0.97374181	3.45607217
H	-2.86865353	0.68375319	-3.20952573
H	-1.40471439	1.05650742	-4.15004697
H	-1.89056669	-1.39229952	-2.46889638
H	-3.61279410	-2.99140359	0.39721932
H	-3.09106893	-4.34152633	1.54747958
H	-1.99515112	-3.73050508	-1.25249285

MP2 Electronic Energy(Ha): 1237.819107915316

B3LYP Electronic Energy(Ha): 1241.006990540654

M06-L Electronic Energy(Ha): 1240.848972142870

Zero point energy correction(kcal/mol): 278.903

Enthalpy correction(kcal/mol): 297.192

Entropy correction(cal/mol): 192.400

Imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.05801786	-1.47782403	0.27417967
C	0.05845979	0.71376471	1.42047457

C	-1.07661086	0.10337173	2.03119577
H	-2.10455987	0.39991927	1.87578823
C	1.18536133	-0.03637746	1.89122384
H	2.21653267	0.14990594	1.62614117
C	0.74415608	-1.10701673	2.70566558
H	1.36880942	-1.83775037	3.19888987
C	-0.66935311	-1.02168928	2.78682439
H	-1.31387090	-1.68185759	3.34983079
B	0.03377618	1.72892682	0.12542319
C	0.11052605	3.31159489	0.42642765
C	1.22255025	1.14842032	-0.85752568
C	-1.28575555	1.25342932	-0.75228920
N	-1.54567719	0.00506549	-0.99150063
N	1.33217538	-0.12601261	-1.06367187
O	2.11204372	1.91243685	-1.50933079
O	-2.14948271	2.13458690	-1.28822442
C	-2.79537855	-0.08288516	-1.76802104
C	-3.10842194	1.39045053	-2.09105678
C	2.46555735	-0.38726005	-1.96451702
C	2.95648838	1.03434588	-2.31323392
N	0.90839959	-3.11750862	-0.10434463
H	-2.65545845	-0.68856164	-2.66674076
H	3.22338598	-0.98557913	-1.45218489
C	1.69832053	-4.31321809	0.01928695
H	2.54022988	-4.30071240	-0.68598216
H	2.13152869	-4.37880949	1.02860505
C	0.80985945	-5.55103553	-0.23723576
C	-0.59063422	-5.17522282	0.24115063
H	-1.32795048	-5.92819652	-0.06279979
H	-0.63267928	-5.09952986	1.33232593
C	-0.98344204	-3.85941827	-0.38012196
C	-1.94388101	-2.96446690	0.17235911
C	0.18077126	3.80328946	1.73789893

H	0.18011372	3.10026339	2.56493931
C	0.11605803	4.26544429	-0.60616207
H	0.06383031	3.93458725	-1.63840930
C	0.18698867	5.63127892	-0.34665329
H	0.18909753	6.33921050	-1.16967789
C	0.25217551	5.16991414	2.01115615
H	0.30566954	5.51364590	3.03939644
C	0.25549592	6.09119276	0.96796008
H	0.31112479	7.15495083	1.17426129
H	0.77751193	-5.76927213	-1.31030820
H	1.19850978	-6.44107696	0.26431027
H	-2.93490925	1.64878626	-3.13775884
H	-4.10886189	1.71013100	-1.80151712
H	-3.58021842	-0.55193248	-1.16672229
H	2.80770347	1.30282809	-3.36008879
H	3.99264693	1.22691138	-2.03534585
H	2.13772693	-0.94827717	-2.84267628
H	-2.68957842	-2.55502910	-0.49913603
H	-2.30386453	-3.17768952	1.17573229
H	-0.94115689	-3.88297813	-1.46695528

MP2 Electronic Energy(Ha): 1237.833178391669

B3LYP Electronic Energy(Ha): 1241.004248688438

M06-L Electronic Energy(Ha): 1240.856906353615

Zero point energy correction(kcal/mol): 279.199

Enthalpy correction(kcal/mol): 296.396

Entropy correction(cal/mol): 179.121

Imaginary Frequencies: -279.43

Product geometry

Zr	0.13823822	-1.40870966	0.22805355
C	1.33785576	0.70713089	0.54776130
C	1.43385686	0.02659194	1.80287738
H	0.89514108	0.28824339	2.70156041

C	2.24432802	0.01758237	-0.31859715
H	2.41436370	0.25573018	-1.35890101
C	2.80521813	-1.08629015	0.35014751
H	3.49623260	-1.80410625	-0.06673789
C	2.29379771	-1.09302406	1.67402566
H	2.55979165	-1.79238690	2.45465970
B	0.15755254	1.73989672	0.07025175
C	0.51238696	3.31379083	0.06143727
C	-0.32961048	1.13080159	-1.39664392
C	-1.15729724	1.31911598	0.97987134
N	-1.38873835	0.08519192	1.31155087
N	-0.36662618	-0.15327349	-1.62213111
O	-0.79018240	1.88681319	-2.39620300
O	-2.11197078	2.19527844	1.33037282
C	-2.70809395	-0.00325006	1.96110102
C	-3.12355929	1.47486008	2.09621812
C	-0.94274923	-0.41100373	-2.95364039
C	-1.17533685	1.01209030	-3.50133754
N	0.59261158	-3.32997737	-0.37038856
H	-3.38910507	-0.58515222	1.33498380
H	-0.24591330	-0.98894394	-3.56418972
C	1.55657271	-4.41325473	-0.50093406
H	1.89798269	-4.50485629	-1.54190118
H	2.44358423	-4.21716337	0.10739660
C	0.80913243	-5.71621989	-0.06755652
C	-0.61084717	-5.24604819	0.31570430
H	-1.38597461	-5.97409602	0.06273891
H	-0.67427018	-5.04907456	1.39132942
C	-0.77262676	-3.91601120	-0.44106070
C	-1.69553876	-2.82976751	0.12424653
C	1.77831445	3.76690825	0.46111756
H	2.52150830	3.04229962	0.77835337
C	-0.41273021	4.29363618	-0.33894748

H	-1.40597620	3.99309360	-0.65393973
C	-0.09224997	5.64869474	-0.34093814
H	-0.83148507	6.37843531	-0.65605408
C	2.11047137	5.12197846	0.46356055
H	3.10030931	5.43543175	0.77991457
C	1.17447394	6.07017878	0.06125867
H	1.42686257	7.12534887	0.06087353
H	0.77294390	-6.42688820	-0.89726081
H	1.31429545	-6.21628659	0.76168279
H	-4.09635671	1.70944792	1.66546519
H	-3.08312564	1.84436579	3.12227664
H	-2.63110734	-0.50630108	2.92741423
H	-2.21464909	1.22954801	-3.74581776
H	-0.54179226	1.26313505	-4.35231229
H	-1.86671587	-0.98649270	-2.85869999
H	-2.56778268	-2.61915593	-0.50060138
H	-2.06302725	-3.10467402	1.12245042
H	-1.02114004	-4.14186445	-1.49268926

MP2 Electronic Energy(Ha): 1237.841055407549

B3LYP Electronic Energy(Ha): 1241.015895414307

M06-L Electronic Energy(Ha): 1240.867975109608

Zero point energy correction(kcal/mol): 279.804

Enthalpy correction(kcal/mol): 297.313

Entropy correction(cal/mol): 186.174

Imaginary Frequencies: -0.00

Axial Reaction H2

Reactant geometry

Zr	-0.47332064	0.65317216	0.05609527
C	0.72557450	-1.21533984	1.13602741
C	1.74362762	-0.23181085	0.95932140
H	2.54527381	-0.28742808	0.23628429

C	-0.09734093	-0.71717234	2.19546053
H	-0.97850719	-1.20475157	2.58558465
C	0.37593986	0.54187150	2.61924702
H	-0.05865930	1.16161754	3.38991980
C	1.51998258	0.84877808	1.84968237
H	2.13336249	1.73133061	1.95889859
B	0.35821343	-2.46184728	0.14403448
C	0.97122000	-3.90472724	0.53123518
C	-1.28795561	-2.39202932	0.04272613
C	0.70114062	-1.93986678	-1.38089641
N	0.55493763	-0.70122431	-1.73889325
N	-1.88949316	-1.24598082	-0.02018370
O	-2.08763570	-3.46691622	-0.04151670
O	0.97181948	-2.80058253	-2.38105902
C	0.64185947	-0.62268610	-3.20987273
C	1.12266904	-2.03022030	-3.60541741
C	-3.33999218	-1.45888450	-0.15174812
C	-3.46067964	-2.99708246	-0.18934215
N	1.01280203	2.24455600	-1.11267605
N	-1.85391287	1.99750315	0.80583988
C	-2.36664073	2.88235255	1.83192301
H	-1.59980177	3.12131573	2.57355022
H	-0.34155868	-0.37495671	-3.62032946
H	-3.86416544	-1.01654548	0.69927434
C	1.92270224	3.28844465	-0.57297462
H	2.66124989	2.78872395	0.05741440
H	2.47118777	3.77127905	-1.38914445
C	1.17013484	4.33895228	0.23733911
C	-2.89382175	4.14585966	1.07579564
C	-2.89223551	3.74103178	-0.42062495
H	-2.05016122	4.20414290	-0.94501166
H	-3.19934462	2.40627264	2.37346908
C	-2.69613726	2.21064877	-0.39799493

H	-3.68586295	1.75117931	-0.22149127
H	-3.80571439	4.03579241	-0.94384765
C	-1.96963972	1.50821909	-1.55558755
H	-1.59862769	2.23817599	-2.28787260
H	0.35074669	2.66923383	-1.75818245
H	-2.61533717	0.81770994	-2.10403186
C	0.67331322	-5.06955171	-0.19763050
H	0.00647214	-5.00809002	-1.05043522
C	1.83840290	-4.05087434	1.62432789
H	2.09173117	-3.17706726	2.21624804
C	1.21039778	-6.30805957	0.14408505
H	0.95718682	-7.18676397	-0.44099568
C	2.38329641	-5.28640810	1.97573204
H	3.05039567	-5.36017368	2.82895391
C	2.07085662	-6.42269275	1.23520581
H	2.49040138	-7.38654164	1.50410433
C	2.09789467	5.42496820	0.81621875
H	2.86896275	4.96200667	1.44204673
H	1.49814969	6.05903413	1.48015139
C	2.74538124	6.29254706	-0.22826365
H	2.06045906	6.82716055	-0.88628680
C	4.05472867	6.45482528	-0.39583590
H	4.77653683	5.94763859	0.23766463
H	4.45381781	7.10723235	-1.16424476
H	2.17672710	-2.06049256	-3.89003296
H	1.34054366	0.15480820	-3.53262438
H	0.52535953	-2.50900958	-4.38053762
H	-3.84214111	-3.38480415	-1.13489726
H	-4.04341441	-3.41388274	0.63234936
H	-3.71497949	-0.98239424	-1.05987715
H	-3.89493617	4.41462584	1.42156722
H	-2.25082629	5.01065733	1.25579185
H	0.40919501	4.81104046	-0.39589833

H 0.62926400 3.84609232 1.04878074

H 1.55689370 1.58763705 -1.66712817

MP2 Electronic Energy(Ha): 1489.173242207166

B3LYP Electronic Energy(Ha): 1492.999576728057

M06-L Electronic Energy(Ha): 1492.819406467995

Zero point energy correction(kcal/mol): 378.833

Enthalpy correction(kcal/mol): 401.565

Entropy correction(cal/mol): 220.200

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.404

Deuterated enthalpy correction(kcal/mol): 397.312

Deuterated entropy correction(cal/mol): 221.319

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr -0.26812026 0.66144700 0.05766371

C 0.61677167 -1.30304333 1.22169579

C 1.72384415 -0.40068777 1.19899850

H 2.60334294 -0.50669633 0.58068888

C -0.31099801 -0.73425798 2.15026806

H -1.27534537 -1.14818564 2.40624933

C 0.18884207 0.49764601 2.63072076

H -0.29998975 1.15636913 3.33309376

C 1.45720184 0.70614488 2.03749536

H 2.10594423 1.55397230 2.20481939

B 0.30908333 -2.50425468 0.14819376

C 0.75535290 -3.99247812 0.57562916

C -1.29288102 -2.31566691 -0.19496077

C 0.92514887 -1.96461168 -1.28158918

N 0.83698326 -0.72029841 -1.63440470

N -1.77680012 -1.13045253 -0.39816961

O -2.17353172 -3.32229212 -0.29961869

O 1.43377610 -2.79341752 -2.20909042

C	1.29172897	-0.58346404	-3.03012784
C	1.80913087	-1.99579114	-3.36788579
C	-3.22566982	-1.22982009	-0.64007689
C	-3.45889320	-2.75306025	-0.69200288
N	1.09410427	2.20730084	-0.92220120
N	-1.85012008	1.87336840	0.60488598
C	-2.64026605	2.49148956	1.65368324
H	-2.07749239	2.56931475	2.58609100
H	0.45811393	-0.27249299	-3.66682091
H	-3.77196189	-0.74487029	0.17332368
C	1.83479501	3.35828975	-0.39029877
H	2.60809984	3.02388883	0.31992941
H	2.36632876	3.86076695	-1.20680158
C	0.94245720	4.37726889	0.31522236
C	-3.06875335	3.87972816	1.08761874
C	-2.80469185	3.78189724	-0.43743801
H	-1.95167999	4.40097988	-0.72333546
H	-3.53861492	1.88964077	1.86638338
C	-2.47022950	2.29406686	-0.67260094
H	-3.43125133	1.76024150	-0.79055537
H	-3.65967970	4.10217991	-1.03856643
C	-1.49907377	1.95433087	-1.81690875
H	-1.47119955	2.76037946	-2.55831629
H	-0.09123885	2.24225801	-1.47686014
H	-1.80603267	1.06047316	-2.37198833
C	0.49674158	-5.11026454	-0.23621054
H	-0.01992445	-4.97531637	-1.18049033
C	1.42406786	-4.23187227	1.78494309
H	1.64002911	-3.39623841	2.44321840
C	0.88523249	-6.39417109	0.13602070
H	0.66896163	-7.23467331	-0.51589456
C	1.81889937	-5.51387274	2.16848630
H	2.33518258	-5.66088254	3.11186606

C	1.55075694	-6.60221483	1.34349590
H	1.85514352	-7.60147057	1.63636061
C	1.73688259	5.53461002	0.95002430
H	2.46425853	5.13820805	1.66749848
H	1.03572621	6.15195742	1.52556135
C	2.44048265	6.41079322	-0.04949135
H	1.80216766	6.86634250	-0.80660002
C	3.74515937	6.66791604	-0.07200902
H	4.42169265	6.23832503	0.66101718
H	4.18465780	7.32015134	-0.81838562
H	2.89458710	-2.04701104	-3.46755172
H	2.07575426	0.17345727	-3.12008508
H	1.34423071	-2.44255667	-4.24631375
H	-3.69033085	-3.12089265	-1.69316038
H	-4.21049772	-3.11396921	0.00927546
H	-3.49984810	-0.72914552	-1.57096153
H	-4.11793975	4.08679981	1.31117625
H	-2.47984875	4.68215433	1.53695656
H	0.21980036	4.78140223	-0.40163292
H	0.35715616	3.87439188	1.09082197
H	1.68772648	1.70696107	-1.57483761

MP2 Electronic Energy(Ha): 1489.142981072868

B3LYP Electronic Energy(Ha): 1492.967907349017

M06-L Electronic Energy(Ha): 1492.787102220639

Zero point energy correction(kcal/mol): 375.194

Enthalpy correction(kcal/mol): 397.796

Entropy correction(cal/mol): 222.564

Imaginary Frequencies: -1511.60

Deuterated zero point energy correction(kcal/mol): 371.809

Deuterated enthalpy correction(kcal/mol): 394.565

Deuterated entropy correction(cal/mol): 223.439

Deuterated imaginary Frequencies: -1102.74

Product geometry

Zr	0.02318084	0.64912025	0.10946822
C	0.51697418	-1.46210083	1.31294638
C	1.70255546	-0.66978828	1.43456896
H	2.62927952	-0.84703491	0.90868674
C	-0.44039756	-0.84209897	2.17058929
H	-1.46158442	-1.16823161	2.30993509
C	0.11502563	0.32682520	2.73544567
H	-0.37171451	0.99556468	3.42859453
C	1.45330211	0.43740528	2.27557270
H	2.15825816	1.21031794	2.54446259
B	0.20162813	-2.58124632	0.15679375
C	0.41704891	-4.12849464	0.55615909
C	-1.32056030	-2.18862367	-0.34836898
C	1.04155132	-2.06971706	-1.15903791
N	1.12797889	-0.80826459	-1.44722839
N	-1.64424690	-0.95977335	-0.61560168
O	-2.30862032	-3.08667683	-0.48076451
O	1.57764025	-2.90438040	-2.06304876
C	1.76871390	-0.65546578	-2.76543698
C	2.18715432	-2.09775119	-3.11289398
C	-3.08689568	-0.90310257	-0.91831314
C	-3.47826710	-2.38973346	-1.00015121
N	1.30681365	2.02850190	-0.82439356
N	-1.55428145	2.02936114	0.38188535
C	-2.19307289	2.56772225	1.58884590
H	-1.54159708	2.49417410	2.45686197
H	1.05786979	-0.23550171	-3.48291579
H	-3.61164963	-0.37193585	-0.11907079
C	1.43815607	3.48016925	-0.75398547
H	1.48692099	3.91655119	-1.76639662
H	0.53726227	3.88505742	-0.28814353
C	2.67257073	3.95681396	0.02741550

C	-2.55866741	4.03447078	1.25185131
C	-2.65070100	4.04913447	-0.29180543
H	-1.87986662	4.69362212	-0.72236505
H	-3.11442974	2.00587752	1.81941904
C	-2.39530792	2.57965078	-0.70310183
H	-3.37068361	2.06023784	-0.66761876
H	-3.61801642	4.40327495	-0.65830453
C	-1.84424178	2.42865088	-2.11882471
H	-2.55637564	2.85116484	-2.83388487
H	-0.89144623	2.94636228	-2.23355654
H	-1.69520385	1.37974056	-2.39522051
C	0.14643926	-5.17612778	-0.34107453
H	-0.22138795	-4.94546987	-1.33555136
C	0.89115806	-4.49236165	1.82501389
H	1.11097052	-3.71414498	2.54903262
C	0.33810802	-6.51054729	0.00679368
H	0.11833044	-7.29396644	-0.71177888
C	1.08753136	-5.82596559	2.18535904
H	1.45587739	-6.06942881	3.17696153
C	0.81117751	-6.84246396	1.27576881
H	0.96148871	-7.88128748	1.55038922
C	2.83068548	5.48988596	0.06743812
H	2.85583744	5.88897737	-0.95299502
H	3.80441369	5.72265510	0.51734214
C	1.75948822	6.18988290	0.85699270
H	1.65575400	5.86995523	1.89379087
C	0.95863669	7.14887063	0.39990012
H	1.02328781	7.50263846	-0.62494259
H	0.21461954	7.61954432	1.03276751
H	3.26560348	-2.25854756	-3.06787108
H	2.62339693	0.02283640	-2.71292697
H	1.80834963	-2.45439185	-4.07022900
H	-3.64091181	-2.73656940	-2.02280808

H -4.33319763 -2.66563941 -0.38425704

H -3.27368091 -0.37042912 -1.85249723

H -3.49204937 4.33597848 1.73362687

H -1.77669491 4.71311654 1.59871039

H 2.62157405 3.56200531 1.04864643

H 3.57146200 3.52190489 -0.42649062

H 2.13955732 1.64128756 -1.26022811

MP2 Electronic Energy(Ha): 1489.188406530259

B3LYP Electronic Energy(Ha): 1493.023704640264

M06-L Electronic Energy(Ha): 1492.840018396700

Zero point energy correction(kcal/mol): 378.354

Enthalpy correction(kcal/mol): 401.330

Entropy correction(cal/mol): 221.895

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.266

Deuterated enthalpy correction(kcal/mol): 397.444

Deuterated entropy correction(cal/mol): 223.207

Deuterated imaginary Frequencies: -0.00

Axial Reaction H3

Reactant geometry

Zr -0.41666062 0.97161308 -0.10666419

C 0.09457245 -1.09162548 -1.35326656

C -1.09240197 -0.62363339 -1.99348066

H -2.06972193 -1.07803965 -1.90708734

C 1.11829543 -0.16541049 -1.73441058

H 2.14918884 -0.21016672 -1.41523513

C 0.55928953 0.87358894 -2.50962984

H 1.08543371 1.71887045 -2.92840987

C -0.82321504 0.58814540 -2.66870091

H -1.52528247 1.18017339 -3.23634308

B 0.18256756 -2.19487046 -0.14443992

C	0.49709535	-3.71890201	-0.56789242
C	1.20989708	-1.53347520	0.95611134
C	-1.22323265	-1.97322219	0.69982952
N	-1.62927043	-0.78369503	1.02567021
N	1.20800821	-0.25909230	1.19822651
O	1.97993653	-2.27361477	1.77142984
O	-2.01545567	-2.98043615	1.09798153
C	-2.92345154	-0.88989120	1.72189464
C	-3.10732889	-2.41234372	1.87861897
C	2.00688912	-0.00592190	2.41269928
C	2.69804130	-1.35896963	2.65070824
N	0.66978051	2.65908621	0.51262903
N	-2.20756275	2.07093842	-0.10859268
C	-2.57774323	2.73605840	1.15286437
H	-2.17416540	3.75990379	1.19960947
H	-2.89173548	-0.37241131	2.68364001
H	2.71546291	0.80720595	2.26074049
C	2.07485225	3.02008505	0.64363290
H	2.30125998	3.37654341	1.66295179
H	2.68429112	2.12548489	0.49118546
C	2.52718317	4.10107391	-0.34971619
C	-4.13063313	2.78000676	1.20057247
C	-4.57757624	2.30590580	-0.20133908
H	-5.38078875	2.91946727	-0.61679988
H	-2.15328388	2.20967105	2.01633517
C	-3.29113325	2.35730162	-1.05871359
H	-4.94480924	1.27719392	-0.15815285
C	0.69715488	-4.07199549	-1.91063562
H	0.63602435	-3.30193942	-2.67316808
C	0.58635154	-4.75575236	0.37716141
H	0.44206445	-4.53265726	1.42893134
C	0.97196984	-5.38442868	-2.29644574
H	1.12104584	-5.61956886	-3.34560546

C	0.86007189	-6.06904834	0.00451199
H	0.92207634	-6.84435343	0.76179500
C	1.05466327	-6.39041903	-1.33827307
H	1.26802459	-7.41284952	-1.63204629
C	4.01272075	4.48989765	-0.21200991
H	4.21793918	4.82322378	0.81167148
H	4.20383113	5.35130458	-0.86459556
C	4.96350649	3.38593188	-0.58409817
H	4.85015486	2.98803961	-1.59249591
C	5.91020198	2.87867358	0.20113652
H	6.06512212	3.24365839	1.21242676
H	6.57044232	2.08908260	-0.13991080
H	-4.04278344	-2.79500388	1.47166446
H	-3.70893463	-0.42769337	1.11873719
H	-2.99177677	-2.75939313	2.90705765
H	2.61508778	-1.73825659	3.66833567
H	3.74647486	-1.36350500	2.34495380
H	1.34329947	0.27797107	3.23651588
H	-4.52721748	2.13259665	1.98548149
H	-4.48073667	3.79179034	1.41714568
H	2.32615691	3.75206131	-1.36895812
H	1.91230146	4.99732232	-0.20336135
H	0.09973587	3.50145676	0.54411850
H	-3.31362490	1.57704515	-1.82254849
C	-3.11474663	3.71402870	-1.76309892
H	-3.10944797	4.54052356	-1.04611270
H	-2.16911473	3.74022332	-2.30962302
H	-3.92870550	3.89264854	-2.47308111

MP2 Electronic Energy(Ha): 1489.189261686411

B3LYP Electronic Energy(Ha): 1493.026932221217

M06-L Electronic Energy(Ha): 1492.840246213654

Zero point energy correction(kcal/mol): 378.226

Enthalpy correction(kcal/mol): 401.261

Entropy correction(cal/mol): 222.981

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.168

Deuterated enthalpy correction(kcal/mol): 397.403

Deuterated entropy correction(cal/mol): 224.299

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.35129175	-0.68337798	-0.23594825
C	0.05007804	1.47705354	-1.41008981
C	1.31609089	1.04404733	-1.89842599
H	2.26904423	1.48325773	-1.63851368
C	-0.90309233	0.57636154	-1.98971736
H	-1.97188626	0.61062359	-1.83412198
C	-0.23169319	-0.41916879	-2.73530883
H	-0.69001617	-1.23046370	-3.28123007
C	1.15910607	-0.13110019	-2.66871912
H	1.94735895	-0.68833879	-3.15408234
B	-0.19748259	2.47357790	-0.12872472
C	-0.47484506	4.02907429	-0.44975354
C	-1.37130381	1.71870266	0.74809764
C	1.09271302	2.18046244	0.86707286
N	1.53846676	0.98164530	1.10088670
N	-1.34057228	0.43042674	0.90422353
O	-2.36005527	2.34648559	1.39495717
O	1.72257350	3.16753190	1.52120729
C	2.68063976	1.07081728	2.03209060
C	2.73309571	2.57029169	2.38294103
C	-2.43489084	0.00969907	1.79431550
C	-3.16333323	1.33904338	2.08503374
N	-0.44443826	-2.43229129	0.13318578
N	2.10961618	-2.23643391	0.14367311
C	2.78368875	-2.33758571	1.44028756

H	2.05918546	-2.25745556	2.25839997
H	2.51553953	0.44018040	2.90787935
H	-3.07108145	-0.72413299	1.29632106
C	-1.32886023	-3.56498835	0.21999586
H	-0.75682495	-4.50554318	0.29391036
H	-1.92510754	-3.50937106	1.14217535
C	-2.28482621	-3.68051244	-0.97794017
C	3.49219976	-3.69654746	1.39490960
C	4.01246006	-3.73197414	-0.05105049
H	4.08459067	-4.74739803	-0.44789222
H	3.53567871	-1.54591877	1.58789465
C	3.00005484	-2.86162845	-0.86449743
H	5.01292960	-3.29316263	-0.10280271
C	-0.47846911	4.50707595	-1.76835335
H	-0.28512513	3.81393190	-2.58096329
C	-0.73269426	4.96862146	0.56347499
H	-0.74212260	4.64739836	1.59975436
C	-0.72503779	5.84753114	-2.06702263
H	-0.72026354	6.18096355	-3.09993477
C	-0.98078512	6.30848442	0.27794413
H	-1.17750344	7.00628655	1.08583193
C	-0.97803859	6.75530134	-1.04287980
H	-1.17173801	7.79859467	-1.26895435
C	-3.29280439	-4.84112186	-0.85910816
H	-2.76098429	-5.78064037	-0.67055039
H	-3.79793653	-4.95780983	-1.82644089
C	-4.33695776	-4.62786778	0.20154163
H	-4.94925527	-3.73375453	0.08133542
C	-4.56888256	-5.42599534	1.24017865
H	-3.98777085	-6.32874737	1.40382640
H	-5.34959211	-5.21065592	1.96131982
H	3.68701541	3.04679782	2.15839617
H	3.59381560	0.72598082	1.54087627

H	2.45575486	2.78698211	3.41596087
H	-3.19197053	1.60784390	3.14080485
H	-4.17153421	1.38613617	1.67232325
H	-2.03141310	-0.45811597	2.69576433
H	4.28765392	-3.79604670	2.13836628
H	2.76544849	-4.49571338	1.56761025
H	-2.82445906	-2.73254887	-1.09049472
H	-1.68964624	-3.80703127	-1.88801902
H	0.82249742	-2.68642762	0.20369566
H	3.56460029	-2.08661040	-1.40446663
C	2.22646608	-3.68528877	-1.89853822
H	1.71303683	-4.52327115	-1.41713568
H	1.47437092	-3.08735056	-2.41724723
H	2.91132981	-4.08953639	-2.65001595

MP2 Electronic Energy(Ha): 1489.140159190950

B3LYP Electronic Energy(Ha): 1492.975636734328

M06-L Electronic Energy(Ha): 1492.784896769089

Zero point energy correction(kcal/mol): 374.959

Enthalpy correction(kcal/mol): 397.962

Entropy correction(cal/mol): 230.574

Imaginary Frequencies: -1590.54

Deuterated zero point energy correction(kcal/mol): 371.187

Deuterated enthalpy correction(kcal/mol): 394.439

Deuterated entropy correction(cal/mol): 233.283

Deuterated imaginary Frequencies: -1146.59

Product geometry

Zr	-0.14135111	0.81554135	-0.23881688
C	0.29402308	-1.35136153	-1.41394822
C	-0.93199347	-0.93676316	-1.99984160
H	-1.89379397	-1.39958992	-1.82499629
C	1.27857223	-0.42954069	-1.90588234
H	2.33205121	-0.45006763	-1.66679309

C	0.66004487	0.54886057	-2.71474714
H	1.14954490	1.36792171	-3.22061234
C	-0.72228115	0.24256805	-2.76364449
H	-1.45805110	0.77674965	-3.34729976
B	0.48084035	-2.34236975	-0.12135717
C	0.79048953	-3.89650091	-0.43299588
C	1.60819131	-1.56992393	0.80681969
C	-0.83356881	-2.08632586	0.85450714
N	-1.33308238	-0.91089834	1.09552933
N	1.52419755	-0.29139561	0.99825756
O	2.63470072	-2.17555745	1.42436736
O	-1.37088449	-3.09535962	1.56724365
C	-2.31541834	-1.03461167	2.18945356
C	-2.46021568	-2.55654698	2.36216679
C	2.64850783	0.15882989	1.83286719
C	3.35150546	-1.16554116	2.19820380
N	0.53361205	2.52921407	0.13366554
N	-2.40275474	1.84892358	-0.17336466
C	-2.57064664	2.62003206	1.09803694
H	-1.87088495	3.45287390	1.10705290
H	-1.92884317	-0.54656073	3.09129380
H	3.28771258	0.83766962	1.26259191
C	1.16215010	3.80688761	0.26424325
H	0.44164918	4.56701339	0.62205556
H	1.94838221	3.77261583	1.03467872
C	1.78255510	4.32779825	-1.04434440
C	-4.05112577	2.99828218	1.14116074
C	-4.72557036	1.73441400	0.58843152
H	-5.70837205	1.92832663	0.15424482
H	-2.31737728	1.97003216	1.94017421
C	-3.72999176	1.18526660	-0.47160179
H	-4.86662928	1.00750081	1.39301238
C	0.78838784	-4.38296627	-1.74881553

H	0.58005441	-3.69582359	-2.56272834
C	1.07355075	-4.82725444	0.58188900
H	1.09129890	-4.49967444	1.61587530
C	1.04955220	-5.72181610	-2.04266451
H	1.03951847	-6.06079824	-3.07390719
C	1.33705381	-6.16538091	0.30144508
H	1.55335769	-6.85535103	1.11127664
C	1.32527819	-6.62066667	-1.01646584
H	1.53081701	-7.66266311	-1.23870559
C	2.45545185	5.70873704	-0.91554188
H	1.73776622	6.44027175	-0.52607883
H	2.73312712	6.05019209	-1.92145527
C	3.68918676	5.70728647	-0.05644164
H	4.47066946	5.01098283	-0.36116323
C	3.89659559	6.47425744	1.01051611
H	3.14843768	7.18237300	1.35487510
H	4.82014439	6.42597697	1.57681061
H	-3.39537033	-2.94850190	1.95569202
H	-3.26228537	-0.55647169	1.93334670
H	-2.33739212	-2.90736285	3.38630555
H	3.25747266	-1.43249125	3.25227453
H	4.40088199	-1.20918292	1.90774747
H	2.28624767	0.70268071	2.70769316
H	-4.39282832	3.26220422	2.14401855
H	-4.23994015	3.85780797	0.48974160
H	2.51060390	3.59102307	-1.40285546
H	0.99586393	4.37900421	-1.80506447
H	-2.23431826	2.53947292	-0.90250614
H	-3.59288747	0.11004655	-0.34858205
C	-4.18442022	1.46700728	-1.90193788
H	-4.37717600	2.53484529	-2.05124458
H	-3.43861738	1.14571346	-2.62943863
H	-5.11051456	0.92770292	-2.11457750

MP2 Electronic Energy(Ha): 1489.173555752585

B3LYP Electronic Energy(Ha): 1493.006712688731

M06-L Electronic Energy(Ha): 1492.818551374688

Zero point energy correction(kcal/mol): 379.007

Enthalpy correction(kcal/mol): 401.970

Entropy correction(cal/mol): 224.158

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.702

Deuterated enthalpy correction(kcal/mol): 397.824

Deuterated entropy correction(cal/mol): 225.187

Deuterated imaginary Frequencies:

Axial Reaction H4

Reactant geometry

Zr	-0.44460769	0.28300981	0.56223180
C	-1.02207872	-2.12274781	0.78205631
C	-0.81866265	-1.70466918	2.13206866
H	0.03531517	-1.95763430	2.74221182
C	-2.25629803	-1.52661511	0.38358281
H	-2.71946882	-1.62922556	-0.58744368
C	-2.76417867	-0.74158211	1.44586222
H	-3.67604189	-0.16121004	1.43811217
C	-1.87424297	-0.85877640	2.53479262
H	-1.97273172	-0.36957127	3.49211540
B	0.06778628	-2.85634309	-0.18738511
C	0.00520733	-4.46826861	-0.26103471
C	-0.15148893	-2.08094477	-1.61902735
C	1.51733816	-2.24671584	0.27478819
N	1.67549515	-1.00972628	0.63853600
N	-0.21774278	-0.78766678	-1.67139941
O	-0.38169804	-2.72395532	-2.77850573
O	2.64540316	-2.97806641	0.20906605

C	3.12215570	-0.75555611	0.79971389
C	3.73565901	-2.16192678	0.71286399
C	-0.66216945	-0.39966927	-3.02395869
C	-0.55550745	-1.71576455	-3.81321530
N	0.19172207	1.57783034	2.18064614
H	3.48389926	-0.10486262	-0.00583619
H	-1.68560687	-0.01574740	-2.97266046
C	-0.78826957	2.35820273	2.93800389
H	-1.68160682	2.54706755	2.33996117
H	-1.12143358	1.84137376	3.85743266
C	-0.03875009	3.64517778	3.32230625
C	1.40110192	3.14805775	3.56872726
H	2.14558390	3.82159921	3.13661154
H	1.61828682	3.08039316	4.63840009
C	1.45690268	1.72898931	2.90977943
C	-0.88594296	-5.19871789	0.53867291
H	-1.54797376	-4.66467564	1.21290882
C	0.83506982	-5.21015266	-1.11924195
H	1.54096756	-4.69063637	-1.75925910
C	0.78130512	-6.60028546	-1.17598283
H	1.43727773	-7.14020996	-1.85186952
C	-0.94907660	-6.59194813	0.49158480
H	-1.65218137	-7.12288272	1.12575325
C	-0.11381411	-7.29996951	-0.36751805
H	-0.15900218	-8.38328596	-0.40914811
H	4.57287477	-2.24823407	0.02129473
H	4.02713882	-2.55986825	1.68739723
H	3.33630273	-0.26747777	1.75085828
H	0.32051010	-1.75495526	-4.46543400
H	-1.44474415	-1.97279334	-4.38746518
H	-0.03416886	0.38591740	-3.44562837
H	-0.06745470	4.35037102	2.48612000
H	-0.46888177	4.14704274	4.19365516

N	-1.86600295	1.59600411	-0.30985835
H	-2.80918478	1.22664998	-0.30940822
C	-1.86378720	2.83197239	-1.07884876
H	-0.83677798	3.18510819	-1.21825936
H	-2.25712624	2.66409831	-2.09388322
C	-2.66232719	3.98449504	-0.43842980
H	-2.22596249	4.21938288	0.53763497
H	-2.54421355	4.87881923	-1.06490380
C	-4.16479936	3.69796897	-0.25115962
H	-4.30108319	2.83858351	0.41293992
H	-4.61123569	4.55760946	0.26465504
C	-4.90426959	3.47030836	-1.54029504
H	-4.83136641	4.27237919	-2.27483367
C	-5.62659146	2.39363442	-1.83950443
H	-5.73634179	1.56972457	-1.14015144
H	-6.14575873	2.29989817	-2.78682518
N	1.23762776	1.80663493	-0.44257742
C	1.79897364	1.82231892	-1.81005976
H	1.99180020	1.69437989	0.23085811
H	0.81952521	2.70164818	-0.20333206
H	2.08207568	0.79708107	-2.05615523
H	0.99138589	2.09965596	-2.49127699
C	2.99625156	2.75982109	-2.00975049
H	3.79509531	2.48336911	-1.30916868
H	3.40082330	2.59036477	-3.01351576
C	2.66771002	4.25590395	-1.85339688
H	2.26552938	4.43751410	-0.84801341
H	1.88125506	4.53416279	-2.56366866
C	3.86783000	5.13779112	-2.05822502
H	4.69280502	4.98445926	-1.36355660
C	3.98929879	6.05837212	-3.00940040
H	3.19332587	6.24734573	-3.72367651
H	4.88532613	6.66049025	-3.10701206

H	2.30412815	1.68934533	2.20871710
C	1.69877612	0.63418020	3.96708677
H	0.89190999	0.62587578	4.70537080
H	1.73748892	-0.35443023	3.50511200
H	2.63980767	0.80464898	4.50296193

MP2 Electronic Energy(Ha): 1740.500860173526

B3LYP Electronic Energy(Ha): 1744.990379872832

M06-L Electronic Energy(Ha): 1744.774175549172

Zero point energy correction(kcal/mol): 477.027

Enthalpy correction(kcal/mol): 505.244

Entropy correction(cal/mol): 257.871

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.026

Deuterated enthalpy correction(kcal/mol): 496.743

Deuterated entropy correction(cal/mol): 262.249

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.50100428	0.25929475	0.38633424
C	-0.88866698	-2.11431448	0.92750576
C	-0.52395652	-1.54192503	2.18400649
H	0.41780508	-1.69876566	2.68639578
C	-2.20318329	-1.62373913	0.65778050
H	-2.78702892	-1.84707180	-0.22348176
C	-2.59975706	-0.74570689	1.69122142
H	-3.53692844	-0.21108079	1.75714858
C	-1.55203160	-0.68783730	2.63875899
H	-1.54941394	-0.10554769	3.54792532
B	0.11313193	-2.89058996	-0.10744144
C	0.09051466	-4.50365700	-0.06759271
C	-0.22392197	-2.21459796	-1.56447402
C	1.58104793	-2.21121161	0.18480559
N	1.72045817	-0.94647851	0.43881474

N	-0.42950383	-0.93904883	-1.65847133
O	-0.27698052	-2.89287925	-2.72171312
O	2.72016315	-2.92872876	0.15713956
C	3.14564020	-0.69884834	0.74877871
C	3.82728390	-1.99627286	0.29348398
C	-0.72411744	-0.59406446	-3.05908923
C	-0.51160351	-1.93312931	-3.79408745
N	0.46092049	1.90560131	1.78400966
H	3.52595535	0.18282255	0.23202238
H	-1.74914829	-0.22411160	-3.14295605
C	-0.42107367	3.00889800	2.22977595
H	-0.91531172	3.45348183	1.36378130
H	-1.22169267	2.64739186	2.88864164
C	0.47968949	4.02462058	2.98836304
C	1.87347624	3.36302388	3.00448838
H	2.48813837	3.74998050	2.18691672
H	2.41650791	3.53750825	3.93688662
C	1.57533693	1.86764041	2.75360271
C	-0.71646122	-5.19724010	0.84620290
H	-1.33846859	-4.63391754	1.53468647
C	0.87452516	-5.28307778	-0.93574038
H	1.51507781	-4.79246147	-1.66087846
C	0.85508293	-6.67459768	-0.89473260
H	1.47394826	-7.24446429	-1.58078700
C	-0.74411258	-6.59142244	0.89728252
H	-1.38128681	-7.09348960	1.61855110
C	0.04332554	-7.33725225	0.02516954
H	0.02597082	-8.42155009	0.05992532
H	4.30913938	-1.90696054	-0.68385195
H	4.53435464	-2.41111528	1.01016091
H	3.26362948	-0.53418601	1.82420570
H	0.36806331	-1.93945576	-4.44013624
H	-1.37805157	-2.27279065	-4.36088897

H	-0.05362029	0.19040463	-3.41508961
H	0.50055858	4.99830609	2.49413537
H	0.10818936	4.19041950	4.00239355
N	-2.10983995	1.39949196	-0.36733632
H	-3.00756860	1.11312218	0.00381538
C	-2.36559557	2.31871299	-1.47219144
H	-1.45065524	2.45956428	-2.05524107
H	-3.09365336	1.87539247	-2.16740794
C	-2.89021544	3.70557143	-1.05287493
H	-2.13685522	4.20764836	-0.43715282
H	-3.01288875	4.31381839	-1.95860369
C	-4.22107021	3.68131329	-0.27660600
H	-4.09755492	3.12304883	0.65664170
H	-4.46446941	4.71216230	0.01052687
C	-5.36957856	3.11415043	-1.06397794
H	-5.57055318	3.59598079	-2.02077452
C	-6.14107848	2.09818561	-0.68579057
H	-5.98767310	1.58918863	0.26154801
H	-6.96229122	1.74551371	-1.29958527
N	0.80403192	1.88638992	-0.71044019
C	1.91655440	1.72418259	-1.65106230
H	0.91672276	2.11804790	0.53368574
H	0.19726109	2.63119535	-1.03781561
H	2.35674314	0.73661592	-1.50004363
H	1.53910268	1.72569895	-2.68440675
C	3.02204412	2.78735791	-1.54060107
H	3.43014207	2.77659425	-0.52243864
H	3.84350440	2.51102254	-2.21264751
C	2.55536702	4.21176094	-1.88762144
H	1.74150099	4.49148359	-1.20673056
H	2.14134022	4.22521568	-2.90272929
C	3.65357159	5.23122058	-1.77862684
H	4.10449251	5.33666562	-0.79238069

C	4.10895608	5.98336843	-2.77617399
H	3.69220712	5.91347452	-3.77678087
H	4.91088809	6.69826649	-2.63071341
H	2.43514666	1.38643372	2.28090827
C	1.27001067	1.12727174	4.06455077
H	0.41617078	1.57006760	4.58563292
H	1.04286294	0.07644693	3.88429350
H	2.13025654	1.17601230	4.73987719

MP2 Electronic Energy(Ha): 1740.484557156017

B3LYP Electronic Energy(Ha): 1744.973191753952

M06-L Electronic Energy(Ha): 1744.752375207278

Zero point energy correction(kcal/mol): 474.386

Enthalpy correction(kcal/mol): 502.216

Entropy correction(cal/mol): 254.730

Imaginary Frequencies: -1327.65

Deuterated zero point energy correction(kcal/mol): 466.311

Deuterated enthalpy correction(kcal/mol): 494.588

Deuterated entropy correction(cal/mol): 258.688

Deuterated imaginary Frequencies: -953.25

Product geometry

Zr	-0.45281774	0.31822873	0.20743493
C	-1.02732772	-2.01892404	0.85061894
C	-0.73212680	-1.42157430	2.11314138
H	0.15472635	-1.61671471	2.69572881
C	-2.29967626	-1.48987893	0.47180671
H	-2.82838181	-1.72064482	-0.44164120
C	-2.73414829	-0.56615243	1.44469103
H	-3.65393047	0.00214433	1.42551650
C	-1.75733608	-0.52078675	2.46688192
H	-1.80746694	0.07391054	3.36705116
B	0.00164998	-2.89770279	-0.06644996
C	-0.10871712	-4.50460921	0.04622528

C	-0.21087588	-2.28297525	-1.57261278
C	1.47839867	-2.27711880	0.30947516
N	1.65113348	-1.00927160	0.51619184
N	-0.41163621	-1.01377034	-1.73228574
O	-0.15867830	-3.00241115	-2.70559920
O	2.58546117	-3.03809104	0.40910160
C	3.05782478	-0.78354695	0.89910616
C	3.71515640	-2.14824179	0.62835106
C	-0.57773038	-0.71758942	-3.16381171
C	-0.30817240	-2.08321887	-3.82829101
N	0.24508238	2.08294903	1.92504170
H	3.50422103	0.02258329	0.31669448
H	-1.59005884	-0.34922425	-3.35089313
C	-0.77541366	3.00446991	2.50177082
H	-1.31688370	3.48097190	1.68642647
H	-1.49941871	2.42023011	3.07086196
C	-0.01563062	4.00421247	3.41631222
C	1.45417443	3.52285714	3.38583626
H	2.02824416	4.09949249	2.65491561
H	1.95449448	3.62723811	4.35084816
C	1.36178097	2.05357803	2.92232889
C	-1.01852115	-5.11101015	0.92486612
H	-1.65970508	-4.48298592	1.53533228
C	0.69573267	-5.36444269	-0.72159379
H	1.41375877	-4.94263457	-1.41693108
C	0.59863245	-6.74967204	-0.61887222
H	1.23579685	-7.38317651	-1.22820638
C	-1.12467609	-6.49784966	1.03717335
H	-1.84085762	-6.93119151	1.72842634
C	-0.31470568	-7.32458310	0.26410400
H	-0.39300917	-8.40367976	0.34659545
H	4.32599101	-2.15767683	-0.27753265
H	4.29778728	-2.54112352	1.46077182

H	3.11329159	-0.50335337	1.95673095
H	0.61935342	-2.11182576	-4.40288378
H	-1.12776771	-2.44621920	-4.44802269
H	0.12461757	0.05387205	-3.48253538
H	-0.10750303	5.03126419	3.05853297
H	-0.41913952	3.98248019	4.43076816
N	-1.95953469	1.56762531	-0.58905017
H	-2.89026558	1.35114651	-0.25216288
C	-2.08685994	2.51090808	-1.69545502
H	-1.14120794	2.55473245	-2.24272164
H	-2.83431347	2.14719857	-2.41528911
C	-2.47538889	3.94327385	-1.28271033
H	-1.70010016	4.34931910	-0.62289117
H	-2.48105225	4.57309017	-2.18191334
C	-3.83973862	4.06288166	-0.57584761
H	-3.83751007	3.46839005	0.34346375
H	-3.97464005	5.10809947	-0.26909992
C	-5.00296249	3.65831756	-1.43840748
H	-5.09777971	4.19158669	-2.38418306
C	-5.90169784	2.72464348	-1.13764634
H	-5.85395970	2.16813990	-0.20596759
H	-6.72371418	2.48793160	-1.80377870
N	0.92745340	1.62589174	-0.84410417
C	2.04829610	1.38686908	-1.74115342
H	0.65494343	2.53105297	1.10144702
H	0.47450315	2.49352782	-1.11751370
H	2.38021052	0.35290576	-1.61530299
H	1.74835609	1.47435508	-2.80128922
C	3.25992116	2.31752030	-1.53540646
H	3.60770999	2.22697733	-0.49894107
H	4.08174578	1.98138055	-2.18014298
C	2.96522859	3.79574500	-1.84158419
H	2.14328766	4.12927838	-1.19448230

H	2.61583839	3.89457263	-2.87605979
C	4.15067492	4.69170009	-1.62215386
H	4.55394243	4.70231166	-0.60967825
C	4.73611226	5.44134090	-2.55169183
H	4.37382402	5.46239162	-3.57542319
H	5.59587683	6.06205239	-2.32566703
H	2.26479525	1.74415605	2.39189410
C	1.10484187	1.09322624	4.08186750
H	0.20278652	1.35792751	4.63979254
H	0.99572422	0.06814198	3.73144129
H	1.94513070	1.12879431	4.78028080

MP2 Electronic Energy(Ha): 1740.497363470435

B3LYP Electronic Energy(Ha): 1744.992539532694

M06-L Electronic Energy(Ha): 1744.772741040318

Zero point energy correction(kcal/mol): 477.154

Enthalpy correction(kcal/mol): 505.523

Entropy correction(cal/mol): 263.043

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.164

Deuterated enthalpy correction(kcal/mol): 497.028

Deuterated entropy correction(cal/mol): 267.720

Deuterated imaginary Frequencies: -0.00

Axial Reaction H5

Reactant geometry

Zr	-1.10952430	0.99091699	-0.19493864
C	-1.80175814	-1.38485509	-0.25356697
C	-2.65629938	-0.78090673	0.72689096
H	-2.58851933	-0.93150089	1.79523357
C	-2.26718928	-0.88850836	-1.50437716
H	-1.83716864	-1.11517515	-2.46912445
C	-3.32111811	0.03244131	-1.29585430

H	-3.84996844	0.58208694	-2.06067996
C	-3.57438522	0.08499992	0.09522930
H	-4.31835553	0.69675763	0.58399858
B	-0.37127702	-2.14092326	0.01829017
C	-0.39609313	-3.75492015	0.06922792
C	0.61207469	-1.50896368	-1.14518272
C	0.18612613	-1.43100774	1.39671774
N	0.06523342	-0.15540329	1.60887494
N	0.57421574	-0.25142264	-1.45902326
O	1.45291421	-2.26020093	-1.88064485
O	0.76471784	-2.12379578	2.39276819
C	0.54195379	0.15382687	2.96927584
C	1.14423170	-1.18554882	3.43757430
C	1.40567189	-0.03619941	-2.65593847
C	2.16164470	-1.36924158	-2.78940403
N	0.99158514	2.33625814	0.23635221
N	-1.89984992	2.78440264	0.50935694
C	-2.57319226	3.68409744	1.41441774
H	-2.23266609	3.55013605	2.44564410
H	1.27838374	0.96172652	2.96235281
H	0.75866035	0.17244072	-3.51391373
C	2.39194526	1.87520972	0.32265398
H	2.41900498	1.00222787	0.97808581
H	2.68891608	1.52213239	-0.66424154
C	3.37604253	2.94048245	0.81605006
C	-2.27616140	5.11784849	0.86434263
C	-1.79682402	4.88472909	-0.59312313
H	-0.72129602	5.06829037	-0.68635328
H	-3.66565053	3.51582582	1.41256950
C	-2.09161849	3.38956194	-0.85041364
C	-1.27667714	2.58357015	-1.87619043
H	-2.30174522	5.53009002	-1.31737643
H	0.70284484	2.78581124	1.10276481

C	0.76982276	-4.51467924	0.26612368
H	1.72288298	-4.00889586	0.38386759
C	-1.59451023	-4.46762236	-0.08063867
H	-2.51741352	-3.91827527	-0.23709230
C	0.74285564	-5.90591049	0.31218089
H	1.66345418	-6.46058069	0.46516052
C	-1.63477596	-5.86178816	-0.03637655
H	-2.58132621	-6.37934493	-0.15680885
C	-0.46398666	-6.58796420	0.16092020
H	-0.48907138	-7.67213190	0.19571553
C	4.83316833	2.43936886	0.87940268
H	4.89194220	1.54585824	1.51082521
H	5.43757224	3.21037085	1.37249584
C	5.42961380	2.14657074	-0.47016201
H	5.45065456	2.98432061	-1.16691137
C	5.92914416	0.97610721	-0.85764200
H	5.93740721	0.11389194	-0.19736122
H	6.36099003	0.84027542	-1.84276317
H	0.73830313	-1.55115659	4.38007834
H	-0.29699249	0.47697497	3.59366036
H	2.23459385	-1.17436161	3.49454623
H	3.19906874	-1.30777949	-2.45210969
H	2.12893536	-1.81043210	-3.78458994
H	2.07678296	0.81613993	-2.53710047
H	-3.16806345	5.74800708	0.90623352
H	-1.50487236	5.61244933	1.46028391
H	3.32147218	3.81922703	0.16142066
H	3.07328003	3.28049891	1.81368758
H	0.90774798	3.06361317	-0.46932691
H	-3.16261758	3.30727373	-1.11154740
H	-0.34473161	3.09252011	-2.15061717
H	-1.83266477	2.38956474	-2.79335114

MP2 Electronic Energy(Ha): 1489.156061724598

B3LYP Electronic Energy(Ha): 1492.983715903073

M06-L Electronic Energy(Ha): 1492.801619542903

Zero point energy correction(kcal/mol): 378.331

Enthalpy correction(kcal/mol): 401.163

Entropy correction(cal/mol): 221.113

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.456

Deuterated enthalpy correction(kcal/mol): 396.585

Deuterated entropy correction(cal/mol): 224.052

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-1.01703304	-0.66038530	-0.00814713
C	-1.45338685	1.70679591	-0.45146756
C	-1.77786399	1.03903904	-1.67556402
H	-1.19536710	1.07806349	-2.58449577
C	-2.50212314	1.36177619	0.45142829
H	-2.56356553	1.66985504	1.48474779
C	-3.39939641	0.47071879	-0.17404028
H	-4.27088809	0.02215164	0.27840561
C	-2.94947301	0.26621707	-1.50136271
H	-3.42443762	-0.35681375	-2.24547233
B	-0.01961818	2.39212044	-0.05150775
C	0.06551360	4.00113316	-0.13471364
C	0.33471153	1.75023408	1.42350583
C	1.05702143	1.58448647	-0.99813144
N	0.98951907	0.29959505	-1.16163097
N	0.02905696	0.52201759	1.71342235
O	1.02256554	2.40320120	2.37127450
O	2.04452247	2.20782337	-1.66119474
C	2.06104995	-0.11540526	-2.09159609
C	2.77173885	1.21062615	-2.43150580
C	0.57048379	0.17764187	3.03706344

C	1.16907696	1.51464008	3.51942619
N	0.43736363	-2.45776599	0.47902656
N	-1.79720678	-2.71108047	-0.63063558
C	-2.31255895	-3.65632038	-1.61181680
H	-1.51728923	-4.00017867	-2.27969199
H	2.73065876	-0.83014627	-1.61359050
H	-0.22329631	-0.19235201	3.68876616
C	1.75187202	-2.83414842	-0.03984256
H	1.70329070	-2.83350113	-1.13548829
H	2.51932148	-2.09741387	0.23320051
C	2.21008008	-4.22295693	0.42437096
C	-2.92978548	-4.81960204	-0.76384655
C	-2.98900229	-4.27243109	0.68769063
H	-2.17923389	-4.68594435	1.29571707
H	-3.09075194	-3.19855423	-2.24021980
C	-2.76894017	-2.75534729	0.50658435
C	-2.21362787	-1.85196205	1.61472589
H	-3.93344831	-4.49915375	1.18905242
H	-0.62105994	-2.95077999	-0.09812125
C	1.24051286	4.70365198	0.18435604
H	2.12191612	4.15452080	0.49830010
C	-1.03894197	4.76835318	-0.53294190
H	-1.96640569	4.26583674	-0.78895306
C	1.30977574	6.09220474	0.11061150
H	2.23407270	6.60174810	0.36437620
C	-0.98168715	6.16038539	-0.61092502
H	-1.85708828	6.72083800	-0.92362116
C	0.19542378	6.82920516	-0.28861486
H	0.24612412	7.91139221	-0.34720076
C	3.57730939	-4.65193166	-0.14384338
H	3.54267683	-4.65107220	-1.23925562
H	3.76161635	-5.69033321	0.15985107
C	4.72753705	-3.80465911	0.32576940

H	4.84484613	-3.72925055	1.40691819
C	5.59591077	-3.17054571	-0.45771669
H	5.52512675	-3.22009733	-1.54050453
H	6.41452616	-2.58943590	-0.04808639
H	2.70553734	1.49043759	-3.48355911
H	1.63135403	-0.59696286	-2.97504982
H	3.81518211	1.24086863	-2.11589534
H	2.22899505	1.46503562	3.76742320
H	0.62283455	1.96111416	4.35146513
H	1.32361882	-0.60950625	2.94038212
H	-3.92331491	-5.08197349	-1.13520808
H	-2.31531306	-5.72048211	-0.82530768
H	2.25432376	-4.23610349	1.52165813
H	1.45340536	-4.96092712	0.13855042
H	0.40412515	-2.63588285	1.47914944
H	-3.72327670	-2.33080023	0.15658538
H	-1.57399708	-2.41041528	2.30773342
H	-3.00062365	-1.36732717	2.19332912

MP2 Electronic Energy(Ha): 1489.135366453465

B3LYP Electronic Energy(Ha): 1492.962273845746

M06-L Electronic Energy(Ha): 1492.775866282626

Zero point energy correction(kcal/mol): 375.524

Enthalpy correction(kcal/mol): 398.095

Entropy correction(cal/mol): 224.414

Imaginary Frequencies: -1389.53

Deuterated zero point energy correction(kcal/mol): 371.599

Deuterated enthalpy correction(kcal/mol): 394.424

Deuterated entropy correction(cal/mol): 227.028

Deuterated imaginary Frequencies: -996.69

Product geometry

Zr	-0.76802324	-0.73346364	-0.08824929
C	-1.23559965	1.63377869	-0.69126312

C	-1.30932296	0.90667181	-1.92442015
H	-0.57126816	0.93031971	-2.71234836
C	-2.43567014	1.31466307	0.00517820
H	-2.70066417	1.67629450	0.98848950
C	-3.19074243	0.39177800	-0.74298946
H	-4.14625887	-0.02485974	-0.46151924
C	-2.48979763	0.13258481	-1.94763703
H	-2.81524650	-0.51569641	-2.74882777
B	0.04777552	2.42856096	-0.07553916
C	0.02574954	4.04037869	-0.16868075
C	0.19926126	1.81530668	1.44233653
C	1.32384153	1.69884199	-0.79724806
N	1.36124105	0.41643943	-0.97002552
N	-0.07140536	0.56895055	1.68731615
O	0.69660729	2.50058415	2.48211998
O	2.40203172	2.38462258	-1.22353541
C	2.66460969	0.07133165	-1.57770925
C	3.28708330	1.44454846	-1.88969879
C	0.30000615	0.24457240	3.07374758
C	0.72313366	1.61409330	3.64038634
N	0.60460140	-2.33917532	0.23543741
N	-2.16032203	-2.76697304	-0.57706235
C	-3.05163163	-3.58554156	-1.42061036
H	-2.47723107	-4.12210033	-2.17753352
H	3.26762389	-0.50472546	-0.87309819
H	-0.54758710	-0.19034263	3.60564398
C	1.92537006	-2.81390305	-0.15847180
H	2.12945341	-2.49577570	-1.18457498
H	2.72267281	-2.37718960	0.46278407
C	2.05418198	-4.34281242	-0.10322249
C	-3.79940380	-4.53415208	-0.42475288
C	-3.47446767	-3.97491507	0.98968754
H	-2.69903417	-4.57155898	1.48143446

H	-3.75401048	-2.92682195	-1.93665846
C	-2.93618900	-2.56269680	0.69181800
C	-2.06173136	-1.73878435	1.62197005
H	-4.34581655	-3.95952741	1.64774171
H	-1.34645298	-3.33847203	-0.34444558
C	1.06379241	4.83379500	0.35036965
H	1.90982791	4.35570941	0.83244128
C	-1.03872953	4.71879294	-0.78045945
H	-1.86118018	4.14430718	-1.19480070
C	1.04097502	6.22341458	0.26484610
H	1.86047973	6.80402618	0.67703796
C	-1.07265428	6.11075206	-0.87291299
H	-1.91354217	6.60033950	-1.35429626
C	-0.03078764	6.87049179	-0.34911462
H	-0.05162374	7.95319413	-0.41750756
C	3.43368876	-4.87315918	-0.54151738
H	3.65224411	-4.54257864	-1.56332821
H	3.38238097	-5.96915365	-0.57439609
C	4.56138766	-4.47478280	0.37004190
H	4.43447836	-4.74266854	1.41903371
C	5.67607307	-3.85086730	-0.00094257
H	5.85057926	-3.56598325	-1.03446887
H	6.45742047	-3.60844655	0.71059722
H	3.28970643	1.68759584	-2.95459857
H	2.52813462	-0.53631802	-2.47564914
H	4.29066854	1.58067706	-1.48715837
H	1.73221986	1.63446742	4.05120359
H	0.02438429	2.01486011	4.37641695
H	1.11402927	-0.48576209	3.07908851
H	-4.87375085	-4.52517008	-0.62059181
H	-3.46173853	-5.56665927	-0.53564272
H	1.84543743	-4.68383725	0.91997859
H	1.28103150	-4.78562275	-0.74104457

H 0.31670174 -2.85655122 1.06403390

H -3.79486164 -1.95070604 0.40068549

H -1.43719166 -2.37352198 2.26434188

H -2.65243945 -1.08743365 2.26848267

MP2 Electronic Energy(Ha): 1489.148165591143

B3LYP Electronic Energy(Ha): 1492.982712669380

M06-L Electronic Energy(Ha): 1492.798014011082

Zero point energy correction(kcal/mol): 379.033

Enthalpy correction(kcal/mol): 401.729

Entropy correction(cal/mol): 219.263

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.196

Deuterated enthalpy correction(kcal/mol): 397.206

Deuterated entropy correction(cal/mol): 222.445

Deuterated imaginary Frequencies: -0.00

Axial Reaction H6

Reactant geometry

Zr -0.05954630 0.76024270 0.23379540

C 0.49426966 -1.41246239 1.27022622

C 1.71109940 -0.68186960 1.45102392

H 2.62821572 -0.85120454 0.90470463

C -0.43110450 -0.83233841 2.19033899

H -1.45646084 -1.14370726 2.32274017

C 0.17911428 0.25001970 2.86308539

H -0.27572495 0.87909417 3.61582993

C 1.51735307 0.33091147 2.41267414

H 2.25144467 1.04230244 2.75834155

B 0.14946620 -2.47641840 0.07916627

C 0.48152514 -4.02936135 0.37450147

C -1.41699068 -2.15647540 -0.30824569

C 0.87674384 -1.83930565 -1.25446359

N	0.90777983	-0.55566050	-1.43475467
N	-1.89558292	-0.95402639	-0.28785188
O	-2.25335443	-3.11334469	-0.76042174
O	1.38012793	-2.56814259	-2.26330798
C	1.47732058	-0.25435105	-2.75718584
C	1.88137863	-1.64860351	-3.27937736
C	-3.27004805	-0.98630773	-0.82168228
C	-3.53335766	-2.48893410	-1.04712535
N	1.28171848	2.35744439	-0.00300448
N	-1.98560455	1.97907826	0.93720810
C	-1.97359433	3.20007203	1.79247683
H	-0.95057366	3.57740770	1.84966243
H	0.72705358	0.23413485	-3.38451916
H	-3.97707191	-0.54880510	-0.11011780
C	2.61521013	2.78847296	0.40223840
H	3.02119535	2.05398750	1.09852000
H	3.29686086	2.78820264	-0.46375239
C	2.69319828	4.17758409	1.06797293
C	-2.87574749	4.20276237	1.06279991
C	-2.54240540	3.92325864	-0.40807686
H	-1.59622875	4.40347120	-0.67276491
H	-2.30147988	2.95638339	2.80465075
C	-2.38297391	2.39340055	-0.50460640
H	-3.36422422	1.94390417	-0.68565574
H	-3.30217228	4.28544328	-1.10342398
C	-1.31986058	1.85057483	-1.45229591
H	-0.80077832	2.65837812	-1.97680597
H	-2.67983045	1.33304275	1.29875402
H	-1.73974900	1.18299148	-2.20786640
C	0.99339894	-4.43716795	1.61534991
H	1.17032503	-3.69072209	2.38323789
C	0.27340208	-5.03709089	-0.58356178
H	-0.12083726	-4.77166633	-1.55833670

C	1.28330129	-5.77367756	1.89249204
H	1.67859525	-6.05085240	2.86484250
C	0.55958193	-6.37391044	-0.31889345
H	0.38663915	-7.12520774	-1.08328582
C	1.06724502	-6.74979338	0.92417527
H	1.29143568	-7.79066639	1.13327945
C	2.66757435	5.38065286	0.10286494
H	3.49714040	5.29190301	-0.60799119
H	2.86195140	6.28652442	0.69275932
C	1.38487273	5.58492242	-0.65267986
H	0.48990324	5.70004938	-0.04237587
C	1.27241640	5.66434519	-1.97701134
H	2.13637018	5.56111107	-2.62701617
H	0.31750589	5.84074397	-2.45930105
H	2.96078665	-1.79174112	-3.34863077
H	2.32690699	0.42472642	-2.66021337
H	1.41976577	-1.91971190	-4.22878162
H	-3.81078889	-2.74289158	-2.07048490
H	-4.27116401	-2.90809726	-0.36038076
H	-3.32905813	-0.40603493	-1.74670605
H	-3.93001960	3.98861087	1.26976475
H	-2.68010990	5.23460856	1.36360196
H	1.88166644	4.26360597	1.79959291
H	3.63123735	4.23362813	1.63359512
H	0.97589061	2.94151871	-0.77654400

MP2 Electronic Energy(Ha): 1489.175466402491

B3LYP Electronic Energy(Ha): 1493.004537690609

M06-L Electronic Energy(Ha): 1492.824143940955

Zero point energy correction(kcal/mol): 379.167

Enthalpy correction(kcal/mol): 401.631

Entropy correction(cal/mol): 217.251

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.779

Deuterated enthalpy correction(kcal/mol): 397.437

Deuterated entropy correction(cal/mol): 218.325

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.17318241	0.66820553	0.24335725
C	0.37853498	-1.46978770	1.35558700
C	1.49771306	-0.62355865	1.66266219
H	2.48689804	-0.71582137	1.23664858
C	-0.69624336	-0.96409454	2.13734442
H	-1.70270085	-1.35695211	2.14832723
C	-0.27159820	0.19212883	2.84330849
H	-0.87370245	0.78902106	3.51403893
C	1.10169491	0.38471582	2.56324552
H	1.72006317	1.18501978	2.94157871
B	0.28376058	-2.53756676	0.12069039
C	0.69268246	-4.06323041	0.45810643
C	-1.23066607	-2.34620768	-0.50333038
C	1.15570414	-1.82805230	-1.08660427
N	1.09174414	-0.54691300	-1.28559907
N	-1.79155561	-1.18640223	-0.62766874
O	-1.92996843	-3.39088104	-0.99396981
O	1.92441569	-2.49956602	-1.95540951
C	1.92738426	-0.18025776	-2.44064743
C	2.47249418	-1.54430039	-2.91312869
C	-3.07640098	-1.35864754	-1.33237176
C	-3.19537997	-2.88747376	-1.49840213
N	0.75900489	2.34894084	0.03149738
N	-2.34948434	1.63638097	0.49947635
C	-2.63770558	2.71969602	1.48921299
H	-1.69305828	3.17350520	1.79281354
H	1.32690984	0.32208902	-3.20283108
H	-3.90555120	-0.94471875	-0.74913160

C	1.65997995	3.46600210	0.05369861
H	2.60886305	3.16693014	0.52753426
H	1.92445021	3.79041112	-0.96551953
C	1.11742994	4.68352427	0.82540882
C	-3.50100328	3.73543953	0.73308897
C	-2.89405055	3.68825143	-0.67380680
H	-1.96781546	4.26969229	-0.70014655
H	-3.11423900	2.29934366	2.37639735
C	-2.57483595	2.20222783	-0.91605549
H	-3.47067512	1.70722595	-1.30826953
H	-3.55558453	4.08222928	-1.44800837
C	-1.33703404	1.93628224	-1.76785341
H	-1.16701581	2.75096918	-2.47812203
H	-3.00341941	0.87551134	0.64926770
H	-1.42868000	1.02159114	-2.36058129
C	0.72154680	-5.06879711	-0.52359297
H	0.46462401	-4.82049528	-1.54765437
C	1.03544108	-4.44802472	1.76300554
H	1.02752922	-3.70230185	2.55161765
C	1.07239883	-6.38199583	-0.22184581
H	1.08474454	-7.13203365	-1.00655373
C	1.38757910	-5.76096951	2.07802665
H	1.64719372	-6.02094196	3.09956286
C	1.40790765	-6.73548062	1.08455964
H	1.68220662	-7.75787305	1.32289923
C	2.11217388	5.85842495	0.91481122
H	3.04831900	5.51960327	1.37274204
H	1.69030693	6.61273859	1.59206567
C	2.40461968	6.51335027	-0.40664754
H	1.53536771	6.88862974	-0.94710384
C	3.61020737	6.67201084	-0.94569391
H	4.50677331	6.31544684	-0.44716035
H	3.74656570	7.16546287	-1.90157334

H	3.55878517	-1.62429784	-2.87321339
H	2.71592895	0.50859645	-2.12900920
H	2.12468113	-1.83713521	-3.90447403
H	-3.30021600	-3.21413955	-2.53336241
H	-3.99412324	-3.32955677	-0.90000951
H	-3.05557722	-0.83260225	-2.29192977
H	-4.54758745	3.41273462	0.71406730
H	-3.46590818	4.72835874	1.18642369
H	0.18916773	5.02696812	0.35250982
H	0.85224505	4.36040806	1.83745388
H	-0.15426284	2.28847269	-0.98045864

MP2 Electronic Energy(Ha): 1489.133349915775

B3LYP Electronic Energy(Ha): 1492.958811781172

M06-L Electronic Energy(Ha): 1492.774643107168

Zero point energy correction(kcal/mol): 375.776

Enthalpy correction(kcal/mol): 398.271

Entropy correction(cal/mol): 219.977

Imaginary Frequencies: -1596.50

Deuterated zero point energy correction(kcal/mol): 372.237

Deuterated enthalpy correction(kcal/mol): 394.862

Deuterated entropy correction(cal/mol): 220.648

Deuterated imaginary Frequencies: -1165.26

Product geometry

Zr	0.05092961	0.68447919	-0.20659904
C	-0.36985677	-1.49182828	-1.39152633
C	-1.47772732	-0.63286995	-1.69634220
H	-2.47954181	-0.73715044	-1.30459498
C	0.72197131	-0.97404317	-2.13852772
H	1.72762064	-1.37315767	-2.13018979
C	0.32101683	0.20269804	-2.82156653
H	0.93054836	0.79816896	-3.48742732
C	-1.05507615	0.40945629	-2.55414861

H	-1.67094860	1.20256698	-2.95133892
B	-0.27009284	-2.53882962	-0.13456363
C	-0.54671839	-4.09671192	-0.46125326
C	1.19991114	-2.23859998	0.56430673
C	-1.24735692	-1.88629366	1.01988883
N	-1.22944593	-0.61087367	1.25048346
N	1.66260124	-1.04546845	0.78305669
O	1.98440353	-3.25132629	0.98481401
O	-2.07773863	-2.59573086	1.79949993
C	-2.19095955	-0.28603432	2.31548905
C	-2.70992455	-1.67564654	2.74038107
C	2.99136906	-1.16976931	1.41433492
C	3.12549606	-2.68092750	1.67606703
N	-0.76989666	2.29009455	0.30448420
N	2.22617780	1.83482445	-0.51678986
C	2.10355383	3.01349055	-1.42873884
H	1.27628287	3.62604423	-1.06713391
H	-1.69766484	0.24881017	3.12989208
H	3.77065756	-0.80233351	0.73686104
C	-1.51612585	3.48212035	0.56352111
H	-2.06722721	3.39483505	1.51666612
H	-0.84239096	4.34540980	0.70006223
C	-2.53069583	3.82955672	-0.54050214
C	3.44113405	3.74378594	-1.30868482
C	3.72800844	3.64317183	0.19581719
H	3.25519279	4.47825398	0.72035578
H	1.85919148	2.67863344	-2.43586375
C	3.07494651	2.30822503	0.65470665
H	3.84616796	1.55015143	0.80576651
H	4.79355374	3.67247854	0.43161053
C	2.27881930	2.46672750	1.94606638
H	2.93130761	2.87114100	2.72612109
H	2.78655181	1.14432311	-1.01171021

H	1.88365350	1.51256976	2.30113738
C	-0.79495304	-4.52726810	-1.77294845
H	-0.80112428	-3.79494304	-2.57398743
C	-0.55492019	-5.08539131	0.53806099
H	-0.37156766	-4.80256778	1.56936010
C	-1.03617885	-5.86739438	-2.07815646
H	-1.22483126	-6.16226643	-3.10575536
C	-0.79527417	-6.42548840	0.24668981
H	-0.79508017	-7.16131711	1.04497477
C	-1.03716025	-6.82419187	-1.06746430
H	-1.22535286	-7.86761011	-1.29827032
C	-3.34481556	5.10964827	-0.26635242
H	-3.84931079	5.03092145	0.70362259
H	-4.13624377	5.18184771	-1.02387964
C	-2.52987332	6.37222865	-0.30951856
H	-1.98958387	6.54856799	-1.24000648
C	-2.42847317	7.26916797	0.66782719
H	-2.94680288	7.13932012	1.61339768
H	-1.82919908	8.16644462	0.55889481
H	-3.78894788	-1.79634929	2.64638171
H	-2.97766921	0.36178866	1.92144558
H	-2.40016210	-1.96915694	3.74473457
H	3.04183686	-2.94406152	2.73287569
H	4.02986073	-3.12884286	1.26478759
H	3.04684424	-0.58144417	2.33312004
H	4.20978628	3.22568063	-1.89256638
H	3.39305701	4.77464336	-1.66514754
H	-1.99473969	3.92739636	-1.49211727
H	-3.21499397	2.98303493	-0.65850491
H	1.43435469	3.14265772	1.80549530

MP2 Electronic Energy(Ha): 1489.173589837018

B3LYP Electronic Energy(Ha): 1493.004779525575

M06-L Electronic Energy(Ha): 1492.818549807742

Zero point energy correction(kcal/mol): 378.979

Enthalpy correction(kcal/mol): 401.975

Entropy correction(cal/mol): 224.621

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.656

Deuterated enthalpy correction(kcal/mol): 397.813

Deuterated entropy correction(cal/mol): 225.639

Deuterated imaginary Frequencies: -0.00

Axial Reaction H7

Reactant geometry

Zr	0.21437633	0.30796382	0.16248819
C	-0.33029823	-1.78191602	1.37954780
C	0.79179779	-1.31476399	2.13267092
H	1.78553323	-1.73777518	2.10241896
C	-1.40803057	-0.91678739	1.73271258
H	-2.41451596	-0.98562078	1.34843827
C	-0.94873488	0.06719413	2.63901792
H	-1.53900126	0.85510970	3.08711967
C	0.41487692	-0.19203803	2.89576755
H	1.05309609	0.38127432	3.55408300
B	-0.31211488	-2.90021744	0.19430536
C	-0.57923068	-4.43121347	0.63814002
C	-1.35058559	-2.31021737	-0.93074155
C	1.11851848	-2.63299719	-0.57259109
N	1.57744085	-1.42931495	-0.71465449
N	-1.46374917	-1.04053497	-1.16776917
O	-2.06977962	-3.12041443	-1.73473193
O	1.85785855	-3.60006065	-1.14156502
C	2.84157259	-1.47244716	-1.46740650
C	2.99063048	-2.96949805	-1.80773027
C	-2.32767322	-0.86890671	-2.35180530

C	-2.89751626	-2.27872890	-2.58035226
N	-0.52001178	3.40273941	-2.23629899
H	2.78078000	-0.83948442	-2.35507907
H	-3.11036835	-0.12911833	-2.16835029
C	0.59866730	4.28387656	-2.66532243
H	0.21576898	5.29088686	-2.84660363
H	1.33437013	4.36186270	-1.86302677
C	1.22512952	3.64597173	-3.93895300
C	0.30198156	2.45379459	-4.26017653
H	-0.49960562	2.77215209	-4.93838168
H	0.83014125	1.62550495	-4.73626974
C	-0.29645210	2.06729873	-2.88203414
H	-1.28443767	1.61703806	-3.01415358
C	0.58307216	1.11111563	-2.05956308
H	1.61714654	1.48576488	-2.06731080
H	0.62536869	0.17810424	-2.63892692
C	-0.85804495	-4.76027452	1.97304754
H	-0.88937353	-3.96869602	2.71502882
C	-0.54917308	-5.49543084	-0.28009967
H	-0.33728181	-5.29207388	-1.32408983
C	-0.78381110	-6.81123636	0.11068259
H	-0.75188115	-7.60778447	-0.62633361
C	-1.09548585	-6.07481487	2.37661385
H	-1.30787415	-6.29034629	3.41923157
C	-1.05915953	-7.10817111	1.44495714
H	-1.24217844	-8.13251930	1.75264985
H	2.90852462	-3.18565548	-2.87425051
H	3.90118701	-3.42408931	-1.41729337
H	3.65878857	-1.09929135	-0.84426705
H	-2.81268033	-2.63849409	-3.60528768
H	-3.93212814	-2.38339503	-2.24455055
H	-1.72982134	-0.52260827	-3.19959050
H	1.28723310	4.35527077	-4.76696803

H	2.24106989	3.30270935	-3.73198157
H	-1.36887918	3.78472218	-2.64439629
N	1.77320617	1.56782789	0.81659108
H	1.99418690	1.44601085	1.79776232
C	2.64977279	2.60262153	0.28326430
H	2.33690372	2.84749825	-0.73193506
H	2.54968695	3.52757081	0.87164374
C	4.13973702	2.21476705	0.24229933
H	4.26030546	1.34704654	-0.41469040
H	4.69878374	3.04059009	-0.21741700
C	4.76464039	1.88671594	1.61231295
H	4.25838996	1.02438045	2.05803004
H	5.80524945	1.57952057	1.44552750
C	4.75152542	3.04021020	2.57652846
H	5.21198771	3.96084755	2.21806617
C	4.23884332	3.01834263	3.80408867
H	3.77585924	2.12387306	4.21105215
H	4.27399764	3.88635596	4.45292747
N	-1.29015622	2.19267179	0.29433652
C	-2.76703830	2.11699550	0.27801318
H	-0.96992807	2.78942407	-0.49400363
H	-0.97532721	2.64504701	1.14894126
H	-3.05677216	1.66211285	-0.67165323
H	-3.08905376	1.42981381	1.06481486
C	-3.48354758	3.46520912	0.43431847
H	-3.13705965	4.15164995	-0.34700287
H	-4.55352609	3.30804775	0.25921228
C	-3.30266825	4.12195005	1.81528232
H	-2.23358867	4.28856334	2.00350187
H	-3.65969283	3.44099486	2.59580350
C	-4.01789356	5.43924239	1.92830746
H	-3.69575757	6.21366973	1.23319668
C	-4.99603241	5.71000077	2.78684997

H -5.34984692 4.96953460 3.49815792

H -5.47633597 6.68142363 2.81420911

MP2 Electronic Energy(Ha): 1740.468554957307

B3LYP Electronic Energy(Ha): 1744.964460738781

M06-L Electronic Energy(Ha): 1744.740532989748

Zero point energy correction(kcal/mol): 477.974

Enthalpy correction(kcal/mol): 505.861

Entropy correction(cal/mol): 256.309

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 469.140

Deuterated enthalpy correction(kcal/mol): 497.385

Deuterated entropy correction(cal/mol): 258.361

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr 0.32716675 -0.12306128 -0.61266292

C 0.17800529 2.18877593 -1.40712834

C 1.51338621 1.81135737 -1.76024366

H 2.41207348 2.16059609 -1.27227981

C -0.66420202 1.47861319 -2.31611746

H -1.74291040 1.51487601 -2.32534536

C 0.11960599 0.64961520 -3.14753998

H -0.24378610 -0.02090374 -3.91276918

C 1.47621434 0.86702796 -2.80693459

H 2.32548769 0.38666475 -3.27134705

B -0.29273986 2.99774120 -0.06710689

C -0.44649942 4.59881899 -0.20109098

C -1.64191671 2.19942445 0.42885785

C 0.76377068 2.48930664 1.09015291

N 1.14957913 1.25125229 1.13539513

N -1.75620815 0.91296874 0.31497712

O -2.65301711 2.81996749 1.06400299

O 1.24815591 3.27588968 2.06207843

C	2.06836680	1.06477680	2.27153727
C	2.07402118	2.45482214	2.94045478
C	-2.99330141	0.48865494	1.00082236
C	-3.67214897	1.82376253	1.35707025
N	-0.48148891	-4.09882938	1.49071850
H	1.70249135	0.27886362	2.93547067
H	-3.61216111	-0.13129697	0.34996902
C	0.49606804	-4.59893289	2.49174927
H	0.33528084	-5.66727203	2.65771537
H	1.51599242	-4.48698276	2.11413319
C	0.29829097	-3.77084640	3.79260143
C	-1.01313870	-3.00426666	3.55112571
H	-1.86816672	-3.61371542	3.86752360
H	-1.06111414	-2.05736439	4.09391803
C	-1.05100082	-2.82992331	2.01317610
H	-2.08882611	-2.76103129	1.66718234
C	-0.26605615	-1.60613854	1.49651690
H	0.79713377	-1.76305594	1.70387866
H	-0.57764967	-0.72999117	2.07295118
C	-0.20388876	5.25162030	-1.41872296
H	0.09233596	4.66463205	-2.28236916
C	-0.82666265	5.40773754	0.88397101
H	-1.02661605	4.94927883	1.84639110
C	-0.95708507	6.78853754	0.76130153
H	-1.25256460	7.38203182	1.62088068
C	-0.33161839	6.63453908	-1.55396895
H	-0.13542626	7.10449981	-2.51258904
C	-0.70936277	7.41024480	-0.46194642
H	-0.80998253	8.48603785	-0.56065371
H	1.61353762	2.46545857	3.92947326
H	3.05949659	2.91680070	2.99636284
H	3.05510076	0.76541938	1.90877186
H	-3.94718866	1.92229759	2.40677274

H	-4.54080185	2.04533586	0.73362620
H	-2.74570007	-0.10438469	1.88555221
H	0.25563996	-4.40146667	4.68318791
H	1.12918622	-3.07451903	3.92976957
H	-1.23188935	-4.77531798	1.41233611
N	2.02416577	-1.33613176	-0.81116399
H	2.70725593	-0.99974135	-1.47949225
C	2.43999438	-2.66373973	-0.36053673
H	1.60299289	-3.15448320	0.13947973
H	2.68398954	-3.28616106	-1.23369579
C	3.65451424	-2.66110881	0.58571172
H	3.39377349	-2.11809216	1.50080704
H	3.86227474	-3.69759868	0.88199437
C	4.93542608	-2.04021843	-0.00530646
H	4.76402463	-0.98491974	-0.24098370
H	5.71271794	-2.06211331	0.76958944
C	5.44884617	-2.75463841	-1.22456098
H	5.62828438	-3.82316320	-1.10664723
C	5.69743498	-2.19092067	-2.40385884
H	5.54156659	-1.12869168	-2.57028780
H	6.07732915	-2.76414131	-3.24207837
N	-1.05949665	-1.82958028	-1.13498700
C	-2.36648581	-1.80711839	-1.79351425
H	-0.82310065	-1.78114575	0.15141685
H	-0.52596558	-2.64435091	-1.42161529
H	-2.83993009	-0.84405873	-1.58940872
H	-2.23012919	-1.84760558	-2.88456585
C	-3.32832473	-2.93197739	-1.37960724
H	-3.54089155	-2.85067687	-0.30655865
H	-4.28135625	-2.78399780	-1.90148605
C	-2.80139849	-4.34467028	-1.68753170
H	-1.86295563	-4.49459618	-1.13914646
H	-2.56733657	-4.42665666	-2.75533480

C	-3.77096856	-5.42531996	-1.30108044
H	-4.05301046	-5.45374137	-0.24849457
C	-4.30556272	-6.31785519	-2.12930339
H	-4.05999771	-6.32951400	-3.18719050
H	-5.00438729	-7.07067264	-1.78232719

MP2 Electronic Energy(Ha): 1740.433826862529

B3LYP Electronic Energy(Ha): 1744.925782881934

M06-L Electronic Energy(Ha): 1744.705183870128

Zero point energy correction(kcal/mol): 474.383

Enthalpy correction(kcal/mol): 502.226

Entropy correction(cal/mol): 256.595

Imaginary Frequencies: -1484.85

Deuterated zero point energy correction(kcal/mol): 466.257

Deuterated enthalpy correction(kcal/mol): 494.548

Deuterated entropy correction(cal/mol): 260.319

Deuterated imaginary Frequencies: -1075.07

Product geometry

Zr	1.29584662	0.11049845	-0.50305157
C	1.49847716	2.56434619	-0.52217325
C	2.50648948	2.17819416	0.41238774
H	2.45648333	2.32893931	1.48173759
C	1.98516363	2.13657598	-1.79911182
H	1.46456526	2.25683840	-2.73764112
C	3.20384439	1.43931491	-1.63828144
H	3.79751321	0.99157099	-2.42212479
C	3.52641058	1.46568853	-0.25476721
H	4.40957881	1.03355480	0.19398065
B	-0.03309026	3.01825584	-0.15990931
C	-0.31412162	4.60183243	-0.03551957
C	-0.98069790	2.21213107	-1.23433127
C	-0.41415279	2.12185979	1.17890066
N	-0.12937679	0.85602957	1.23872613

N	-0.71183368	0.99867515	-1.60750573
O	-2.16383600	2.69730746	-1.65020641
O	-1.04821137	2.61562594	2.25193799
C	-0.54985140	0.32242994	2.54957211
C	-1.32796210	1.50368925	3.15655781
C	-1.88496670	0.45955698	-2.32263048
C	-2.76485910	1.70371849	-2.52745558
N	-2.65548264	-2.53794995	1.64722837
H	-1.16910289	-0.56889289	2.42549537
H	-1.60120957	-0.00859541	-3.26451110
C	-2.64271912	-3.70986930	2.55312697
H	-1.67696676	-4.21420752	2.48597910
H	-2.75327852	-3.36988882	3.58617122
C	-3.83618617	-4.62949687	2.15257406
C	-4.54868980	-3.86689330	1.01083539
H	-4.23627129	-4.26081014	0.03917626
H	-5.63692298	-3.95128670	1.06119919
C	-4.04763590	-2.41036296	1.15794146
H	-4.02733799	-1.89647674	0.19238376
C	-4.89438552	-1.58587431	2.13102403
H	-4.94279512	-2.05431379	3.11832773
H	-5.91833270	-1.48356818	1.76130124
C	0.70078460	5.53875353	-0.28041005
H	1.69042002	5.18527117	-0.55217523
C	-1.57497427	5.11514673	0.31517558
H	-2.39255861	4.43076716	0.51409726
C	-1.81003391	6.48387976	0.41486277
H	-2.79673128	6.84443685	0.68852537
C	0.47739254	6.91269018	-0.18407954
H	1.28790709	7.60733356	-0.38114493
C	-0.78181635	7.39186180	0.16475468
H	-0.96170374	8.45905818	0.24190073
H	-2.40897941	1.34942751	3.15838247

H	-1.00217611	1.79660733	4.15389258
H	0.33565912	0.05728198	3.13401819
H	-3.80522995	1.57762487	-2.23036198
H	-2.72323016	2.09370681	-3.54695311
H	-2.37268304	-0.30218077	-1.70483452
H	-3.49968411	-5.61525546	1.82565634
H	-4.50452934	-4.78689044	3.00205683
H	-2.06166047	-2.74368452	0.84974241
N	2.27879066	-1.17503040	0.83381984
H	3.18376428	-0.92060780	1.21073300
C	1.93104818	-2.53443596	1.23482933
H	0.91151886	-2.74988422	0.89594747
H	2.58006881	-3.26535687	0.72533774
C	1.99953259	-2.80483973	2.74789272
H	1.31317654	-2.12680863	3.26423930
H	1.63548993	-3.82391096	2.93205440
C	3.40352337	-2.65978023	3.36873652
H	3.77635238	-1.63903578	3.23169108
H	3.30892234	-2.80383922	4.45255591
C	4.40659482	-3.64439501	2.83509191
H	4.13829494	-4.69533191	2.94174071
C	5.56618388	-3.33507596	2.26156688
H	5.88031152	-2.30317122	2.13396592
H	6.24847270	-4.09892695	1.90593832
N	1.12295342	-1.47099347	-1.88717728
C	0.76905072	-1.64892084	-3.28975416
H	-4.47049455	-0.58705200	2.25424504
H	1.71214239	-2.24460437	-1.59023428
H	0.35647917	-0.71067905	-3.67006039
H	1.66903179	-1.84428215	-3.89467765
C	-0.24310203	-2.77721678	-3.56040315
H	-1.15874921	-2.57690460	-2.99160792
H	-0.51547878	-2.76258462	-4.62291880

C 0.28211178 -4.17789395 -3.20149467

H 0.55822326 -4.18556631 -2.13934554

H 1.19578248 -4.38602777 -3.77017892

C -0.72515013 -5.26410492 -3.45006359

H -1.65962577 -5.17733110 -2.89579836

C -0.56896217 -6.28788312 -4.28434439

H 0.34231045 -6.41640588 -4.86111493

H -1.34217233 -7.03561553 -4.42073490

MP2 Electronic Energy(Ha): 1740.468136303356

B3LYP Electronic Energy(Ha): 1744.987570694652

M06-L Electronic Energy(Ha): 1744.746698881941

Zero point energy correction(kcal/mol): 475.900

Enthalpy correction(kcal/mol): 504.941

Entropy correction(cal/mol): 277.825

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.521

Deuterated enthalpy correction(kcal/mol): 496.955

Deuterated entropy correction(cal/mol): 280.340

Deuterated imaginary Frequencies: -0.00

Axial Reaction C1-S

Reactant geometry

Zr -0.05219385 0.45242549 -0.74150432

C 1.22336418 2.56992801 -0.95013433

C 2.25171395 1.61935109 -0.66721434

H 2.79775751 1.54960796 0.26347954

C 0.78074051 2.26113063 -2.27529912

H -0.00230440 2.77879486 -2.80964566

C 1.44796995 1.10837053 -2.74734553

H 1.31400298 0.63634690 -3.71023468

C 2.36970960 0.71183220 -1.74006657

H 3.04938504 -0.12453773 -1.80530867

B	0.45287670	3.52682626	0.13725578
C	1.03332614	5.01726782	0.34465143
C	-1.13335556	3.44234514	-0.29660714
C	0.39162769	2.60065019	1.50374542
N	0.08123524	1.34148197	1.43980723
N	-1.66620400	2.32582920	-0.67537978
O	-1.97224799	4.49180327	-0.22041406
O	0.62212235	3.06856300	2.73910191
C	0.10227556	0.75961539	2.79156625
C	0.40746423	1.97989913	3.68537413
C	-3.09922269	2.54142808	-0.94292584
C	-3.30615878	4.02462134	-0.57156006
N	-1.72450282	-0.44276373	-1.64875895
H	-0.86075721	0.29953798	3.02720133
C	-1.93501401	-1.73327495	-2.29673570
H	-1.71190788	-1.68140880	-3.37507461
H	-1.22078068	-2.44825119	-1.87615550
C	-3.35702980	-2.30107677	-2.15273285
C	-3.82678411	-2.53874650	-0.69637103
H	-4.41494776	-3.46573570	-0.67448244
H	-2.95792108	-2.70370788	-0.05287661
C	-4.69314320	-1.45285201	-0.12049237
H	-5.58168514	-1.20877500	-0.70335653
C	-4.49315318	-0.81455782	1.02962813
H	-3.62023474	-1.01279307	1.64409301
C	2.13026036	5.47913325	-0.39747342
H	2.59410627	4.81560148	-1.12047610
C	0.47141522	5.91728679	1.26669330
H	-0.38030131	5.60743676	1.86320657
C	0.97459100	7.20396983	1.43913125
H	0.51506911	7.87240942	2.16059243
C	2.64330292	6.76641111	-0.23416154
H	3.49359069	7.08873645	-0.82696424

C	2.06641572	7.63578059	0.68694621
H	2.46101625	8.63787549	0.81854997
H	-3.70785478	1.86222395	-0.34199053
H	-3.32173372	2.34590029	-1.99721214
H	-3.94804610	4.17003815	0.29893391
H	-3.67024623	4.64104154	-1.39363894
H	0.86959350	-0.01618006	2.85234550
H	-0.42304881	2.26534722	4.33271244
H	1.31260015	1.87748575	4.28376513
H	-4.06609029	-1.63777345	-2.66505642
H	-3.38560935	-3.24886516	-2.70183725
H	-2.49497250	0.17622764	-1.88164821
H	-5.19159667	-0.07114833	1.39820833
N	0.65031509	-1.39006368	-0.06681026
H	-0.10345723	-2.02376636	0.20984753
C	1.91809737	-2.04805219	0.22022295
H	2.72406773	-1.30838399	0.19217285
H	1.91668350	-2.45762444	1.24248671
C	2.25199671	-3.18766180	-0.75609100
H	2.26595458	-2.78242609	-1.77416245
H	1.44710965	-3.92991978	-0.72904114
C	3.59403239	-3.87340018	-0.44368091
H	3.57607300	-4.28466750	0.57172843
H	4.38801723	-3.11376320	-0.45977282
C	3.93970804	-4.96154784	-1.42001438
H	4.01946185	-4.65340836	-2.46207969
C	4.14016211	-6.24014400	-1.11177135
H	4.07282915	-6.59310273	-0.08680687
H	4.38461297	-6.97763216	-1.86807334
N	-1.04352063	-3.74111133	1.85874885
H	-2.05124945	-3.64593038	1.95151502
H	-0.63416728	-3.19307140	2.60932630
C	-0.65955054	-5.15629229	1.99619873

H	0.43242365	-5.20943349	1.99389080
H	-0.99476703	-5.60281897	2.94621159
C	-1.21356694	-5.98164907	0.83591048
H	-0.84117700	-5.56257953	-0.10477370
H	-2.30510497	-5.87744935	0.81101226
C	-0.86274366	-7.47917117	0.92096770
H	-1.24687535	-7.90137663	1.85643126
H	-1.38697876	-7.99621899	0.10757771
C	0.60957685	-7.76388647	0.80414682
H	1.09488286	-7.38680643	-0.09552633
C	1.33862908	-8.42937855	1.69567536
H	0.90159490	-8.82364845	2.60859471
H	2.39615581	-8.61307258	1.54236908

MP2 Electronic Energy(Ha): 1740.444189212528

B3LYP Electronic Energy(Ha): 1744.972131593027

M06-L Electronic Energy(Ha): 1744.730883426056

Zero point energy correction(kcal/mol): 473.589

Enthalpy correction(kcal/mol): 502.727

Entropy correction(cal/mol): 283.777

Imaginary Frequencies: -11.21 -6.39

Deuterated zero point energy correction(kcal/mol): 465.160

Deuterated enthalpy correction(kcal/mol): 494.693

Deuterated entropy correction(cal/mol): 286.410

Deuterated imaginary Frequencies: -11.18 -6.35

Transition State geometry

Zr	0.21245994	0.38483990	0.48194899
C	-1.16729320	2.40845030	0.67596088
C	-2.09864208	1.41811043	0.23459025
H	-2.50977185	1.34270801	-0.76172960
C	-0.91624903	2.10105933	2.04984205
H	-0.23816915	2.64012915	2.69496970
C	-1.63732004	0.94981153	2.42213268

H	-1.61375445	0.46278955	3.38632700
C	-2.37230771	0.52358814	1.29487497
H	-3.03685465	-0.32568788	1.26245601
B	-0.36114039	3.49498560	-0.23920427
C	-1.02114766	4.96369829	-0.37020244
C	1.16431872	3.47621280	0.37583102
C	-0.11076289	2.70578237	-1.65784451
N	0.16079631	1.43975719	-1.66288803
N	1.71925648	2.38358033	0.79671773
O	1.93855021	4.57799026	0.41967605
O	-0.11202515	3.29946745	-2.86424172
C	0.40195218	0.99537521	-3.04420460
C	0.17816703	2.28244420	-3.86676743
C	3.10733743	2.68196674	1.19539487
C	3.20909125	4.21054015	1.02108308
N	1.35257084	-0.40600495	2.23169865
H	1.41686594	0.60153036	-3.14559210
C	1.31688588	-1.70631605	2.89215673
H	1.06700356	-1.60545395	3.95538371
H	0.53401595	-2.31316814	2.43143306
C	2.67657264	-2.39652191	2.70104754
C	3.03788558	-2.20192425	1.22679216
H	4.08579578	-2.46811495	1.04134130
H	2.42594488	-2.84771285	0.59063806
C	2.85714979	-0.76194389	0.80848129
H	3.51572603	-0.06836995	1.32177584
C	2.40966299	-0.39078652	-0.47174717
H	2.14906226	-1.17980950	-1.16848830
C	-2.20790346	5.28933370	0.30303967
H	-2.68979622	4.53453582	0.91632914
C	-0.44095014	5.97806153	-1.15176044
H	0.47716694	5.77474387	-1.69247260
C	-1.01053082	7.24453661	-1.25460122

H	-0.53408069	8.00356579	-1.86742503
C	-2.78794883	6.55499483	0.20825480
H	-3.70695103	6.77010247	0.74460588
C	-2.19012315	7.54010727	-0.57235072
H	-2.63625201	8.52620391	-0.64977025
H	3.81247877	2.14345122	0.55504320
H	3.29114709	2.37086296	2.22780705
H	4.00554443	4.52862805	0.34800348
H	3.29957809	4.74999925	1.96559632
H	-0.29502930	0.19691350	-3.31051214
H	1.05594458	2.60801579	-4.42602021
H	-0.67795597	2.22801596	-4.54046622
H	3.43011364	-1.91796223	3.33875544
H	2.64335997	-3.45558439	2.97468308
H	1.79078955	0.28347428	2.83445849
H	2.79886172	0.51855204	-0.91430180
N	-0.45152567	-1.48768624	-0.18466097
H	0.31278633	-2.08752007	-0.49242693
C	-1.69177955	-2.23114592	-0.38277424
H	-2.52694298	-1.53168245	-0.47746639
H	-1.65179004	-2.78325027	-1.33371432
C	-2.00219669	-3.23033772	0.74386294
H	-2.05828462	-2.68157000	1.69071282
H	-1.16779472	-3.93353472	0.84072284
C	-3.30753803	-4.01332303	0.51565169
H	-3.24086045	-4.58825386	-0.41453046
H	-4.12861592	-3.29515231	0.38246662
C	-3.64327645	-4.93312665	1.65486470
H	-3.77417397	-4.45346533	2.62450825
C	-3.77647424	-6.25399859	1.57024616
H	-3.65885156	-6.77658203	0.62533954
H	-4.01494532	-6.85970890	2.43738765
N	1.55720899	-3.92315255	-1.91531249

H	2.57216006	-3.86842317	-1.93857798
H	1.22284859	-3.31164983	-2.65411798
C	1.11975428	-5.30624442	-2.16909985
H	0.02682826	-5.31223331	-2.19124765
H	1.45829219	-5.69255620	-3.14415349
C	1.61167776	-6.24573928	-1.06930536
H	1.27864279	-5.86039178	-0.09970417
H	2.70847157	-6.23480308	-1.04998003
C	1.13341610	-7.69990954	-1.24840170
H	1.44074421	-8.07727096	-2.23027451
H	1.64350312	-8.32134904	-0.50206639
C	-0.35223445	-7.86664716	-1.08289402
H	-0.75795592	-7.54657814	-0.12362013
C	-1.18079290	-8.36307715	-1.99724473
H	-0.82479841	-8.69419455	-2.96850103
H	-2.24349387	-8.46401828	-1.80733608

MP2 Electronic Energy(Ha): 1740.440893774566

B3LYP Electronic Energy(Ha): 1744.948340919801

M06-L Electronic Energy(Ha): 1744.721983757041

Zero point energy correction(kcal/mol): 474.850

Enthalpy correction(kcal/mol): 503.501

Entropy correction(cal/mol): 267.038

Imaginary Frequencies: -304.69

Deuterated zero point energy correction(kcal/mol): 466.095

Deuterated enthalpy correction(kcal/mol): 495.210

Deuterated entropy correction(cal/mol): 270.617

Deuterated imaginary Frequencies: -302.96

Product geometry

Zr	-0.21567463	0.37580150	-0.38483246
C	1.08894867	2.42911521	-0.81048658
C	2.11595468	1.49679666	-0.45928396
H	2.66274345	1.49152664	0.47304850

C	0.65666738	2.03626717	-2.11366743
H	-0.11493668	2.52615604	-2.68852392
C	1.35183479	0.87378357	-2.51723021
H	1.23389258	0.34627625	-3.45374587
C	2.27115233	0.55038961	-1.49236729
H	2.96560708	-0.27512502	-1.50976657
B	0.37227902	3.51895919	0.17260425
C	1.03563593	4.99115762	0.23047094
C	-1.21267513	3.48273803	-0.26520520
C	0.25796339	2.74177925	1.62073205
N	0.01908583	1.46815217	1.66885251
N	-1.79585909	2.38849876	-0.63511590
O	-2.00877177	4.56849677	-0.16877107
O	0.29833218	3.35885915	2.81311319
C	-0.17666387	1.05375056	3.06617926
C	0.10282015	2.35267979	3.85043765
C	-3.23334615	2.66097763	-0.81834237
C	-3.34206440	4.18326430	-0.59755627
N	-1.74369429	-0.46066155	-2.01503272
H	-1.19555810	0.68290278	3.20609173
C	-1.50866915	-1.64163678	-2.89583736
H	-1.31866043	-1.31687760	-3.92064123
H	-0.62614195	-2.17490719	-2.53866727
C	-2.76043079	-2.51317836	-2.73561482
C	-3.09567713	-2.32409585	-1.25104936
H	-4.12516593	-2.58910740	-1.00090713
H	-2.43342819	-2.94143262	-0.63735866
C	-2.82088162	-0.83623003	-0.96272119
H	-3.71056627	-0.25297727	-1.22186956
C	-2.27560035	-0.47464515	0.41369563
H	-2.17708312	-1.35744192	1.05059767
C	2.14784085	5.31530862	-0.56073971
H	2.56537013	4.55865117	-1.21738925

C	0.53642858	6.00835608	1.06286578
H	-0.32290924	5.80682727	1.69286104
C	1.11360245	7.27496901	1.10369473
H	0.70120105	8.03590176	1.75913702
C	2.73433253	6.58108745	-0.52898963
H	3.59439084	6.79434960	-1.15618503
C	2.21860477	7.56839415	0.30550073
H	2.67058930	8.55442174	0.33518939
H	-3.82033169	2.08827172	-0.09479198
H	-3.56368014	2.36756946	-1.81955085
H	-4.04455112	4.47024145	0.18532035
H	-3.57363263	4.73794086	-1.50891670
H	0.51378460	0.24753886	3.32371824
H	-0.72541250	2.68028551	4.47887352
H	1.01527609	2.31316785	4.44732976
H	-3.57270462	-2.13774724	-3.36785092
H	-2.57765132	-3.55468628	-3.00965282
H	-2.08906020	0.30801945	-2.58022842
H	-2.90478294	0.25083357	0.93392385
N	0.55994329	-1.47421255	0.20645474
H	-0.15640313	-2.05313953	0.64435694
C	1.81627962	-2.20883178	0.28492539
H	2.65709624	-1.51241609	0.22332689
H	1.90081115	-2.70022342	1.26575902
C	1.97687010	-3.28375014	-0.80304454
H	1.92175187	-2.80025867	-1.78551331
H	1.13101247	-3.97740457	-0.74703770
C	3.29435623	-4.07025708	-0.68103291
H	3.35000212	-4.55148907	0.30162949
H	4.13200010	-3.36073030	-0.72999218
C	3.46497517	-5.10419854	-1.75711228
H	3.46613922	-4.72684543	-2.77941434
C	3.60060454	-6.41246520	-1.55652669

H	3.60915568	-6.83419757	-0.55559070
H	3.71606889	-7.10735539	-2.38083947
N	-1.04036868	-3.76900813	2.19352978
H	-2.03132670	-3.57627959	2.31100019
H	-0.56028862	-3.25796238	2.92791666
C	-0.78225974	-5.21200038	2.31985163
H	0.29970939	-5.36392168	2.27893600
H	-1.12332505	-5.63028243	3.28087081
C	-1.44843627	-5.98128426	1.17996251
H	-1.08915180	-5.57840652	0.22699416
H	-2.52958839	-5.79808504	1.20753753
C	-1.20227658	-7.50112142	1.23359337
H	-1.55239755	-7.90422542	2.19054425
H	-1.81463724	-7.97210649	0.45449992
C	0.23523931	-7.88695282	1.01648876
H	0.68042181	-7.54229277	0.08355307
C	0.97791688	-8.60134267	1.85736382
H	0.57966534	-8.96572861	2.79990145
H	2.00776038	-8.85525849	1.63251100

MP2 Electronic Energy(Ha): 1740.465268127464

B3LYP Electronic Energy(Ha): 1744.968153462246

M06-L Electronic Energy(Ha): 1744.739193284156

Zero point energy correction(kcal/mol): 476.079

Enthalpy correction(kcal/mol): 503.918

Entropy correction(cal/mol): 267.908

Imaginary Frequencies: -10.19 -8.24

Deuterated zero point energy correction(kcal/mol): 467.406

Deuterated enthalpy correction(kcal/mol): 495.607

Deuterated entropy correction(cal/mol): 270.232

Deuterated imaginary Frequencies: -10.17 -8.14

Axial Reaction C2-S

Reactant geometry

Zr	-0.10826364	0.64284118	-0.48956592
C	-1.14703193	-1.54435547	-1.12571963
C	-2.28882744	-0.75567813	-0.82376754
H	-2.92529745	-0.89235179	0.04128045
C	-0.61512542	-0.98599818	-2.33649551
H	0.25718537	-1.34563080	-2.86297925
C	-1.37411032	0.14411986	-2.71992392
H	-1.21100664	0.76225390	-3.59076251
C	-2.41297769	0.29708807	-1.76828879
H	-3.19131800	1.04755934	-1.79902907
B	-0.35038131	-2.53936678	-0.09213268
C	-0.72458135	-4.10886692	-0.15906372
C	1.24028482	-2.18334972	-0.34455708
C	-0.50768080	-1.86351630	1.41611911
N	-0.39034542	-0.58980740	1.64801004
N	1.62382077	-0.95151294	-0.46689908
O	2.21942071	-3.09845317	-0.41042190
O	-0.65804277	-2.63312532	2.50947518
C	-0.40745751	-0.36659271	3.10624146
C	-0.68654596	-1.77074408	3.67829650
C	3.07546517	-0.91250992	-0.71508604
C	3.48878960	-2.38576023	-0.53046593
N	-1.60550408	2.00987103	0.90074130
N	0.97413139	2.08970212	-1.01647883
C	1.71830629	3.10335551	-1.70430899
H	1.33678251	4.11122616	-1.45387494
H	0.55480344	0.03731870	3.43649637
H	3.26612159	-0.54424537	-1.72708837
C	-2.11964758	3.32661283	0.42391149
H	-2.34319312	3.23017913	-0.64089601
H	-3.05445544	3.57660139	0.93636437
C	-1.08701034	4.42735248	0.64106816

C	3.24081893	3.12009304	-1.44760835
C	3.69208827	3.61348541	-0.05524220
H	3.14780360	4.54257984	0.16669384
H	1.57561787	3.00419675	-2.79295477
C	3.48131209	2.64416115	1.07455727
H	2.45937337	2.30336688	1.21084401
H	4.75379939	3.88148647	-0.09549240
C	4.44207293	2.18818277	1.87628298
H	4.23076257	1.49342053	2.68244928
H	-1.14831317	2.14810296	1.79990731
H	5.47719591	2.49760302	1.75970313
C	-0.05361078	-5.07681655	0.60856210
H	0.74935252	-4.77004540	1.27026888
C	-1.74782803	-4.57186030	-0.99953234
H	-2.28721982	-3.85790065	-1.61378652
C	-0.38527504	-6.42748115	0.54381271
H	0.15606283	-7.14698314	1.15031124
C	-2.09024996	-5.92260329	-1.07253533
H	-2.88778227	-6.24300154	-1.73562377
C	-1.40924956	-6.85796589	-0.29906527
H	-1.66987802	-7.90988517	-0.35250852
C	-1.52542871	5.78629178	0.06309887
H	-1.71128951	5.68666118	-1.01162094
H	-0.68513725	6.48266408	0.17030593
C	-2.73425951	6.37458118	0.73788243
H	-2.63800198	6.54729975	1.80990873
C	-3.87645770	6.69533861	0.13671825
H	-4.01874274	6.54672957	-0.92967385
H	-4.70688068	7.12685939	0.68416158
H	-1.67122650	-1.86551943	4.13924863
H	-1.18307559	0.35150145	3.39101918
H	0.07262354	-2.12442880	4.37579547
H	4.05252120	-2.56525880	0.38717742

H	4.02931127	-2.81094401	-1.37536268
H	3.57108261	-0.23755525	-0.01633995
H	3.64861699	2.12193375	-1.63757635
H	3.68774340	3.78905118	-2.19379919
H	-0.89629906	4.53775360	1.71759070
H	-0.14958944	4.11143355	0.17898382
H	-2.38603794	1.38462959	1.08477428

MP2 Electronic Energy(Ha): 1489.145127649422

B3LYP Electronic Energy(Ha): 1492.989762208731

M06-L Electronic Energy(Ha): 1492.795728280970

Zero point energy correction(kcal/mol): 377.593

Enthalpy correction(kcal/mol): 401.298

Entropy correction(cal/mol): 230.762

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.170

Deuterated enthalpy correction(kcal/mol): 397.052

Deuterated entropy correction(cal/mol): 231.883

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.33123265	-0.77532428	-0.28688326
C	0.86077057	1.25958133	-1.14648410
C	1.92917765	0.34506117	-0.99934760
H	2.69991310	0.39879426	-0.24275166
C	0.09554029	0.77198039	-2.26391237
H	-0.79747812	1.23395309	-2.66029482
C	0.68703586	-0.40033530	-2.77323912
H	0.31055311	-1.00257393	-3.58650630
C	1.80298584	-0.69545624	-1.96603231
H	2.48851214	-1.51741315	-2.11893544
B	0.39332144	2.41630478	-0.10069425
C	0.89992274	3.91817773	-0.42957928
C	-1.24294713	2.24779542	-0.03630320

C	0.80403260	1.86532393	1.39411637
N	0.72285051	0.61980917	1.73886282
N	-1.81258798	1.07935441	-0.03968274
O	-2.08114967	3.29432158	0.03014073
O	1.16942081	2.72135740	2.37568218
C	1.01479392	0.51973780	3.18324490
C	1.47968702	1.93954639	3.55701881
C	-3.27613101	1.25861728	-0.00912484
C	-3.44323307	2.78749952	0.09564051
N	1.25725912	-2.28508038	0.86551971
N	-1.43928226	-2.05591363	-1.11570664
C	-2.44950294	-2.95646025	-1.53856021
H	-2.20574417	-4.00123350	-1.26507519
H	0.11400246	0.22080140	3.72981176
H	-3.72202582	0.84710405	-0.91790962
C	1.85408327	-3.50961237	0.26203324
H	2.26962480	-3.22421422	-0.70522483
H	2.68015599	-3.87403314	0.88214761
C	0.81317138	-4.60692997	0.06937232
C	-3.79023460	-2.57340248	-0.88576750
C	-3.65169977	-2.38065779	0.65000053
H	-4.15450729	-3.20919714	1.16367941
H	-2.56738825	-2.95585899	-2.63305383
C	-2.24699725	-2.37143811	1.20185506
H	-1.71177922	-3.30834706	1.08558796
H	-4.16924129	-1.47349777	0.96914930
C	-1.74038910	-1.44889469	2.05760340
H	-0.85244450	-1.65473734	2.64018094
H	0.86677006	-2.53187500	1.77294972
H	-2.26953675	-0.53505710	2.29744450
C	0.54123860	5.02840826	0.35472647
H	-0.09973265	4.88599623	1.21793490
C	1.73177053	4.17026415	-1.53089105

H	2.03099577	3.34077449	-2.16343083
C	0.98641921	6.31422675	0.05863298
H	0.68839730	7.14778073	0.68731350
C	2.18493996	5.45393322	-1.83767527
H	2.82754640	5.60865576	-2.69895709
C	1.81334336	6.53396538	-1.04243378
H	2.16192875	7.53469749	-1.27608304
C	1.39494868	-5.87370823	-0.58740519
H	1.84455208	-5.61566449	-1.55224851
H	0.56077509	-6.55140925	-0.80486776
C	2.39947147	-6.59791612	0.26642296
H	2.03754380	-6.93063889	1.23937456
C	3.65812261	-6.86062926	-0.07353292
H	4.06366310	-6.55436868	-1.03331834
H	4.32640208	-7.39924410	0.58883440
H	2.55593761	2.00773041	3.73161670
H	1.78580092	-0.23115636	3.38289746
H	0.95033584	2.37625339	4.40392516
H	-3.87570443	3.11692882	1.04200366
H	-4.00381642	3.22950317	-0.72835807
H	-3.71491800	0.73700601	0.84410167
H	-4.11890059	-1.63273125	-1.33562828
H	-4.56156391	-3.31839472	-1.11044196
H	0.37836856	-4.87468313	1.04219823
H	0.00431882	-4.20916267	-0.54759401
H	1.99561322	-1.61372636	1.06652189

MP2 Electronic Energy(Ha): 1489.141486078920

B3LYP Electronic Energy(Ha): 1492.969059116628

M06-L Electronic Energy(Ha): 1492.792249969307

Zero point energy correction(kcal/mol): 377.756

Enthalpy correction(kcal/mol): 400.667

Entropy correction(cal/mol): 220.617

Imaginary Frequencies: -47.86

Deuterated zero point energy correction(kcal/mol): 373.325

Deuterated enthalpy correction(kcal/mol): 396.413

Deuterated entropy correction(cal/mol): 221.722

Deuterated imaginary Frequencies: -47.78

Product geometry

Zr	-0.35133174	-0.70354671	-0.02507436
C	0.69713457	1.20984858	-1.18104692
C	1.75995716	0.26275806	-1.09911588
H	2.61644178	0.34359101	-0.44440913
C	-0.19294156	0.68953359	-2.17512631
H	-1.11618581	1.15197508	-2.49163496
C	0.28485802	-0.55092329	-2.64303536
H	-0.18700228	-1.18388077	-3.38017742
C	1.49898524	-0.82251038	-1.97113895
H	2.12912417	-1.68477080	-2.13444632
B	0.38092575	2.43867296	-0.15214824
C	0.92677551	3.89951055	-0.57151779
C	-1.24815369	2.32681955	0.07354312
C	0.85846631	1.91194871	1.33493769
N	0.77348391	0.66651295	1.69033545
N	-1.81821774	1.16670761	0.17166129
O	-2.06051559	3.38437800	0.22698878
O	1.19249499	2.76949955	2.31799471
C	0.99053764	0.57524435	3.14697523
C	1.46154292	1.99299891	3.51812679
C	-3.25316033	1.35210238	0.44671901
C	-3.41753976	2.88554563	0.41476623
N	1.26449893	-2.24486976	1.01372485
N	-1.66825214	-2.16262387	-0.67336370
C	-2.40069243	-2.85297987	-1.71524929
H	-1.95996486	-3.84534361	-1.90949518
H	0.05484698	0.29301873	3.63856514

H	-3.85507098	0.84800063	-0.31276232
C	1.98966538	-3.39407989	0.40912313
H	2.59631318	-3.00570418	-0.41158679
H	2.67814113	-3.83299796	1.13941811
C	1.03195864	-4.46085313	-0.11242507
C	-3.85185209	-3.03268546	-1.16423381
C	-3.75622248	-2.65427157	0.33611211
H	-4.27857266	-3.35944014	0.98811929
H	-2.37062546	-2.29963521	-2.65694696
C	-2.24003978	-2.60641910	0.62138164
H	-1.90633189	-3.64179559	0.82250509
H	-4.18468223	-1.66356576	0.51108560
C	-1.68680536	-1.63795179	1.67924031
H	-1.26786137	-2.16060544	2.54806656
H	0.71113949	-2.56926538	1.80458122
H	-2.46727209	-0.97416756	2.06125277
C	0.66527681	5.04933286	0.19417856
H	0.07484805	4.96326289	1.09957232
C	1.69442461	4.07754592	-1.73220663
H	1.91654216	3.21615103	-2.35412052
C	1.14294226	6.30372883	-0.17643064
H	0.92029798	7.17004002	0.43878296
C	2.17908761	5.32929518	-2.11327183
H	2.76953633	5.42776085	-3.01887813
C	1.90475549	6.45008514	-1.33501937
H	2.27784397	7.42637935	-1.62653536
C	1.76019417	-5.63964171	-0.78674358
H	2.37729040	-5.27213354	-1.61417446
H	0.99942792	-6.29166897	-1.23242687
C	2.60516510	-6.45358112	0.15464495
H	2.07662800	-6.89240576	1.00088238
C	3.91037207	-6.67567056	0.02816231
H	4.47971069	-6.26434073	-0.80023588

H 4.45619081 -7.28406532 0.74043834

H 2.53340980 2.05205422 3.71920962

H 1.73775880 -0.18388349 3.39588917

H 0.91390754 2.44757611 4.34295500

H -3.80260785 3.31003134 1.34209123

H -4.01892130 3.24285192 -0.42235003

H -3.51086132 0.92076844 1.41658554

H -4.55544348 -2.38613076 -1.69366848

H -4.19463624 -4.06099584 -1.30306009

H 0.42261886 -4.83922286 0.71774543

H 0.33762544 -3.99975231 -0.81902359

H 1.94045941 -1.58867708 1.39743110

MP2 Electronic Energy(Ha): 1489.174742662367

B3LYP Electronic Energy(Ha): 1493.000966715972

M06-L Electronic Energy(Ha): 1492.819590164491

Zero point energy correction(kcal/mol): 378.900

Enthalpy correction(kcal/mol): 401.619

Entropy correction(cal/mol): 220.218

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.469

Deuterated enthalpy correction(kcal/mol): 397.367

Deuterated entropy correction(cal/mol): 221.331

Deuterated imaginary Frequencies: -0.00

Axial Reaction C3-S

Reactant geometry

Zr 0.01437576 -0.26162198 -0.16129207

C -1.59334186 1.62929447 -0.27545919

C -1.82537778 0.95227923 -1.51236492

H -1.51329827 1.30608233 -2.48445263

C -2.19234040 0.80267632 0.72334353

H -2.19993987 1.00786183 1.78382474

C	-2.73024617	-0.35206892	0.12318854
H	-3.24731960	-1.15071061	0.63165262
C	-2.49825241	-0.26419554	-1.26894097
H	-2.80933415	-0.98637682	-2.00990790
B	-0.63296488	2.92529693	-0.01728104
C	-1.36069587	4.36611541	0.05151297
C	0.21163201	2.50797198	1.33017168
C	0.52739337	2.79074638	-1.17173239
N	0.99375432	1.63680461	-1.52681104
N	0.56277745	1.27685171	1.53414954
O	0.62153468	3.38089227	2.26476391
O	1.07170059	3.85649373	-1.79206331
C	1.98564078	1.83691690	-2.59840090
C	2.12427159	3.37020144	-2.66987788
C	1.28565586	1.17753762	2.81313983
C	1.42417816	2.65184590	3.24065961
N	-0.19509490	-2.01540792	0.97907023
N	2.13029606	-0.77452451	-0.11630986
C	3.34563925	-0.02105668	0.14977340
H	3.64781727	-0.08320509	1.20968322
H	2.92645299	1.33964322	-2.35951816
H	0.69874437	0.58650138	3.52232081
C	-1.16059635	-2.95175341	1.54404623
H	-2.11506209	-2.84719128	1.02246381
H	-0.83614661	-3.98771081	1.37318998
C	-1.39644733	-2.75226193	3.04989044
C	4.56714457	-0.44277210	-0.69041864
C	5.05629162	-1.88364247	-0.44082577
H	5.87642888	-2.09087186	-1.14046806
H	3.14574562	1.03770748	-0.04016150
H	2.29881990	-1.75243947	0.10589657
C	5.54670656	-2.12536025	0.95950160
H	6.33928231	-1.46092750	1.30330655

H	4.26131558	-2.59711405	-0.68258693
C	5.10207424	-3.06995081	1.78428197
H	5.51140534	-3.19731258	2.78021871
H	0.73053961	-2.29021199	1.30006499
H	4.31693527	-3.75965125	1.48773938
C	-0.64929823	5.55230789	0.30263603
H	0.42310234	5.50732770	0.45951103
C	-2.74444860	4.49070933	-0.14145721
H	-3.33159675	3.59896686	-0.33689834
C	-1.28181015	6.79155915	0.35815263
H	-0.70041524	7.68702277	0.55496803
C	-3.38942042	5.72700832	-0.08893031
H	-4.46246341	5.78403901	-0.24334592
C	-2.65912615	6.88501442	0.16176034
H	-3.15508241	7.84916399	0.20445288
C	-2.40131466	-3.74950322	3.66054801
H	-3.35521779	-3.69447997	3.12355938
H	-2.60779552	-3.43730016	4.69229405
C	-1.91347827	-5.17172920	3.67935234
H	-0.96917118	-5.33673695	4.19846538
C	-2.53413959	-6.21405834	3.13375988
H	-3.47782848	-6.10179265	2.60793777
H	-2.12746196	-7.21716503	3.19766751
H	4.32594637	-0.34224202	-1.75504374
H	5.39307441	0.25147687	-0.48436562
H	-0.43656817	-2.83191612	3.57594823
H	-1.75354570	-1.73037902	3.21254491
H	3.07739679	3.73479751	-2.28088677
H	1.95634708	3.78945395	-3.66161809
H	1.61362777	1.41326171	-3.53877715
H	2.44662802	3.02834156	3.17250095
H	1.02388766	2.87007963	4.23021120
H	2.24726090	0.68234413	2.67762810

N	0.37054437	-1.41722819	-2.32549321
C	0.35228472	-2.89471488	-2.47540892
H	1.34032625	-1.10254007	-2.34782212
H	-0.12309213	-0.98386798	-3.10213900
H	0.89059510	-3.30837526	-1.61990816
H	0.89538615	-3.19135485	-3.38218629
C	-1.06246395	-3.46243634	-2.51965142
H	-1.62175256	-3.00331723	-3.34382998
H	-1.58240331	-3.19887019	-1.59510884
C	-1.06708015	-4.99041734	-2.70433749
H	-0.48788367	-5.44273821	-1.88839823
H	-0.55911429	-5.25645211	-3.63783574
C	-2.45396783	-5.56976193	-2.70293125
H	-3.02838747	-5.41802447	-1.79018825
C	-3.01186038	-6.22650432	-3.71522678
H	-2.47609915	-6.40225674	-4.64356829
H	-4.02135270	-6.61668541	-3.65332123

MP2 Electronic Energy(Ha): 1740.468700672987

B3LYP Electronic Energy(Ha): 1744.980655714334

M06-L Electronic Energy(Ha): 1744.751632540315

Zero point energy correction(kcal/mol): 475.254

Enthalpy correction(kcal/mol): 504.508

Entropy correction(cal/mol): 272.229

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 466.697

Deuterated enthalpy correction(kcal/mol): 496.355

Deuterated entropy correction(cal/mol): 274.716

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.20413384	-0.20097930	-0.22512861
C	-1.16220058	1.95180311	-0.98789267
C	-0.89877529	1.27382637	-2.21089837

H	-0.11128084	1.52568469	-2.90671465
C	-2.30220862	1.28813587	-0.43075892
H	-2.77658379	1.53881522	0.50696333
C	-2.70892542	0.24009364	-1.27845121
H	-3.52904032	-0.43798187	-1.10090328
C	-1.82728936	0.21180107	-2.37735110
H	-1.88922797	-0.46523644	-3.21948263
B	-0.22836502	3.05032374	-0.22115938
C	-0.66774296	4.59957123	-0.38110240
C	-0.23863983	2.52136515	1.33671781
C	1.29766986	2.72979658	-0.73487551
N	1.73377843	1.52744088	-0.93389198
N	-0.26175303	1.25595214	1.63588237
O	-0.26311471	3.35489616	2.38627805
O	2.16708629	3.72417573	-1.02031874
C	3.08073748	1.62252627	-1.53367995
C	3.42911518	3.11481448	-1.39603452
C	-0.40582992	1.10926716	3.09789059
C	-0.26359191	2.55596171	3.60438565
N	-1.10839004	-1.91715942	0.23296701
N	1.59458001	-1.09650901	1.07290092
C	2.68286173	-0.23958226	1.59372170
H	2.22656554	0.55318343	2.18721924
H	3.79927829	0.97672657	-1.02373561
H	-1.38175619	0.67241083	3.32771527
C	-2.21232089	-2.81166658	-0.07377465
H	-2.68638511	-2.52379138	-1.01958403
H	-1.82344242	-3.82917038	-0.21683120
C	-3.28401037	-2.85732642	1.02622392
C	3.61518320	-1.11797780	2.46669014
C	2.81815687	-2.40458739	2.75249522
H	2.88630191	-2.71613523	3.79707534
H	3.21837014	0.25100548	0.78392616

H	2.02113873	-1.74335879	0.40949234
C	1.34557524	-2.17938998	2.38506080
H	0.87902231	-1.49188210	3.09357539
H	3.19372392	-3.24075493	2.15317412
C	0.51446258	-3.32552855	2.07896256
H	-0.33118883	-3.47245241	2.74788845
H	-0.43676985	-2.51394875	0.89216955
H	1.05889784	-4.25354197	1.89808455
C	0.03578132	5.64293301	0.24572913
H	0.90369856	5.41103605	0.85370577
C	-1.77884248	4.96580769	-1.15436883
H	-2.35115106	4.19188283	-1.65591597
C	-0.34688568	6.97447961	0.10990509
H	0.22065085	7.75376595	0.60906277
C	-2.17233552	6.29717871	-1.29835432
H	-3.03863823	6.54219081	-1.90481886
C	-1.45679692	7.30892917	-0.66520085
H	-1.75829752	8.34565458	-0.77261724
C	-4.42805294	-3.84496614	0.72081539
H	-4.90792997	-3.58216714	-0.22937296
H	-5.19466516	-3.73078596	1.49816407
C	-3.99326277	-5.28428104	0.68294016
H	-3.48702739	-5.64521279	1.57787104
C	-4.17702835	-6.12446834	-0.33189534
H	-4.67158095	-5.81149161	-1.24700408
H	-3.84227828	-7.15483008	-0.28598848
H	4.54924329	-1.33764569	1.94170725
H	3.88856358	-0.59106049	3.38439526
H	-2.80316269	-3.12777614	1.97198509
H	-3.69773996	-1.85233909	1.16210532
H	4.14964157	3.31353456	-0.59894732
H	3.77185349	3.58440015	-2.31737148
H	3.04693448	1.30665467	-2.58452436

H	0.67875198	2.74308299	4.12290159
H	-1.09113191	2.89637617	4.22556721
H	0.35749319	0.44804628	3.50767687
N	0.97006470	-1.28816101	-2.13073844
C	1.98761045	-2.37659333	-2.11566827
H	1.34339791	-0.48594367	-2.63217499
H	0.17265021	-1.60717071	-2.67680121
H	2.80136255	-2.06906654	-1.45119391
H	2.42767915	-2.48826232	-3.11426201
C	1.39472546	-3.70648698	-1.65970292
H	0.60668557	-4.00915090	-2.35962297
H	0.91618582	-3.58642018	-0.68280175
C	2.45355799	-4.81983184	-1.57889645
H	3.25606130	-4.48956656	-0.90452354
H	2.91446856	-4.98616760	-2.55912944
C	1.88371618	-6.10965637	-1.05714339
H	1.40246701	-6.04620989	-0.08312350
C	1.92169034	-7.27703207	-1.69166573
H	2.38868185	-7.38244378	-2.66671023
H	1.49033032	-8.17194709	-1.25777885

MP2 Electronic Energy(Ha): 1740.418159829800

B3LYP Electronic Energy(Ha): 1744.910929838010

M06-L Electronic Energy(Ha): 1744.692290448555

Zero point energy correction(kcal/mol): 474.718

Enthalpy correction(kcal/mol): 502.886

Entropy correction(cal/mol): 262.253

Imaginary Frequencies: -411.93

Deuterated zero point energy correction(kcal/mol): 466.273

Deuterated enthalpy correction(kcal/mol): 494.767

Deuterated entropy correction(cal/mol): 264.158

Deuterated imaginary Frequencies: -405.27

Product geometry

Zr	-0.17504912	-0.45899691	-0.33765814
C	-0.49478147	1.77295789	-1.48862299
C	0.34101251	1.07846341	-2.38932318
H	1.37518631	1.32642770	-2.57927499
C	-1.76204004	1.09284733	-1.54632803
H	-2.64630218	1.37104153	-0.99056429
C	-1.68514515	0.00996259	-2.44657065
H	-2.47633117	-0.68598542	-2.68363663
C	-0.36724503	-0.02682107	-2.94956702
H	0.00479039	-0.73304195	-3.68101281
B	-0.11863457	2.93649345	-0.41994470
C	-0.70159724	4.40591941	-0.82395609
C	-0.76062814	2.37814658	0.99448780
C	1.51160747	2.95591176	-0.15714024
N	2.33162301	1.95876928	-0.18507442
N	-0.93517856	1.11436402	1.26137301
O	-1.18015224	3.21738827	1.95782724
O	2.06588797	4.16421056	0.15106002
C	3.68671175	2.46872996	0.11242082
C	3.48507705	3.97838637	0.34766604
C	-1.65910869	0.98843230	2.54208959
C	-1.69916224	2.43423582	3.06583800
N	-1.15920578	-2.03732251	-0.13663796
N	1.19449498	-1.06521306	1.74849570
C	1.92067116	-0.02836313	2.53500433
H	1.24509393	0.81030286	2.71011646
H	4.10451147	1.96304782	0.99056719
H	-2.65499962	0.57558402	2.35880398
C	-2.13583104	-3.05023435	-0.40609186
H	-2.43961956	-3.03658100	-1.46823266
H	-1.71479074	-4.05419833	-0.23305242
C	-3.40656455	-2.90753213	0.45091299
C	2.30090077	-0.71389233	3.84861082

C	1.05771490	-1.56798736	4.14507320
H	0.32219463	-0.97636972	4.69784737
H	2.76059958	0.35253443	1.95644486
H	1.90969729	-1.64743031	1.32169228
C	0.49523530	-1.96357614	2.75018718
H	-0.57052202	-1.75119172	2.68250398
H	1.28348420	-2.44665727	4.75252594
C	0.70096436	-3.43133289	2.39338543
H	0.13423582	-4.06839520	3.07676180
H	0.34285714	-3.61706644	1.37941907
H	1.75682751	-3.71696752	2.47163734
C	-0.63645685	5.52085304	0.03133975
H	-0.18105875	5.41485482	1.00840655
C	-1.29639237	4.61661895	-2.07750212
H	-1.37035604	3.78634029	-2.77185307
C	-1.13670629	6.76616143	-0.33983575
H	-1.06829155	7.60215331	0.34982291
C	-1.79793491	5.86104738	-2.46273653
H	-2.24915807	5.98095047	-3.44297169
C	-1.72212356	6.94413331	-1.59287684
H	-2.11244581	7.91374119	-1.88479478
C	-4.47429579	-3.98437044	0.17383883
H	-4.73839674	-3.98243334	-0.88973712
H	-5.38622022	-3.71163192	0.72122118
C	-4.06642216	-5.37026161	0.58981226
H	-3.78478227	-5.48132536	1.63726782
C	-4.03331458	-6.44209723	-0.19753350
H	-4.30391558	-6.38346505	-1.24770680
H	-3.73945312	-7.41632507	0.17743048
H	3.18136291	-1.34888257	3.70233121
H	2.53531098	-0.00585935	4.64649273
H	-3.12253797	-2.93143242	1.51007274
H	-3.83613338	-1.91741604	0.26633016

H	3.73671243	4.30411763	1.35925408
H	4.01353509	4.60831318	-0.37017619
H	4.35909088	2.26462180	-0.72741161
H	-1.04987730	2.60320871	3.92777046
H	-2.70029494	2.79905427	3.29360605
H	-1.14310828	0.31379322	3.22611112
N	2.06914382	-1.08772870	-1.19603026
C	2.86970310	-2.32324647	-1.02378649
H	2.56479461	-0.24853424	-0.87736188
H	1.92771480	-0.94204582	-2.19126068
H	3.03151807	-2.50063035	0.04440441
H	3.86531585	-2.20043153	-1.46855834
C	2.16385648	-3.52634724	-1.64399383
H	2.04220992	-3.35719901	-2.72041836
H	1.15536088	-3.59755927	-1.22460337
C	2.93175104	-4.84118644	-1.42658039
H	3.05013208	-5.00452156	-0.34663618
H	3.94082831	-4.76239661	-1.84607579
C	2.22816224	-6.02609272	-2.02749849
H	1.22634380	-6.22282025	-1.64886664
C	2.73044789	-6.81698601	-2.97044910
H	3.72435129	-6.65679716	-3.37821571
H	2.16924903	-7.65483988	-3.36799549

MP2 Electronic Energy(Ha): 1740.476161011190

B3LYP Electronic Energy(Ha): 1744.970571135018

M06-L Electronic Energy(Ha): 1744.746658042013

Zero point energy correction(kcal/mol): 477.344

Enthalpy correction(kcal/mol): 505.963

Entropy correction(cal/mol): 268.248

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.103

Deuterated enthalpy correction(kcal/mol): 497.165

Deuterated entropy correction(cal/mol): 272.399

Deuterated imaginary Frequencies: -0.00

Axial Reaction H3-S

Reactant geometry

Zr	-0.22314284	0.51525139	-0.47398875
C	-1.84752188	-1.38047867	-0.44998953
C	-2.50765405	-0.39934313	0.34737041
H	-2.61770772	-0.43935830	1.42156812
C	-1.97949187	-0.92309834	-1.79726916
H	-1.58471172	-1.42363043	-2.66953865
C	-2.67314839	0.30092536	-1.81766640
H	-2.90569599	0.88272918	-2.69594814
C	-2.98966593	0.63962367	-0.48388999
H	-3.54162085	1.51293866	-0.16354327
B	-0.92799657	-2.62748298	0.05873961
C	-1.63939611	-4.07832094	0.10726233
C	0.40606676	-2.54319292	-0.89789236
C	-0.30991321	-2.11015370	1.48797044
N	0.04765278	-0.87833356	1.65430650
N	0.86740983	-1.40324303	-1.31474275
O	1.13613630	-3.61495565	-1.24314917
O	-0.11700661	-2.92431589	2.54554727
C	0.52937012	-0.70953290	3.03696464
C	0.53355008	-2.14877783	3.58922134
C	2.08183060	-1.63391737	-2.11905737
C	2.30839766	-3.15095017	-1.97466520
N	1.74493480	1.11947660	0.18079370
N	-0.00289814	1.97697286	-2.01038383
C	-1.01271714	2.88361615	-2.58218967
H	-1.86245858	3.00116884	-1.91042031
H	1.51714867	-0.24728403	3.05453084
H	1.90237113	-1.33813936	-3.15610551

C	2.94479489	0.44168075	0.64412101
H	2.66319420	-0.53988550	1.04121048
H	3.65112129	0.23711342	-0.17808622
C	3.71854971	1.21666237	1.72372101
C	-0.28853752	4.23368548	-2.84323581
C	1.21802346	3.89008379	-2.75427455
H	1.65072031	4.29257719	-1.83404691
H	-1.41294118	2.49138098	-3.52845493
C	1.24445057	2.34552119	-2.71063929
H	2.10232590	1.97556103	-2.14712490
H	1.79527977	4.29642918	-3.58903447
C	1.32600922	1.74165512	-4.12650497
H	2.28345046	1.99247586	-4.59456801
H	1.23675359	0.65436868	-4.08509325
H	0.53115907	2.11568493	-4.77766303
C	-2.98631004	-4.23739458	-0.25102409
H	-3.55345064	-3.36789238	-0.56774237
C	-0.95283494	-5.23724111	0.50972356
H	0.09067410	-5.16571504	0.79659230
C	-3.61949006	-5.48030518	-0.21251266
H	-4.66371831	-5.56402984	-0.49732639
C	-1.57375290	-6.48295094	0.55160106
H	-1.01191763	-7.35660643	0.86740182
C	-2.91420487	-6.61080248	0.18958874
H	-3.40092066	-7.58009792	0.22108309
C	4.98002975	0.49496128	2.23889502
H	4.71025183	-0.48880000	2.64043892
H	5.38568887	1.07306748	3.07947988
C	6.06104502	0.33563586	1.20567716
H	6.39142214	1.25727482	0.72644340
C	6.63817493	-0.81052615	0.85503258
H	6.34599802	-1.75492914	1.30499206
H	7.42692436	-0.84723987	0.11196520

H	-0.03631779	-2.27685727	4.50929935
H	-0.15101087	-0.05764832	3.59789044
H	1.53808300	-2.55406537	3.72862919
H	3.18888556	-3.40430638	-1.38157259
H	2.34371141	-3.68785290	-2.92219445
H	2.91555144	-1.04358122	-1.73923174
H	-0.55966085	4.64254691	-3.81941936
H	-0.56699954	4.98296106	-2.09823881
H	4.00315134	2.19752930	1.32004256
H	3.04942827	1.41966706	2.56770022
H	2.00328340	2.03292472	-0.18308497
N	-0.73698500	2.13973183	1.30144732
H	0.22444518	2.14359025	1.64536805
C	-1.21316742	3.52175960	1.07817034
H	-1.31373269	1.68327030	2.00367622
H	-0.55740236	3.97265921	0.32944482
H	-2.20883611	3.46006794	0.63474672
C	-1.23951581	4.37728209	2.34861564
H	-0.23466081	4.38687025	2.78710246
H	-1.90358433	3.91300219	3.08744991
C	-1.68973246	5.83558991	2.11628233
H	-1.55878773	6.39449228	3.04758770
H	-1.01965322	6.29551021	1.37824962
C	-3.11494504	5.97547522	1.65286856
H	-3.34312113	5.60281431	0.65611708
C	-4.09550452	6.51682742	2.36980102
H	-3.91936409	6.91361532	3.36550020
H	-5.10762119	6.58893417	1.98819128

MP2 Electronic Energy(Ha): 1740.494974578476

B3LYP Electronic Energy(Ha): 1744.989308577743

M06-L Electronic Energy(Ha): 1744.767811484378

Zero point energy correction(kcal/mol): 476.752

Enthalpy correction(kcal/mol): 505.338

Entropy correction(cal/mol): 264.705

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.917

Deuterated enthalpy correction(kcal/mol): 496.994

Deuterated entropy correction(cal/mol): 269.194

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.10423512	0.25409346	-0.34391686
C	-1.18210627	-1.99038748	-0.77275039
C	-2.29228796	-1.21578796	-0.32823446
H	-2.77786417	-1.32484604	0.63237599
C	-0.89845010	-1.51938241	-2.09047725
H	-0.11344384	-1.89522964	-2.72924213
C	-1.76808094	-0.45733189	-2.41462838
H	-1.77846268	0.10277128	-3.33762713
C	-2.64155516	-0.26720237	-1.31814903
H	-3.45544310	0.44337768	-1.27197573
B	-0.24270689	-2.97202080	0.12854521
C	-0.58447231	-4.54953169	0.10518718
C	1.29043779	-2.57305719	-0.32256096
C	-0.20670827	-2.27156349	1.62223545
N	-0.17139340	-0.98132492	1.76420393
N	1.59974039	-1.34121693	-0.59445985
O	2.32313622	-3.42768321	-0.29639026
O	-0.06099872	-2.97840124	2.75649783
C	0.11009254	-0.66578998	3.17726548
C	0.01077249	-2.03998191	3.86610819
C	3.06476345	-1.22679151	-0.71590325
C	3.51747224	-2.69768185	-0.70894205
N	1.22555634	1.57198560	0.33552990
N	0.59976318	1.78653461	-2.08789669
C	-0.22537852	2.92069016	-2.53156795

H	-0.53896822	3.50713529	-1.66048822
H	1.10355453	-0.21621709	3.26693088
H	3.34323484	-0.70907914	-1.63463032
C	2.23654702	2.11587459	1.20006047
H	2.43611726	1.44672233	2.05676186
H	3.20133378	2.21282852	0.67652683
C	1.87495437	3.50138521	1.77119511
C	0.65632160	3.76386940	-3.50043873
C	1.99045877	2.99169254	-3.57227975
H	2.70769067	3.40195569	-2.85628642
H	-1.14431805	2.59866332	-3.04282031
C	1.60593239	1.55857751	-3.14070450
H	2.46706897	1.05160291	-2.69057912
H	2.44937943	3.03168622	-4.56385027
C	1.12283759	0.71779718	-4.33326488
H	1.91938359	0.61347672	-5.07750496
H	0.82351271	-0.28168997	-4.01623691
H	0.26527261	1.18147850	-4.83007849
C	-1.64791140	-5.04374842	-0.66512922
H	-2.24534858	-4.34736263	-1.24484302
C	0.15876656	-5.49434729	0.83432940
H	0.99148210	-5.16178158	1.44434522
C	-1.95811843	-6.40333758	-0.71048221
H	-2.78775121	-6.74850417	-1.31958643
C	-0.14166471	-6.85369388	0.79711640
H	0.45463441	-7.55499735	1.37259928
C	-1.20448609	-7.31594377	0.02206294
H	-1.44016051	-8.37463210	-0.01006564
C	2.95428307	4.11018407	2.68806273
H	3.17897143	3.42116480	3.51053818
H	2.54205049	5.01862904	3.14693145
C	4.22627873	4.47340038	1.97348102
H	4.11084800	5.14662628	1.12405900

C	5.44676371	4.05597850	2.29814000
H	5.61354705	3.38440793	3.13531619
H	6.32319976	4.37163345	1.74330888
H	-0.89663594	-2.15959042	4.46154651
H	-0.61418161	0.04708511	3.58148202
H	0.87728131	-2.30190210	4.47234174
H	4.30952075	-2.92435356	0.00359238
H	3.80114011	-3.06507435	-1.69711543
H	3.46006492	-0.65177132	0.12561334
H	0.18829332	3.83436127	-4.48540572
H	0.79776556	4.78537720	-3.14060301
H	1.67161539	4.18288444	0.93661762
H	0.93751534	3.41672908	2.33469982
H	1.14671107	1.96730006	-0.90378220
N	-1.64048089	1.48599075	1.13724198
H	-0.98000492	1.69629094	1.88126913
C	-2.30635897	2.74230028	0.72208239
H	-2.32856549	0.83664179	1.51089093
H	-1.52537382	3.41501654	0.36107985
H	-2.95095939	2.50755631	-0.12674665
C	-3.10428901	3.41326146	1.84395788
H	-2.42942666	3.61288088	2.68495237
H	-3.87342182	2.72278442	2.20987631
C	-3.77742148	4.73888260	1.42813354
H	-4.20180674	5.20963942	2.31976570
H	-3.00458851	5.42122372	1.05111477
C	-4.85725516	4.58202313	0.39131087
H	-4.53934248	4.27238279	-0.60241756
C	-6.15192754	4.79449433	0.60861701
H	-6.52038964	5.11504548	1.57888584
H	-6.89045186	4.66182552	-0.17378199

MP2 Electronic Energy(Ha): 1740.443923269775

B3LYP Electronic Energy(Ha): 1744.937713209269

M06-L Electronic Energy(Ha): 1744.709113294691

Zero point energy correction(kcal/mol): 473.324

Enthalpy correction(kcal/mol): 501.866

Entropy correction(cal/mol): 267.133

Imaginary Frequencies: -1512.42

Deuterated zero point energy correction(kcal/mol): 465.616

Deuterated enthalpy correction(kcal/mol): 494.455

Deuterated entropy correction(cal/mol): 269.060

Deuterated imaginary Frequencies: -1089.10

Product geometry

Zr	0.02375508	0.28413556	-0.19975999
C	-1.23151000	-1.91526038	-0.69036526
C	-2.32884613	-1.21322269	-0.11855678
H	-2.71533378	-1.37361034	0.88079353
C	-1.10232272	-1.39727976	-2.01719942
H	-0.39425602	-1.74499801	-2.75601564
C	-2.08158744	-0.40648131	-2.23537229
H	-2.24307605	0.13496172	-3.15705724
C	-2.84048420	-0.28012552	-1.05150815
H	-3.69182703	0.37305100	-0.90655557
B	-0.22605899	-2.95408566	0.05452480
C	-0.62104572	-4.52265988	0.01921163
C	1.25691778	-2.59471466	-0.56459260
C	-0.00840906	-2.33000108	1.56422565
N	0.04249212	-1.04722027	1.77272425
N	1.58761973	-1.36519452	-0.81934293
O	2.23965801	-3.49500774	-0.73561467
O	0.27507561	-3.09067676	2.63621970
C	0.50647429	-0.80612674	3.15141397
C	0.45843543	-2.21009050	3.77912228
C	3.01986334	-1.30902702	-1.15939497
C	3.39404956	-2.79714117	-1.28749266

N	1.45911408	1.37640397	0.37473318
N	0.01482290	2.18603873	-1.96883920
C	-1.10064468	2.97845819	-2.55837910
H	-1.59937193	3.53682734	-1.76561181
H	1.51384857	-0.38004632	3.13138260
H	3.18195044	-0.75650486	-2.08734366
C	2.68446070	1.91175894	0.88108968
H	3.32586826	1.11596358	1.30647804
H	3.28771280	2.36655852	0.07681665
C	2.48934650	2.97668494	1.97831338
C	-0.48081555	3.90377737	-3.64329984
C	1.02625942	3.56308936	-3.63238989
H	1.57138244	4.26316110	-2.99230123
H	-1.83482143	2.29808170	-2.98688058
C	1.08695701	2.15097011	-3.01588190
H	2.03215719	1.97361812	-2.49897748
H	1.47720893	3.60810121	-4.62603632
C	0.86178293	1.04718202	-4.04926671
H	1.66479115	1.07030811	-4.79112258
H	0.85292433	0.06224222	-3.58197176
H	-0.08524982	1.16958847	-4.58124013
C	-1.79758206	-4.95185022	-0.61333755
H	-2.43960699	-4.21206037	-1.08030195
C	0.17797557	-5.51945642	0.60649975
H	1.09887174	-5.23861764	1.10607212
C	-2.16302509	-6.29771121	-0.65968406
H	-3.08133136	-6.59144168	-1.15894973
C	-0.17621900	-6.86597561	0.56655502
H	0.46615972	-7.60820357	1.03075520
C	-1.35237148	-7.26272979	-0.06842629
H	-1.63127025	-8.31098848	-0.10175338
C	3.80308619	3.56036084	2.53558145
H	4.43790061	2.75206642	2.91627559

H	3.55938589	4.19647165	3.39681971
C	4.57569430	4.38164150	1.54112488
H	4.03021553	5.21431963	1.09646714
C	5.84091370	4.18196034	1.18216106
H	6.42656118	3.36633164	1.59600543
H	6.33884895	4.82600330	0.46587974
H	-0.39265600	-2.35291472	4.44863536
H	-0.14371295	-0.10060571	3.67616130
H	1.37365367	-2.50728609	4.28989818
H	4.27074236	-3.09389988	-0.71274851
H	3.51213295	-3.12320705	-2.32297216
H	3.56889915	-0.79562741	-0.36551773
H	-0.92412372	3.69821356	-4.61988444
H	-0.65709920	4.95960133	-3.42924182
H	1.86722158	3.78586952	1.57532982
H	1.92047877	2.52836891	2.80132043
H	0.42610003	2.71419001	-1.19846141
N	-1.44073823	1.47551546	1.38398697
H	-0.77112753	1.64932194	2.12969681
C	-2.16722953	2.72542484	1.07487786
H	-2.09361895	0.76740376	1.71219421
H	-1.43049345	3.45344381	0.72203975
H	-2.84068221	2.50924207	0.24359211
C	-2.93846218	3.30385856	2.26557626
H	-2.23736638	3.46729054	3.09281285
H	-3.67464729	2.56975888	2.61270284
C	-3.65822239	4.63499490	1.96129420
H	-4.05744867	5.03907450	2.89617739
H	-2.91622675	5.35954838	1.60003547
C	-4.77443298	4.51854350	0.95835661
H	-4.49226152	4.25572519	-0.05942842
C	-6.06148050	4.71182964	1.23109035
H	-6.39679745	4.98322469	2.22791574

H -6.82671703 4.60967087 0.47013571

MP2 Electronic Energy(Ha): 1740.462063474580

B3LYP Electronic Energy(Ha): 1744.957951352390

M06-L Electronic Energy(Ha): 1744.731319620281

Zero point energy correction(kcal/mol): 476.769

Enthalpy correction(kcal/mol): 505.668

Entropy correction(cal/mol): 271.129

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.033

Deuterated enthalpy correction(kcal/mol): 497.264

Deuterated entropy correction(cal/mol): 273.262

Deuterated imaginary Frequencies: -0.00

Axial Reaction H6-S

Reactant geometry

Zr	0.34447783	-1.48440590	0.38444425
C	-1.78991861	-0.50860716	1.16307818
C	-2.23605267	-1.64792751	0.42226495
H	-2.71620224	-1.61957615	-0.54559545
C	-1.21356031	-1.04062483	2.35592718
H	-0.77341921	-0.45892441	3.15125385
C	-1.25224352	-2.45193287	2.31630029
H	-0.89407357	-3.12541261	3.08190119
C	-1.90127151	-2.82788589	1.11812749
H	-2.10700283	-3.84044352	0.80853025
B	-1.68370005	1.03968846	0.63683001
C	-2.98463639	1.97120088	0.87485362
C	-0.26228097	1.56783333	1.27076215
C	-1.27765730	0.86466086	-0.95114806
N	-0.39238955	-0.01179313	-1.31894883
N	0.77481361	0.79742977	1.36056917
O	-0.07084408	2.84883699	1.65367849

O	-1.83357047	1.57133337	-1.94495837
C	-0.26560600	0.00782015	-2.78734782
C	-1.28516361	1.08739583	-3.20759076
C	1.92418381	1.60433561	1.82452602
C	1.29159889	2.96729513	2.15352408
N	0.44707629	-3.10621892	-0.94110589
N	2.02985309	-2.40358488	1.81491316
C	2.42246015	-1.95348047	3.17666044
H	1.97247989	-2.59797770	3.93328439
H	0.75623918	0.26150473	-3.08065469
H	2.39427066	1.14671093	2.69779875
C	-0.34128475	-4.20972701	-1.47851371
H	-1.40266577	-4.03520463	-1.27817761
H	-0.24576807	-4.24939116	-2.57181045
C	0.05270274	-5.57851422	-0.89981563
C	3.95517022	-1.96807584	3.17426902
C	4.29035329	-1.48875450	1.75447834
H	5.28577691	-1.79576526	1.42759046
H	2.04691807	-0.94156368	3.33756172
C	3.19039125	-2.08273990	0.84170019
H	3.52555118	-3.04821382	0.45108418
H	4.25684849	-0.39698609	1.70832552
C	2.62157383	-1.20455356	-0.26973110
H	2.87305182	-1.59746521	-1.26045023
H	1.89102746	-3.40904383	1.83302046
H	3.00774352	-0.18486529	-0.21237874
C	-2.95543598	3.37229980	0.76120452
H	-2.01786709	3.87186217	0.54559313
C	-4.22844932	1.39000802	1.16680914
H	-4.29678050	0.31173978	1.27078910
C	-4.09844725	4.14788450	0.93961603
H	-4.03376744	5.22834133	0.85760680
C	-5.38159571	2.15552491	1.33382705

H	-6.32649812	1.66863742	1.55227731
C	-5.32006487	3.54155159	1.22473303
H	-6.21049795	4.14424772	1.36369566
C	-0.75910238	-6.75420746	-1.47991673
H	-1.82996189	-6.57300768	-1.33213941
H	-0.51104912	-7.65927459	-0.91072015
C	-0.48628856	-7.00998530	-2.93630608
H	0.54459087	-7.26600194	-3.18205850
C	-1.38155970	-6.94426069	-3.91784394
H	-2.42022711	-6.69158968	-3.72389945
H	-1.11048657	-7.14367835	-4.94874799
H	-2.11534995	0.69922014	-3.79847909
H	-0.49617410	-0.97870318	-3.19441600
H	-0.84152836	1.93801098	-3.72486206
H	1.76382681	3.80434094	1.64082804
H	1.23417374	3.18193406	3.22236110
H	2.66251817	1.68111688	1.02440505
H	4.38206378	-1.33442472	3.95582037
H	4.31978778	-2.98756026	3.33657036
H	1.12216651	-5.74736146	-1.07767327
H	-0.07910159	-5.54686634	0.18737843
H	1.32910247	-3.06774355	-1.44445356
N	2.33334173	2.23630932	-1.47284784
H	1.74926937	1.41897978	-1.33225755
H	2.93381434	2.05538552	-2.27095864
C	1.52278387	3.44047366	-1.67621079
H	0.95795355	3.44467095	-2.62363532
H	0.77892061	3.47668913	-0.87590604
C	2.39332706	4.69274695	-1.61139099
H	3.15276392	4.65358735	-2.40153663
H	2.93965205	4.68865198	-0.66163460
C	1.58812157	5.99489952	-1.75433432
H	0.83360740	6.03451399	-0.95705813

H 1.04139562 5.99269276 -2.70379267

C 2.46077469 7.21545178 -1.67877630

C 2.66151864 8.07781811 -2.67051989

H 2.16528411 7.96185498 -3.63024051

H 3.32687007 8.92694260 -2.55988109

H 2.98054666 7.36930417 -0.73329120

MP2 Electronic Energy(Ha): 1740.466091509394

B3LYP Electronic Energy(Ha): 1744.963451196441

M06-L Electronic Energy(Ha): 1744.738692284509

Zero point energy correction(kcal/mol): 475.466

Enthalpy correction(kcal/mol): 499.143

Entropy correction(cal/mol): 224.072

Imaginary Frequencies: -58.15 -57.60 -55.01 -51.63 -50.84 -38.82 -26.69 -23.33

Deuterated zero point energy correction(kcal/mol): 466.809

Deuterated enthalpy correction(kcal/mol): 490.864

Deuterated entropy correction(cal/mol): 226.413

Deuterated imaginary Frequencies: -58.09 -57.50 -54.95 -51.48 -50.68 -38.60 -26.50 -23.25

Transition State geometry

Zr -0.45447581 -1.58787563 0.28721988

C -2.58888440 -0.38966150 -0.01422258

C -2.63621020 -1.41447589 -1.01913125

H -2.52835514 -1.25357458 -2.08267899

C -2.76583933 -1.06976942 1.22222492

H -2.76645416 -0.60415488 2.19678620

C -2.84898102 -2.46795112 0.98877131

H -2.98963226 -3.23540646 1.73780824

C -2.79288738 -2.67430978 -0.41027355

H -2.82307608 -3.62902079 -0.91443876

B -2.08567361 1.15223974 -0.23022526

C -3.23235535 2.24474002 -0.54834390

C -1.14346861 1.49231374 1.07593093

C -0.92078994 1.01334746 -1.39183662

N	-0.02989712	0.06886291	-1.32292928
N	-0.34888658	0.62517336	1.61897794
O	-1.09114181	2.73799457	1.58634208
O	-0.81827269	1.81322722	-2.46208172
C	0.82260005	0.10830141	-2.52431055
C	0.33881516	1.38412388	-3.24249009
C	0.42304930	1.30057769	2.68460678
C	-0.09887572	2.74855020	2.65063968
N	0.38013648	-2.99833125	-0.74478426
N	0.21092303	-2.64669914	2.34711868
C	-0.20127394	-2.29113265	3.73520850
H	-1.04867234	-2.90589287	4.04276958
H	1.87887073	0.15346393	-2.24971736
H	0.24823888	0.81954498	3.65123500
C	0.73777104	-4.06107998	-1.63715807
H	-0.11709369	-4.31136623	-2.28713694
H	1.54874492	-3.75176831	-2.31496645
C	1.17543359	-5.34864613	-0.91477538
C	1.05666284	-2.48847486	4.59075794
C	2.17428383	-2.03272841	3.64214314
H	3.15870169	-2.41478006	3.91937119
H	-0.52394053	-1.24933902	3.75211234
C	1.74486325	-2.54317182	2.25193645
H	2.11217302	-3.56531800	2.11798216
H	2.23775565	-0.94130041	3.63112148
C	2.10304586	-1.71941333	1.02160574
H	3.08580179	-1.99460710	0.62724875
H	-0.04273895	-3.61478111	2.17698429
H	2.14090230	-0.64943933	1.24713409
C	-2.93262474	3.58984025	-0.82540309
H	-1.89808773	3.91636641	-0.82464455
C	-4.58891796	1.88789637	-0.56082423
H	-4.86478774	0.85883616	-0.35363917

C	-3.92722686	4.52488331	-1.09934922
H	-3.65802859	5.55544250	-1.30941822
C	-5.59508921	2.81570868	-0.83273451
H	-6.63420267	2.50158432	-0.83335332
C	-5.26768307	4.14084715	-1.10421803
H	-6.04547261	4.86669301	-1.31756547
C	1.49642313	-6.51707209	-1.86743103
H	0.62495611	-6.73215117	-2.49592160
H	1.67267452	-7.41501386	-1.26089263
C	2.70008490	-6.28265578	-2.73739959
H	3.62643129	-6.05855354	-2.20817168
C	2.71881075	-6.33598417	-4.06632888
H	1.82195145	-6.55476435	-4.63842748
H	3.62901638	-6.16726916	-4.63093705
H	0.00459222	1.22065052	-4.26646558
H	0.67030206	-0.79825684	-3.11496312
H	1.06624459	2.19722535	-3.22476858
H	0.67233235	3.47003682	2.38128927
H	-0.59786105	3.06391879	3.56806410
H	1.49069462	1.25933169	2.46201264
H	1.02061369	-1.92094602	5.52335470
H	1.17796955	-3.54586087	4.84923154
H	2.05216304	-5.13165310	-0.29182507
H	0.37278721	-5.65240091	-0.23376865
H	1.39063396	-2.38945076	-0.06164876
N	2.56488394	2.28352106	0.23335878
H	1.82176997	1.67828238	-0.10359460
H	3.42610240	1.74734759	0.17863769
C	2.66785072	3.49777095	-0.58715010
H	2.92775938	3.29365069	-1.63975867
H	1.68408343	3.97807397	-0.59522146
C	3.69863534	4.46406243	-0.00376936
H	4.67917604	3.97365422	0.03289829

H	3.42319686	4.68397357	1.03309816
C	3.82110800	5.76984768	-0.80782871
H	2.83228361	6.24588747	-0.85334118
H	4.10955370	5.54705809	-1.84096728
C	4.80466088	6.73534646	-0.20877951
C	5.89954827	7.19051128	-0.81015798
H	6.16062616	6.88818386	-1.82021648
H	6.57260632	7.88440850	-0.31933476
H	4.58405681	7.06696651	0.80524426

MP2 Electronic Energy(Ha): 1740.420959994869

B3LYP Electronic Energy(Ha): 1744.916994662035

M06-L Electronic Energy(Ha): 1744.687636458303

Zero point energy correction(kcal/mol): 471.662

Enthalpy correction(kcal/mol): 494.358

Entropy correction(cal/mol): 215.783

Imaginary Frequencies: -1599.64 -62.05 -61.65 -57.76 -55.92 -50.99 -49.13 -41.13 -39.16

Deuterated zero point energy correction(kcal/mol): 463.837

Deuterated enthalpy correction(kcal/mol): 486.836

Deuterated entropy correction(cal/mol): 217.627

Deuterated imaginary Frequencies: -1168.96 -62.01 -61.56 -57.69 -55.55 -50.87 -48.78 -40.54 -38.74

Product geometry

Zr	0.88313988	-1.14486365	0.03595518
C	2.73887141	0.50677929	0.37289277
C	2.79795689	-0.40379487	1.48192444
H	2.52086755	-0.17454160	2.50119975
C	3.21883073	-0.22937029	-0.74123705
H	3.28125303	0.14782838	-1.75271957
C	3.49568396	-1.56605086	-0.35035644
H	3.89542066	-2.35181857	-0.97830662
C	3.24540475	-1.67024931	1.04008486
H	3.39445767	-2.54777293	1.65183661
B	1.87183864	1.90056638	0.31252740

C	2.69824610	3.27893884	0.47177115
C	0.94908623	1.80847043	-1.06058183
C	0.69802185	1.65819493	1.44601160
N	0.01711703	0.55199303	1.45508997
N	0.34528538	0.72854392	-1.45733745
O	0.69032247	2.91096021	-1.78672263
O	0.41678718	2.51104134	2.44196878
C	-0.81690090	0.51028408	2.66934726
C	-0.68375405	1.94332084	3.21575724
C	-0.52723898	1.06275047	-2.60377480
C	-0.19587579	2.54080867	-2.87981676
N	-0.14174817	-2.48376468	0.86386511
N	0.88229118	-2.52679133	-2.03134645
C	1.50986896	-2.13854893	-3.32336991
H	2.54116554	-1.82864273	-3.16023502
H	-1.84723636	0.24041658	2.43191855
H	-0.30455332	0.42531587	-3.46266643
C	-0.79599201	-3.52346646	1.59594271
H	-1.53120411	-3.09544701	2.30050833
H	-1.38446401	-4.16803674	0.92169302
C	0.16747541	-4.41268469	2.40214377
C	1.35199849	-3.37452581	-4.21373079
C	-0.04661486	-3.90069816	-3.83341553
H	-0.10134647	-4.99023848	-3.86841540
H	0.96525360	-1.28601374	-3.73328557
C	-0.33091228	-3.35376283	-2.40079245
H	-0.38603875	-4.15951063	-1.66799820
H	-0.79814534	-3.51936205	-4.52968757
C	-1.62338664	-2.54871219	-2.32539198
H	-2.46621953	-3.17995206	-2.62142922
H	1.52900166	-3.18595346	-1.59806021
H	-1.60196656	-1.68920922	-3.00055831
C	2.06442952	4.53249562	0.52544485

H	0.98298185	4.58702724	0.45492398
C	4.09759772	3.27791185	0.56752690
H	4.62618582	2.33058642	0.53524750
C	2.78353702	5.71644339	0.66465463
H	2.25970855	6.66652807	0.70326946
C	4.83000393	4.45760069	0.70608492
H	5.91242191	4.41661679	0.77741546
C	4.17465504	5.68435527	0.75520176
H	4.73852159	6.60494085	0.86408634
C	-0.52900769	-5.53179827	3.20190193
H	-1.28936678	-5.10051188	3.86320833
H	0.21803357	-6.00425207	3.85313165
C	-1.15304396	-6.59657047	2.34349064
H	-0.47440673	-7.09901089	1.65367605
C	-2.43019945	-6.96810643	2.36688811
H	-3.14582552	-6.49890457	3.03569097
H	-2.80708515	-7.75559796	1.72361939
H	-0.41524534	2.00342298	4.26936153
H	-0.42617317	-0.24538071	3.35696713
H	-1.56653745	2.55905307	3.02998160
H	-1.06327012	3.19995568	-2.84485917
H	0.34479087	2.70410207	-3.81398631
H	-1.57266266	0.91893938	-2.32032855
H	1.44667089	-3.14768203	-5.27754819
H	2.12578435	-4.10811868	-3.96503818
H	0.90058258	-4.85073648	1.71385851
H	0.73302263	-3.77442512	3.08886883
H	-1.79505886	-2.20080619	-1.30569626
N	-3.10227022	0.98466760	-0.31248452
H	-2.18156741	0.90619238	0.11069830
H	-3.56947171	0.09577429	-0.15798570
C	-3.87084953	2.07734910	0.29716774
H	-4.05412140	1.93435734	1.37557082

H	-3.28097154	2.99501751	0.19955781
C	-5.21250139	2.26340577	-0.41151314
H	-5.79397968	1.33617291	-0.33961596
H	-5.02370606	2.42950828	-1.47736320
C	-6.04342350	3.42188556	0.16657273
H	-5.44792715	4.34309105	0.10663442
H	-6.24209239	3.24571883	1.22940965
C	-7.34267295	3.62917386	-0.55972980
C	-8.55180930	3.53812991	-0.01455616
H	-8.68472667	3.30666326	1.03828582
H	-9.45272802	3.69507921	-0.59690141
H	-7.25932654	3.86302533	-1.62051476

MP2 Electronic Energy(Ha): 1740.464325826725

B3LYP Electronic Energy(Ha): 1744.966955616364

M06-L Electronic Energy(Ha): 1744.733086257712

Zero point energy correction(kcal/mol): 474.838

Enthalpy correction(kcal/mol): 497.473

Entropy correction(cal/mol): 215.530

Imaginary Frequencies: -62.35 -61.86 -58.12 -56.74 -55.16 -49.46 -45.28 -39.28 -38.41

Deuterated zero point energy correction(kcal/mol): 466.217

Deuterated enthalpy correction(kcal/mol): 489.182

Deuterated entropy correction(cal/mol): 217.629

Deuterated imaginary Frequencies: -62.32 -61.75 -58.02 -56.55 -55.10 -49.29 -44.57 -38.97 -38.09

Axial Reaction C1-S

Reactant geometry

Zr	0.15341711	-0.43118576	-0.93540162
C	-0.89128962	-2.67574618	-1.05602219
C	-2.02239435	-1.80604734	-1.13566487
H	-2.75501308	-1.66165555	-0.35355183
C	-0.20408692	-2.51274695	-2.30028927
H	0.70917192	-3.01652199	-2.58065894

C	-0.83991039	-1.51405643	-3.07195448
H	-0.54199993	-1.17170118	-4.05283441
C	-1.97905405	-1.07753264	-2.34207671
H	-2.68877280	-0.33368024	-2.67168929
B	-0.30333761	-3.38733967	0.29987984
C	-0.81255325	-4.88387505	0.62178646
C	1.32877261	-3.20769274	0.18486759
C	-0.59659152	-2.27520263	1.48713860
N	-0.35663909	-1.01426582	1.29048904
N	1.85597750	-2.11474930	-0.26504923
O	2.19907565	-4.13368680	0.63025839
O	-1.07076776	-2.58158722	2.70346775
C	-0.72858174	-0.24853032	2.49198671
C	-1.12873978	-1.35442191	3.49029563
C	3.31917803	-2.19183359	-0.11486669
C	3.54416821	-3.62860397	0.39925956
N	1.91564569	0.48957544	-1.63534754
H	0.11479336	0.35008525	2.84422536
C	2.15203620	1.73195148	-2.37806805
H	1.59045736	1.73992373	-3.32319708
H	1.76816814	2.57843203	-1.79655769
C	3.62929275	1.96864622	-2.72140221
C	4.57096977	2.15583137	-1.51581187
H	4.44262537	1.33549284	-0.80342773
H	5.60477886	2.09574373	-1.88182845
C	4.41229920	3.47000850	-0.80466371
H	4.44138920	4.35564599	-1.43974519
C	4.28518436	3.63063722	0.51113292
H	4.22919387	4.61603905	0.96098302
C	-1.69422350	-5.55164840	-0.24090571
H	-2.03804519	-5.04563875	-1.13749686
C	-0.39989357	-5.58499843	1.76816051
H	0.28356568	-5.11192778	2.46551765

C	-0.84101327	-6.87757636	2.03882016
H	-0.50119153	-7.38881945	2.93419624
C	-2.14313947	-6.84697019	0.01912772
H	-2.82544514	-7.33164008	-0.67218451
C	-1.71759511	-7.51653217	1.16265039
H	-2.06347543	-8.52373431	1.37050014
H	3.66636198	-1.43119834	0.59097114
H	3.82128321	-2.01310218	-1.06992996
H	4.08976690	-3.68408685	1.34127103
H	4.02260000	-4.28105705	-0.33330045
H	-1.54834980	0.43522821	2.25875345
H	-0.43044030	-1.46420583	4.32167046
H	-2.14172474	-1.25819615	3.88029314
H	3.98581156	1.11892683	-3.31708306
H	3.70407614	2.84711627	-3.37418652
H	2.72713730	-0.11447258	-1.71293310
H	4.25916075	2.78022895	1.18613341
N	-0.80409320	1.39257769	-0.71259860
H	-0.17050562	2.12716650	-0.37565706
C	-2.13817461	1.96940634	-0.80342979
H	-2.87886507	1.16733123	-0.88341783
H	-2.38051231	2.51774014	0.11998629
C	-2.30983597	2.92733212	-1.99406244
H	-2.09149687	2.38039262	-2.91829284
H	-1.56164283	3.72390735	-1.92298713
C	-3.71567215	3.54972320	-2.06877800
H	-3.92900400	4.10028335	-1.14563471
H	-4.45570686	2.73957859	-2.12767869
C	-3.89169694	4.46152090	-3.24967757
H	-3.75483462	4.00028558	-4.22731228
C	-4.17995722	5.75838386	-3.18746826
H	-4.32610792	6.26268636	-2.23647646
H	-4.28574076	6.36271421	-4.08148877

N	0.63359654	4.08011265	0.48231503
H	1.64548487	3.98541455	0.43716967
H	0.38166744	4.81112826	-0.17712540
C	0.20334130	4.44695550	1.83730441
H	-0.88918853	4.49672579	1.84427713
H	0.47458670	3.62342297	2.50737440
C	0.78296207	5.75877462	2.38588258
H	0.52272220	6.57872782	1.70400038
H	1.87709564	5.69314633	2.38524928
C	0.30276177	6.10605755	3.80960025
H	0.53939569	5.28261017	4.49298766
H	0.87286294	6.97535420	4.16064980
C	-1.16429290	6.42673786	3.89202702
H	-1.50248010	7.24575956	3.25735651
C	-2.05120829	5.80716473	4.66540763
H	-1.76293131	4.98725820	5.31680536
H	-3.09492365	6.10001063	4.68266222

MP2 Electronic Energy(Ha): 1740.444685240620

B3LYP Electronic Energy(Ha): 1744.975696364541

M06-L Electronic Energy(Ha): 1744.730314156763

Zero point energy correction(kcal/mol): 474.616

Enthalpy correction(kcal/mol): 504.101

Entropy correction(cal/mol): 271.554

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 466.154

Deuterated enthalpy correction(kcal/mol): 496.033

Deuterated entropy correction(cal/mol): 274.143

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.84380922	-0.28116496	0.10868968
C	0.54760531	-2.31637153	-1.23325721
C	0.28477399	-1.26315202	-2.16231111

H	-0.68993800	-0.98305561	-2.53488642
C	1.96430862	-2.29925076	-1.03808842
H	2.50971408	-2.95391671	-0.37461701
C	2.53950403	-1.25753066	-1.79249058
H	3.58356273	-0.98048964	-1.80919561
C	1.49779124	-0.61146600	-2.49032231
H	1.61766423	0.22116741	-3.16578471
B	-0.53925710	-3.17746326	-0.36891748
C	-1.01117419	-4.58717593	-1.00039782
C	0.13054902	-3.27480604	1.13063808
C	-1.74339032	-2.10220081	-0.06752900
N	-1.46151014	-0.86758199	0.20118577
N	0.79504165	-2.29003371	1.64686210
O	-0.03264961	-4.34972074	1.92660787
O	-3.04932017	-2.41832808	-0.01896820
C	-2.70027030	-0.13897032	0.51462423
C	-3.79416427	-1.20133688	0.27866508
C	1.18227289	-2.64951313	3.02314444
C	0.66366912	-4.09410294	3.17599852
N	2.76292239	0.07583895	1.19584340
H	-2.67704789	0.21766955	1.54819441
C	3.91178733	0.93180142	1.41806233
H	4.84504940	0.46095321	1.08629785
H	3.78919965	1.83961307	0.82125672
C	3.97833490	1.27700689	2.93770604
C	2.55055305	1.11377526	3.51600675
H	2.42976161	0.16233163	4.04132706
H	2.33502559	1.89891438	4.25080215
C	1.53773617	1.22331181	2.40048536
H	1.70575205	2.11319912	1.79694795
C	0.21541121	0.75951707	2.36593683
H	-0.53987887	1.43393117	1.98087127
C	-0.47932331	-5.05456943	-2.21138158

H	0.26058596	-4.45241842	-2.72910139
C	-1.96719332	-5.40572205	-0.37407730
H	-2.40860323	-5.08712946	0.56419223
C	-2.36923217	-6.62041577	-0.92353902
H	-3.11072957	-7.22631771	-0.41191282
C	-0.87368183	-6.27022574	-2.77159593
H	-0.43955588	-6.59877445	-3.71081180
C	-1.82240070	-7.05992494	-2.12856748
H	-2.13359673	-8.00585932	-2.55958760
H	0.72514711	-1.96260438	3.74068919
H	2.26753705	-2.58723833	3.15195770
H	-0.04875875	-4.22423790	3.99119363
H	1.45950147	-4.83446954	3.27256096
H	-2.80424583	0.73071630	-0.13787254
H	-4.41865559	-1.39778112	1.15037667
H	-4.43171363	-0.98613314	-0.58035141
H	4.67278019	0.60668524	3.45176756
H	4.35489225	2.29268389	3.08933651
H	2.88930045	-0.76683137	1.75558011
H	-0.12563086	0.03826428	3.10096188
N	0.45396337	1.65195202	-0.58184327
H	0.21468501	2.30849768	0.16415014
C	0.33220816	2.39091270	-1.83325806
H	0.14443258	1.69882546	-2.65832231
H	-0.54368096	3.05526564	-1.79081721
C	1.56952799	3.24163529	-2.16562482
H	2.44216088	2.58133218	-2.22389263
H	1.76130795	3.93403046	-1.33825626
C	1.42177134	4.03753251	-3.47489207
H	0.55340375	4.70290549	-3.41086279
H	1.21552496	3.33280263	-4.29223209
C	2.64587385	4.83891805	-3.81515850
H	3.56054179	4.26487886	-3.96044156

C	2.69413424	6.16277313	-3.93357470
H	1.80860935	6.77753932	-3.79936682
H	3.61576942	6.68082621	-4.17419321
N	-0.42354294	4.26525270	1.31875958
H	-0.24588466	4.13619803	2.31116208
H	0.22789652	4.97636315	0.99781118
C	-1.80766572	4.71056167	1.10232255
H	-1.96743946	4.79700313	0.02421758
H	-2.47173973	3.90976544	1.44561303
C	-2.19591004	6.02527394	1.79257164
H	-1.52421501	6.82308480	1.45003346
H	-2.03006331	5.92459621	2.87180912
C	-3.65881796	6.44784209	1.54857663
H	-4.33481872	5.64989513	1.87588254
H	-3.87356985	7.31739993	2.18213884
C	-3.95472238	6.80692220	0.11827037
H	-3.34747234	7.60911997	-0.30084113
C	-4.88141637	6.23740419	-0.64686749
H	-5.51260138	5.43603627	-0.27403549
H	-5.04910876	6.55435161	-1.66997167

MP2 Electronic Energy(Ha): 1740.425066780021

B3LYP Electronic Energy(Ha): 1744.934126533416

M06-L Electronic Energy(Ha): 1744.706150353406

Zero point energy correction(kcal/mol): 475.145

Enthalpy correction(kcal/mol): 503.671

Entropy correction(cal/mol): 262.955

Imaginary Frequencies: -334.56

Deuterated zero point energy correction(kcal/mol): 466.586

Deuterated enthalpy correction(kcal/mol): 495.493

Deuterated entropy correction(cal/mol): 265.393

Deuterated imaginary Frequencies: -330.91

Product geometry

Zr	0.75350518	-0.28019019	0.09246176
C	0.56361189	-2.37391864	-1.20213145
C	0.29706420	-1.38299314	-2.19844230
H	-0.67160617	-1.17733623	-2.63158389
C	1.96150398	-2.26456009	-0.92943759
H	2.50791295	-2.86531565	-0.21830169
C	2.51475335	-1.20794431	-1.68839639
H	3.54669288	-0.88567654	-1.68366086
C	1.48014934	-0.67209706	-2.48904513
H	1.58850057	0.13631421	-3.19511119
B	-0.53774777	-3.23173205	-0.35347281
C	-0.99849254	-4.64600688	-0.98409603
C	0.08878612	-3.31457838	1.16452541
C	-1.75312003	-2.15551479	-0.07100655
N	-1.48604651	-0.90890152	0.16671527
N	0.74924975	-2.33320778	1.68867241
O	-0.13921471	-4.36929439	1.97615326
O	-3.05029521	-2.48766628	0.02931832
C	-2.72151039	-0.19687440	0.52699721
C	-3.80570447	-1.27501448	0.32509247
C	1.02767865	-2.65972172	3.10035912
C	0.53985553	-4.11536465	3.23435574
N	2.70543308	0.20950074	1.43297804
H	-2.65907879	0.15578149	1.55995929
C	4.10789246	0.67272571	1.44395819
H	4.79147351	-0.16525913	1.30012861
H	4.24717128	1.36721043	0.61358297
C	4.28973847	1.39395978	2.82020578
C	2.85340101	1.53499879	3.40024283
H	2.66245837	0.77995299	4.17026432
H	2.67662395	2.51378414	3.85128650
C	1.94344272	1.27616776	2.18318471
H	2.00092611	2.15882898	1.53596908

C	0.50247518	0.80045434	2.22415497
H	-0.20198133	1.63349190	2.27753799
C	-0.42727448	-5.13042808	-2.17035507
H	0.33209473	-4.53714684	-2.66985798
C	-1.97808840	-5.45409990	-0.38065795
H	-2.44929835	-5.12282908	0.53820602
C	-2.36514345	-6.67426635	-0.92883763
H	-3.12550766	-7.27164698	-0.43517832
C	-0.80615991	-6.35185686	-2.72869182
H	-0.34105438	-6.69345924	-3.64824082
C	-1.77907687	-7.13058125	-2.10890088
H	-2.07860587	-8.08091424	-2.53853679
H	0.48698584	-1.97316632	3.75827620
H	2.09451866	-2.56316673	3.32686361
H	-0.17390055	-4.27439672	4.04270286
H	1.35463217	-4.83670415	3.32637997
H	-2.86096181	0.67318140	-0.11765127
H	-4.41253148	-1.46929193	1.20934008
H	-4.45962667	-1.07958694	-0.52634676
H	4.93766028	0.81872930	3.48511256
H	4.76195370	2.36839126	2.67895270
H	2.65955409	-0.62573702	2.01845513
H	0.31725585	0.13786116	3.07607392
N	0.39358189	1.62698721	-0.66374006
H	0.11270335	2.26927943	0.08005123
C	0.32261926	2.36851697	-1.91572358
H	0.16900242	1.67867915	-2.75029334
H	-0.55297685	3.03381082	-1.90561341
C	1.57331833	3.21911548	-2.19490599
H	2.44677707	2.55744204	-2.22642502
H	1.73374685	3.90445364	-1.35538788
C	1.47690462	4.02488296	-3.50287878
H	0.60781137	4.69124854	-3.46613629

H	1.30035824	3.32683834	-4.33280792
C	2.71412435	4.82670592	-3.79047024
H	3.63243048	4.25212234	-3.90862268
C	2.76957577	6.15161567	-3.89316988
H	1.88102065	6.76705660	-3.78473678
H	3.70040592	6.66992991	-4.09470181
N	-0.53478964	4.31438121	1.15683386
H	-0.32333459	4.14070346	2.13561365
H	0.10790538	5.03699474	0.84489660
C	-1.92376915	4.76784576	1.00559943
H	-2.11071403	4.92522637	-0.06014338
H	-2.57774319	3.94380605	1.31124727
C	-2.29824009	6.03225311	1.79145193
H	-1.62866431	6.85066704	1.49665305
H	-2.11757604	5.85521670	2.85845535
C	-3.76295900	6.47450224	1.59793720
H	-4.43697390	5.65187595	1.86226077
H	-3.97158898	7.28754958	2.30439002
C	-4.06989012	6.95363242	0.20572122
H	-3.46778892	7.79119551	-0.14633389
C	-4.99865415	6.44820768	-0.60076105
H	-5.62455277	5.61483365	-0.29531796
H	-5.17277198	6.85122910	-1.59203290

MP2 Electronic Energy(Ha): 1740.455189131641

B3LYP Electronic Energy(Ha): 1744.961112418213

M06-L Electronic Energy(Ha): 1744.728231563588

Zero point energy correction(kcal/mol): 476.880

Enthalpy correction(kcal/mol): 505.394

Entropy correction(cal/mol): 263.679

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.176

Deuterated enthalpy correction(kcal/mol): 497.047

Deuterated entropy correction(cal/mol): 265.972

Deuterated imaginary Frequencies: -0.00

Axial Reaction C2-S

Reactant geometry

Zr	-0.85115101	0.71377831	0.75115570
C	0.01168317	-1.51049440	1.51219586
C	1.02490014	-0.62575122	1.96775565
H	2.01766235	-0.54952618	1.54563847
C	-1.13193470	-1.22760267	2.33256028
H	-2.08988912	-1.72339362	2.26823842
C	-0.83852008	-0.16294735	3.21623333
H	-1.50436115	0.26154314	3.95352831
C	0.50417534	0.22290783	2.98025844
H	1.04348933	0.98923123	3.52081189
B	-0.00613644	-2.30678205	0.07647840
C	0.51615764	-3.83474581	0.08252732
C	-1.54901432	-2.09197115	-0.47254908
C	0.77084849	-1.32122889	-1.01180610
N	0.58911693	-0.03474335	-1.07087718
N	-2.10911599	-0.92621596	-0.40028284
O	-2.30014615	-3.05728172	-1.02632565
O	1.54033414	-1.83229155	-1.99077480
C	1.22488173	0.47777485	-2.29879722
C	2.04141270	-0.72801773	-2.79329288
C	-3.47857542	-1.00352797	-0.93148767
C	-3.57175829	-2.46272077	-1.42650053
N	0.70646502	2.59556392	0.67760117
N	-2.20092066	2.02465502	0.78759159
C	-3.23751426	2.98910764	0.98411162
H	-2.87286892	3.85017325	1.57416643
H	0.45316751	0.78300124	-3.01405979
H	-4.19963970	-0.77467581	-0.14256146

C	2.18439229	2.55301745	0.73397479
H	2.46566554	2.03618364	1.65437375
H	2.53397971	1.92828090	-0.08866743
C	2.85305943	3.92969237	0.68246856
C	-3.85345863	3.54210442	-0.31618678
C	-2.96138065	4.49386430	-1.13339642
H	-2.61569840	5.32008860	-0.50094480
H	-4.06080645	2.55915837	1.57854179
C	-1.78994293	3.87956636	-1.84787714
C	-0.59516431	4.45207524	-2.00931606
H	-3.59576014	4.95194641	-1.90574357
H	0.34432041	3.14016186	1.45796435
C	0.47214718	-4.65067399	-1.06141569
H	0.07224059	-4.25016676	-1.98695721
C	1.04023653	-4.41398714	1.24770491
H	1.08697615	-3.81953592	2.15454964
C	0.92624212	-5.96680982	-1.04531381
H	0.87535300	-6.56776919	-1.94803419
C	1.49949458	-5.73129248	1.27643506
H	1.89803755	-6.14486058	2.19762049
C	1.44464245	-6.51477502	0.12743436
H	1.79897071	-7.54023014	0.14380777
C	4.39358337	3.85399326	0.69399500
H	4.73038998	3.27730319	1.56234310
H	4.78391550	4.87052026	0.82367893
C	4.97581494	3.26838872	-0.56345621
H	4.74722986	3.80776803	-1.48260506
C	5.73512287	2.17813043	-0.63043900
H	5.99586536	1.61006136	0.25755191
H	6.13477517	1.82014401	-1.57255498
H	3.11104478	-0.63114629	-2.59447555
H	1.85182414	1.34838222	-2.09529511
H	1.88875861	-0.97736094	-3.84260341

H	-3.64944919	-2.55194129	-2.51130539
H	-4.36903877	-3.04093185	-0.95974093
H	-3.62246105	-0.27505690	-1.73239697
H	-4.16049695	2.69700692	-0.94351697
H	-4.76880591	4.08838477	-0.05671573
H	2.52127907	4.46444249	-0.21605325
H	2.51827377	4.52581474	1.53927736
H	0.38922991	3.10560208	-0.14998340
H	-1.97950755	2.91906652	-2.32288329
H	-0.36338996	5.41902990	-1.57144450
H	0.17693769	3.99338826	-2.61851868

MP2 Electronic Energy(Ha): 1489.148069694713

B3LYP Electronic Energy(Ha): 1492.993618387495

M06-L Electronic Energy(Ha): 1492.799983816541

Zero point energy correction(kcal/mol): 377.525

Enthalpy correction(kcal/mol): 401.094

Entropy correction(cal/mol): 227.988

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.698

Deuterated enthalpy correction(kcal/mol): 396.561

Deuterated entropy correction(cal/mol): 231.012

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.92960508	0.79201609	0.31265734
C	-0.05440548	-1.25714587	1.39853583
C	0.79644887	-0.24997416	1.92636293
H	1.82444506	-0.08833327	1.63720508
C	-1.30435804	-1.09324507	2.08654686
H	-2.19033028	-1.69079356	1.92379816
C	-1.21014558	-0.03016738	3.00479778
H	-2.00913763	0.34731025	3.62629341
C	0.08110851	0.51843546	2.88786895

H	0.47620197	1.34150909	3.47057677
B	0.22306083	-2.22092055	0.11375998
C	0.75118091	-3.71522294	0.44133906
C	-1.18992696	-2.16238623	-0.73311937
C	1.19059558	-1.35487034	-0.89426620
N	1.10915897	-0.06906670	-1.01211309
N	-1.85637285	-1.05386115	-0.85198360
O	-1.72378756	-3.21998406	-1.36422515
O	2.04750724	-1.96718977	-1.74314572
C	1.97914311	0.35515715	-2.12517192
C	2.72113928	-0.93801482	-2.51380482
C	-3.06512404	-1.29510171	-1.65851302
C	-2.94815913	-2.78926639	-2.02344265
N	0.36018205	2.85653899	0.68441051
N	-2.49350560	1.83413311	0.75179563
C	-3.44069192	2.80910936	1.19221835
H	-2.95400575	3.53643903	1.86469241
H	1.37137176	0.75334614	-2.94421488
H	-3.95992548	-1.07384922	-1.07049552
C	1.82608649	3.00940780	0.53868223
H	2.29771597	2.18734601	1.08082478
H	2.06823184	2.87113912	-0.51542701
C	2.36413345	4.35260611	1.03822487
C	-4.04293990	3.57522314	-0.01188168
C	-2.97553043	3.62084354	-1.10491933
H	-2.14731399	4.28411049	-0.82802235
H	-4.24814170	2.34872049	1.78083895
C	-2.47419091	2.22846024	-1.37781203
C	-1.23017125	1.88540691	-1.92057319
H	-3.39616623	4.01893824	-2.03734897
H	0.09116050	3.03398356	1.65048540
C	0.98251991	-4.67207327	-0.56250444
H	0.80368751	-4.40965169	-1.59939435

C	1.00436628	-4.11640129	1.76163124
H	0.83713290	-3.40828784	2.56682536
C	1.43940472	-5.95389977	-0.26674609
H	1.60641747	-6.66665790	-1.06861412
C	1.46315082	-5.39760260	2.07050561
H	1.64747213	-5.67093302	3.10493907
C	1.68289424	-6.32409340	1.05536324
H	2.03873273	-7.32224185	1.28920479
C	3.89112442	4.49237983	0.87552945
H	4.39578123	3.67256853	1.39796658
H	4.20194035	5.41841474	1.37411871
C	4.34366508	4.53753857	-0.55832196
H	3.91821931	5.33906768	-1.16199852
C	5.20989478	3.69972213	-1.12159790
H	5.66614121	2.89026747	-0.55943823
H	5.50517969	3.80029114	-2.15986976
H	3.77337359	-0.93511892	-2.22078188
H	2.66644019	1.14380676	-1.81016919
H	2.64378865	-1.19979502	-3.56929933
H	-2.83215570	-2.97199693	-3.09261866
H	-3.76498647	-3.40112890	-1.63997311
H	-3.07632554	-0.65194579	-2.54290433
H	-4.91573395	3.03551870	-0.39583883
H	-4.38342260	4.57462467	0.27367886
H	1.86475043	5.16997348	0.50218607
H	2.10799070	4.47265348	2.09735205
H	-0.11376895	3.57083846	0.13673840
H	-3.28259283	1.52772601	-1.56338476
H	-0.47561558	2.65486779	-2.06025149
H	-1.16092558	1.03546282	-2.58816310

MP2 Electronic Energy(Ha): 1489.143963144283

B3LYP Electronic Energy(Ha): 1492.970964770738

M06-L Electronic Energy(Ha): 1492.790137712521

Zero point energy correction(kcal/mol): 377.278

Enthalpy correction(kcal/mol): 400.150

Entropy correction(cal/mol): 220.845

Imaginary Frequencies: -226.06

Deuterated zero point energy correction(kcal/mol): 372.859

Deuterated enthalpy correction(kcal/mol): 395.908

Deuterated entropy correction(cal/mol): 221.965

Deuterated imaginary Frequencies: -225.94

Product geometry

Zr	-0.81099317	0.92893997	0.19811651
C	-0.13770567	-1.12329891	1.38978586
C	0.84638982	-0.17263180	1.79045086
H	1.87266395	-0.16302269	1.45452504
C	-1.33284799	-0.73865786	2.07772716
H	-2.28924043	-1.23396249	1.99715301
C	-1.09713507	0.43026416	2.83049630
H	-1.82175928	0.95928126	3.43198753
C	0.25792058	0.78982974	2.64885498
H	0.75598343	1.62790108	3.11710723
B	-0.03481444	-2.18901139	0.15234683
C	0.40057278	-3.69869734	0.52420361
C	-1.49456661	-2.03505159	-0.60372741
C	0.90008435	-1.45151091	-0.98992672
N	0.87379108	-0.16851595	-1.18092682
N	-2.04430862	-0.86830334	-0.73117058
O	-2.16280046	-3.05052922	-1.17337892
O	1.60653558	-2.15326501	-1.89705916
C	1.57986269	0.13917684	-2.43721081
C	2.23788758	-1.20400923	-2.80149521
C	-3.30183715	-0.99638854	-1.48481034
C	-3.37013304	-2.50851424	-1.78690967
N	0.83774332	2.75670273	0.11873721

N	-2.36694211	2.26153709	0.52349860
C	-3.22326266	3.05424730	1.38198949
H	-2.84012402	3.09612264	2.40460468
H	0.85885961	0.47897437	-3.18683130
H	-4.14246235	-0.65007577	-0.87832641
C	2.28069706	2.66700128	0.43802551
H	2.37330960	2.39911758	1.49242489
H	2.69466750	1.83451701	-0.13221930
C	3.05974358	3.95464695	0.15581151
C	-3.30682052	4.46182415	0.70619485
C	-2.71860381	4.25174716	-0.71374881
H	-1.71323155	4.68196185	-0.78322462
H	-4.23213466	2.61454337	1.43316909
C	-2.62717449	2.71776508	-0.86349171
C	-1.52122245	2.09640172	-1.73130351
H	-3.32307633	4.71234937	-1.49954603
H	0.40333785	3.49283848	0.67183275
C	0.45991323	-4.72303132	-0.43700516
H	0.20153645	-4.50237758	-1.46679678
C	0.74484424	-4.04821146	1.83853781
H	0.70920526	-3.28772424	2.61219119
C	0.84177134	-6.02060236	-0.10596006
H	0.87530250	-6.78672690	-0.87441743
C	1.12976044	-5.34467877	2.18204372
H	1.38868706	-5.57736095	3.21029785
C	1.18008902	-6.33842562	1.20884416
H	1.47768851	-7.34872124	1.46979671
C	4.56796762	3.82614132	0.45215620
H	4.71591338	3.49044922	1.48435749
H	5.01469741	4.82507754	0.38172446
C	5.28947505	2.90349800	-0.49203446
H	5.25395626	3.18584833	-1.54414393
C	5.95517973	1.80603189	-0.14326330

H 6.02412604 1.48629703 0.89221434

H 6.46481860 1.19222987 -0.87726232

H 3.31212980 -1.22271634 -2.60529806

H 2.31621704 0.93429585 -2.29630221

H 2.05050666 -1.53621326 -3.82201024

H -3.33578533 -2.74699911 -2.85061589

H -4.22532347 -3.00963988 -1.33266058

H -3.26771567 -0.38483502 -2.38899756

H -4.33978313 4.81632859 0.67024062

H -2.73461279 5.20358881 1.26912360

H 2.91920114 4.24496950 -0.89314707

H 2.64463743 4.76886036 0.76113970

H 0.71159378 3.03852718 -0.85116423

H -3.62333391 2.35278742 -1.17429014

H -0.87643247 2.87281776 -2.16503687

H -1.91718937 1.51936557 -2.57086699

MP2 Electronic Energy(Ha): 1489.174249816735

B3LYP Electronic Energy(Ha): 1493.002315613723

M06-L Electronic Energy(Ha): 1492.818687372232

Zero point energy correction(kcal/mol): 378.519

Enthalpy correction(kcal/mol): 401.441

Entropy correction(cal/mol): 225.894

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.114

Deuterated enthalpy correction(kcal/mol): 397.210

Deuterated entropy correction(cal/mol): 227.033

Deuterated imaginary Frequencies: -0.00

Axial Reaction H3-S

Reactant geometry

Zr 0.36953734 0.69893455 -0.77493909

C -0.74216676 -1.36677783 -1.57399625

C	-1.80776305	-0.41674494	-1.64707467
H	-2.62835118	-0.34502074	-0.94949001
C	0.08121538	-1.09244808	-2.70945612
H	0.97676437	-1.63490763	-2.97451404
C	-0.44329462	-0.00160217	-3.42358351
H	-0.04433205	0.41429457	-4.33506953
C	-1.61186831	0.43224958	-2.75586702
H	-2.25360525	1.24353174	-3.07040391
B	-0.41174006	-2.41369312	-0.36860061
C	-0.93187303	-3.93262662	-0.56170290
C	1.21290258	-2.25965323	-0.16802373
C	-0.98806380	-1.65779630	0.96875014
N	-0.93028798	-0.36945701	1.09345094
N	1.80684702	-1.12982362	-0.39839530
O	2.01058080	-3.24079212	0.28608905
O	-1.53561688	-2.31864864	2.00776554
C	-1.58075374	0.01041986	2.36161818
C	-1.83108453	-1.34532319	3.04712165
C	3.24910467	-1.27158615	-0.13870617
C	3.35328096	-2.69349959	0.44586790
N	1.36503215	1.48134455	0.98246435
N	1.52743059	2.12993146	-1.87712942
C	1.99986511	3.39382504	-1.28072107
H	3.02629795	3.30333985	-0.88250103
H	-0.94431344	0.67189195	2.95024165
H	3.80421070	-1.16118740	-1.07480778
C	1.76190944	0.91422771	2.26433533
H	1.12029047	0.06046799	2.49786253
H	2.78533215	0.50682097	2.23506107
C	1.70310625	1.92030133	3.42676903
C	2.00513005	4.41036970	-2.42558263
C	2.56465054	3.56329891	-3.56760929
H	3.65897552	3.55580926	-3.51831996

H	1.37347499	3.71326510	-0.44425974
C	2.00907523	2.14013537	-3.29004312
H	2.28590064	3.92445198	-4.56017161
H	1.15727214	1.96594093	-3.95025902
C	-1.67448851	-4.30513506	-1.69197287
H	-1.89455449	-3.55724580	-2.44715995
C	-0.67377383	-4.94019571	0.38409014
H	-0.10184190	-4.70134841	1.27415837
C	-2.13803274	-5.60857044	-1.87481190
H	-2.70989065	-5.85941524	-2.76286622
C	-1.13048673	-6.24449278	0.21214271
H	-0.91175083	-6.99724320	0.96327200
C	-1.86731343	-6.58578428	-0.92137741
H	-2.22448971	-7.60122623	-1.05826713
C	2.13123901	1.33670223	4.78849329
H	1.51786127	0.46069887	5.03015928
H	1.92232473	2.08561638	5.56356650
C	3.58673585	0.96655757	4.86588602
H	4.28689014	1.76814846	4.63013753
C	4.06972695	-0.22580382	5.20480735
H	3.41389086	-1.05596960	5.45048087
H	5.13623186	-0.41468290	5.25624892
H	-2.85945720	-1.50023431	3.37190855
H	-2.51590448	0.54338281	2.15902360
H	-1.15525113	-1.53618729	3.88383240
H	3.59009530	-2.70715109	1.51129203
H	4.04390409	-3.34573442	-0.08771747
H	3.59442135	-0.50071606	0.55029544
H	0.98164969	4.73353077	-2.64616080
H	2.60160604	5.30019580	-2.20667849
H	2.34024500	2.78116559	3.18541572
H	0.68333606	2.31413896	3.50695099
H	2.06111704	2.17681537	0.73470304

N	-1.14247040	2.58564391	-0.21116241
H	-0.77957360	3.34750188	-0.78027701
C	-2.61917862	2.64887610	-0.19026199
H	-0.75217483	2.72173273	0.72193407
H	-2.97196251	2.54529938	-1.21896750
H	-2.97633841	1.77397186	0.35346795
C	-3.17150706	3.93529200	0.43113680
H	-2.75800608	4.79575374	-0.10877655
H	-2.82352740	4.01632066	1.46749890
C	-4.71190935	4.03467866	0.40797017
H	-5.00359268	5.02139377	0.77959214
H	-5.05159356	3.97926706	-0.63441483
C	-5.41185034	2.97480652	1.21601389
H	-5.35612939	1.95613814	0.83681102
C	-6.08610935	3.19974660	2.34027677
H	-6.18363438	4.19919141	2.75440064
H	-6.57226754	2.39737921	2.88357900
C	3.06152607	1.06117174	-3.56997504
H	3.92015262	1.18776009	-2.90334363
H	2.65475512	0.06055909	-3.41582463
H	3.41947668	1.12791625	-4.60359248

MP2 Electronic Energy(Ha): 1740.493574284329

B3LYP Electronic Energy(Ha): 1744.987360458535

M06-L Electronic Energy(Ha): 1744.767014219632

Zero point energy correction(kcal/mol): 477.015

Enthalpy correction(kcal/mol): 505.422

Entropy correction(cal/mol): 262.251

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 483.735

Deuterated enthalpy correction(kcal/mol): 511.833

Deuterated entropy correction(cal/mol): 259.757

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.17931280	-0.52500872	-0.64167836
C	-0.34532494	1.85962873	-1.41025645
C	0.97261973	1.53605039	-1.84069916
H	1.87851885	1.89869131	-1.37697043
C	-1.21708510	1.15801147	-2.30696493
H	-2.29646198	1.19453667	-2.29031389
C	-0.45040448	0.38616727	-3.20221955
H	-0.83122024	-0.25022286	-3.98738096
C	0.91681806	0.61665162	-2.91009651
H	1.75612271	0.18550809	-3.43875315
B	-0.75655924	2.61355863	-0.02479093
C	-0.92634745	4.21802431	-0.07180155
C	-2.06943268	1.76515712	0.48839066
C	0.31289969	2.05327237	1.10407379
N	0.76017484	0.83157514	1.08299447
N	-2.10517227	0.47796127	0.33695648
O	-3.10181387	2.29399074	1.16373914
O	0.63942534	2.75774585	2.20040114
C	1.42223338	0.54436804	2.36941395
C	1.51424565	1.93395406	3.02244514
C	-3.28495317	-0.05811385	1.03957367
C	-4.05103526	1.21855094	1.43326931
N	-0.57702635	-2.08836082	0.52713644
N	-0.50630205	-2.58781824	-1.92662619
C	0.59778512	-3.36244704	-2.51446387
H	1.22477216	-3.77787342	-1.71354434
H	0.81285467	-0.15752269	2.94712937
H	-3.86537452	-0.71248454	0.38756176
C	-0.97769736	-2.74083775	1.74152794
H	-1.12838736	-2.01396542	2.56080670
H	-1.95026588	-3.24576931	1.61865974
C	0.03425265	-3.79091142	2.24009946

C	-0.03639368	-4.50192602	-3.36582990
C	-1.54249396	-4.36942175	-3.09595943
H	-1.83889439	-4.97619347	-2.23372993
H	1.24731108	-2.74363151	-3.15418626
C	-1.70006474	-2.88114025	-2.73991941
H	-2.15755106	-4.67031467	-3.94852712
H	-1.67041686	-2.30746155	-3.68288136
C	-0.66738009	4.93499393	-1.24970615
H	-0.35388102	4.39343546	-2.13651782
C	-1.33494226	4.96700444	1.04570461
H	-1.55039428	4.45771973	1.97868911
C	-0.80390410	6.32201692	-1.31570726
H	-0.59526520	6.84219194	-2.24541930
C	-1.47518631	6.35153637	0.99164572
H	-1.79396881	6.89744079	1.87423546
C	-1.20880059	7.03762889	-0.19257079
H	-1.31768561	8.11627454	-0.23795544
C	-0.38360373	-4.50571917	3.54045453
H	-0.56248597	-3.76873461	4.33201120
H	0.45791164	-5.12561297	3.87709297
C	-1.59296301	-5.38634556	3.39019307
H	-1.52550291	-6.14635171	2.61173780
C	-2.70157118	-5.31680164	4.12210211
H	-2.81739419	-4.57698000	4.90884497
H	-3.53138993	-5.99692573	3.96553567
H	2.51669535	2.36471843	2.97571115
H	2.40642485	0.09255003	2.22517387
H	1.14946813	1.97614736	4.04781759
H	-4.32709439	1.27327313	2.48567631
H	-4.93412258	1.39864274	0.81691452
H	-2.96728746	-0.64737394	1.90301710
H	0.17667748	-4.34437792	-4.42645624
H	0.35563374	-5.48596074	-3.10005392

H	0.19271872	-4.53109647	1.44654811
H	1.00040409	-3.29706493	2.40053211
H	-0.63261833	-2.70522760	-0.63879486
N	2.16430113	-1.28392483	-0.50260829
H	2.22488966	-2.05901406	-1.15933472
C	3.39766334	-0.46950346	-0.59071302
H	2.08767419	-1.72535069	0.41267409
H	3.48301488	-0.10988233	-1.61844426
H	3.25350740	0.40910913	0.03846871
C	4.66505559	-1.22922659	-0.18853674
H	4.75921854	-2.12407800	-0.81530836
H	4.56814719	-1.57861541	0.84642141
C	5.96082314	-0.39975595	-0.31717978
H	6.81333591	-1.04860836	-0.09607349
H	6.07128321	-0.08151653	-1.36176802
C	6.01239210	0.80904672	0.57878465
H	5.33721398	1.62676700	0.33395474
C	6.82016043	0.94217197	1.62721540
H	7.52332759	0.16260159	1.90603623
H	6.81716061	1.83730451	2.23885555
C	-3.01060480	-2.54979079	-2.03164293
H	-3.08536045	-3.08288659	-1.07997153
H	-3.09939203	-1.47873553	-1.83079405
H	-3.85984187	-2.83820974	-2.65768996

MP2 Electronic Energy(Ha): 1740.452202004261

B3LYP Electronic Energy(Ha): 1744.942593647808

M06-L Electronic Energy(Ha): 1744.717891883658

Zero point energy correction(kcal/mol): 473.534

Enthalpy correction(kcal/mol): 501.845

Entropy correction(cal/mol): 262.966

Imaginary Frequencies: -1529.47

Deuterated zero point energy correction(kcal/mol): 479.878

Deuterated enthalpy correction(kcal/mol): 508.006

Deuterated entropy correction(cal/mol): 262.817

Deuterated imaginary Frequencies: -1525.81

Product geometry

Zr	0.21456975	0.58805970	-0.40357748
C	0.33548636	-1.80868770	-1.30825723
C	-0.98658767	-1.54901911	-1.75812174
H	-1.88568377	-1.91575663	-1.28193993
C	1.19234955	-1.13491958	-2.23900105
H	2.27352912	-1.15932725	-2.23011770
C	0.40462228	-0.49489707	-3.22094103
H	0.77481537	0.05866040	-4.07340951
C	-0.95108373	-0.74036455	-2.91727598
H	-1.80465401	-0.40886552	-3.49548546
B	0.75690708	-2.57741516	0.06134050
C	0.91890679	-4.18583221	-0.01346777
C	2.08545725	-1.76405549	0.58176305
C	-0.31210619	-2.04737643	1.20241007
N	-0.76259703	-0.82596772	1.21119514
N	2.15885699	-0.47665055	0.44534583
O	3.10471135	-2.32840932	1.25346471
O	-0.66006716	-2.78402845	2.27210355
C	-1.45100871	-0.57989086	2.49141895
C	-1.56049303	-1.99021174	3.09404330
C	3.35185187	0.01676542	1.15428576
C	4.07924386	-1.28445259	1.54198953
N	0.59289715	2.00907884	0.79032480
N	0.50915786	2.51215616	-2.08452336
C	-0.53949588	2.87183716	-3.09362592
H	-1.16531445	3.67426722	-2.68995710
H	-0.85235907	0.10091894	3.10403995
H	3.95783009	0.65424889	0.50682872
C	1.03258557	2.85500109	1.85519659

H	1.44183407	2.26566349	2.69811275
H	1.86246513	3.50583164	1.53074338
C	-0.07773671	3.75796221	2.42818018
C	0.20308659	3.33712475	-4.36446208
C	1.59226872	3.72910762	-3.85099383
H	1.57918807	4.74240848	-3.43233347
H	-1.17213733	2.00721717	-3.29526521
C	1.85044769	2.71147272	-2.73035457
H	2.36147567	3.69803321	-4.62594549
H	2.13425770	1.75575034	-3.18020671
C	0.66482012	-4.87875170	-1.20675706
H	0.35816993	-4.31621140	-2.08252816
C	1.31688902	-4.95920687	1.09131975
H	1.52808913	-4.46973217	2.03594282
C	0.79649282	-6.26484058	-1.29898800
H	0.59145697	-6.76566347	-2.24026714
C	1.45220856	-6.34321223	1.01132457
H	1.76272576	-6.90766270	1.88541338
C	1.19126473	-7.00483871	-0.18789803
H	1.29606863	-8.08299428	-0.25392457
C	0.38096104	4.67331511	3.58086809
H	0.81748336	4.06954739	4.38464549
H	-0.50533862	5.16299114	4.00564003
C	1.35755905	5.73695515	3.16214270
H	1.02066992	6.39217198	2.35846372
C	2.56140179	5.94037007	3.69020684
H	2.94282755	5.31492533	4.49197273
H	3.20816557	6.73904342	3.34436682
H	-2.56074729	-2.41934665	3.00177512
H	-2.43087644	-0.12034422	2.33955916
H	-1.22790115	-2.06693005	4.12845165
H	4.34419282	-1.35579677	2.59656885
H	4.96395761	-1.48103943	0.93276305

H	3.05002570	0.61301260	2.01912043
H	0.28382251	2.50902831	-5.07319069
H	-0.31672288	4.15289141	-4.87041460
H	-0.48924414	4.36898950	1.61452198
H	-0.89603394	3.12019525	2.78282186
H	0.45646449	3.15199429	-1.29401597
N	-2.13512646	1.39636343	-0.36859422
H	-2.17714579	2.21759448	-0.96839082
C	-3.36581020	0.59316701	-0.55334671
H	-2.08670859	1.76966632	0.57832723
H	-3.38995994	0.26484369	-1.59422899
H	-3.25427369	-0.30570139	0.05341293
C	-4.65198772	1.34351292	-0.19698380
H	-4.71230152	2.25625872	-0.80270579
H	-4.61144653	1.66364516	0.85111493
C	-5.93943702	0.52109771	-0.42017411
H	-6.80329051	1.16782654	-0.24026511
H	-5.98533008	0.22154011	-1.47513187
C	-6.04775126	-0.70314874	0.44916143
H	-5.35244087	-1.51346681	0.23898869
C	-6.92674068	-0.85681398	1.43559451
H	-7.65146800	-0.08449874	1.67708538
H	-6.96202954	-1.76187270	2.03138482
C	2.91665094	3.12865728	-1.72556464
H	2.66977388	4.09252781	-1.26915264
H	3.01918288	2.39807132	-0.92198854
H	3.88224295	3.22981782	-2.22773755

MP2 Electronic Energy(Ha): 1740.466997776674

B3LYP Electronic Energy(Ha): 1744.961534663333

M06-L Electronic Energy(Ha): 1744.736331584248

Zero point energy correction(kcal/mol): 476.764

Enthalpy correction(kcal/mol): 505.565

Entropy correction(cal/mol): 268.962

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 483.476

Deuterated enthalpy correction(kcal/mol): 511.961

Deuterated entropy correction(cal/mol): 266.458

Deuterated imaginary Frequencies: -0.00

Axial Reaction H6-S

Reactant geometry

Zr	0.19455717	-1.52599311	0.44770312
C	-2.08642555	-0.65254330	0.78173871
C	-2.30572608	-1.71738721	-0.14771412
H	-2.54978539	-1.59436029	-1.19350913
C	-1.77811256	-1.29334633	2.02083615
H	-1.54953527	-0.78673840	2.94637076
C	-1.74628168	-2.69379279	1.83852023
H	-1.53343829	-3.43438986	2.59651243
C	-2.08753083	-2.95632095	0.49005915
H	-2.16909586	-3.93519486	0.04307188
B	-1.90700430	0.93755961	0.43911782
C	-3.24231218	1.84399198	0.48652016
C	-0.68943241	1.42395949	1.43121246
C	-1.11312053	0.93459836	-1.00507522
N	-0.15788447	0.08361509	-1.22100934
N	0.31689020	0.65544578	1.70864100
O	-0.63988770	2.66452805	1.94610372
O	-1.35200691	1.78987858	-2.01156178
C	0.40838984	0.30182882	-2.56138426
C	-0.46398772	1.44645970	-3.11843223
C	1.25211731	1.40163065	2.57543514
C	0.62135002	2.80269088	2.66466053
N	0.66141800	-2.98500710	-0.99392328
N	1.63403892	-2.67903078	2.03704108

C	1.86043635	-3.21701309	3.39378661
H	1.41502355	-4.20793500	3.49161325
H	1.46564910	0.57114700	-2.48810979
H	1.32891835	0.91456916	3.55305844
C	0.04561457	-3.99304618	-1.85029415
H	-1.04164467	-3.88352691	-1.81813246
H	0.33302328	-3.83245974	-2.89806900
C	0.40808780	-5.43448589	-1.45658619
C	3.41356370	-3.21389634	3.58248710
C	3.96876858	-2.40367454	2.37728500
H	4.36244271	-3.06935987	1.60197716
H	1.37398972	-2.55854648	4.11635318
C	2.73013347	-1.66418897	1.83775750
H	2.49804721	-0.86602656	2.54997103
H	4.77113176	-1.72003880	2.66196619
C	2.56693081	-1.12572180	0.42604657
H	3.12830302	-1.73613727	-0.29421914
H	1.82570124	-3.43359381	1.37542895
H	2.93531790	-0.10045949	0.34393485
C	-3.22551640	3.21933176	0.19632480
H	-2.28729334	3.69781074	-0.06333685
C	-4.48554026	1.28737105	0.82166456
H	-4.54378385	0.22855522	1.05333941
C	-4.38144799	3.99450705	0.23739796
H	-4.33049750	5.05431011	0.00762690
C	-5.65081313	2.05363860	0.86674481
H	-6.59477377	1.58713237	1.13079953
C	-5.60347824	3.41334734	0.57366965
H	-6.50613570	4.01452710	0.60675993
C	-0.21785955	-6.50679193	-2.37086783
H	-1.30639248	-6.38262595	-2.39980743
H	-0.02892116	-7.49105766	-1.92347005
C	0.32825773	-6.50455470	-3.77194192

H	1.40738452	-6.63491685	-3.85478847
C	-0.38721391	-6.36741623	-4.88477937
H	-1.46478390	-6.23530430	-4.85497815
H	0.07518446	-6.38725630	-5.86532135
H	-1.08990314	1.14796402	-3.96028168
H	0.33808247	-0.61335060	-3.15282994
H	0.09599921	2.34264528	-3.38448118
H	1.21519173	3.55552492	2.14754336
H	0.39174107	3.12708582	3.67980939
H	2.24614279	1.43903602	2.12725194
H	3.68061319	-2.74912371	4.53389485
H	3.81089251	-4.23078908	3.60091352
H	1.50027537	-5.54336937	-1.46025348
H	0.08391959	-5.60464471	-0.42403808
H	1.63124963	-2.87253591	-1.27719513
N	2.44434866	2.88543909	-0.27328501
H	1.91115542	2.02918052	-0.39300682
H	3.41617962	2.65146559	-0.45496634
C	1.98821473	3.92348437	-1.20760440
H	2.13816413	3.65314153	-2.26678833
H	0.91032012	4.04887344	-1.06465270
C	2.69342635	5.25185164	-0.93436627
H	3.77701539	5.11952547	-1.04237098
H	2.51759340	5.53280230	0.10930253
C	2.23060890	6.38134737	-1.87072882
H	1.14242204	6.49273387	-1.77193617
H	2.42464463	6.10588880	-2.91322548
C	2.88869336	7.69808597	-1.56830569
C	3.65441152	8.38691341	-2.40904156
H	3.85565421	8.03185958	-3.41564911
H	4.10446896	9.33177959	-2.12600950
H	2.71511837	8.09447285	-0.56852389

MP2 Electronic Energy(Ha): 1740.456984823679

B3LYP Electronic Energy(Ha): 1744.959233711757

M06-L Electronic Energy(Ha): 1744.730087963545

Zero point energy correction(kcal/mol): 475.025

Enthalpy correction(kcal/mol): 498.412

Entropy correction(cal/mol): 221.687

Imaginary Frequencies: -61.88 -61.66 -58.35 -55.36 -53.83 -48.07 -43.18 -39.06 -37.28

Deuterated zero point energy correction(kcal/mol): 466.364

Deuterated enthalpy correction(kcal/mol): 490.115

Deuterated entropy correction(cal/mol): 223.953

Deuterated imaginary Frequencies: -61.85 -61.60 -58.29 -55.33 -53.48 -47.99 -42.51 -38.78 -36.90

Transition State geometry

Zr	0.39128859	1.58911070	0.30212068
C	2.49387735	0.31586548	0.24183002
C	2.68650070	1.34575378	-0.74017033
H	2.69577474	1.19582035	-1.81055618
C	2.54693674	0.98278431	1.49741874
H	2.41760455	0.51284025	2.46138312
C	2.69648759	2.37915597	1.29052458
H	2.76236527	3.13707775	2.05874548
C	2.80666932	2.59690880	-0.10365638
H	2.92205858	3.55368821	-0.59115791
B	1.96294129	-1.20749774	-0.04232554
C	3.09830832	-2.33616343	-0.25604493
C	0.89411379	-1.51226258	1.17345326
C	0.92273056	-1.02796211	-1.30958629
N	0.09086070	-0.03036006	-1.34539585
N	0.04600643	-0.62977404	1.59810975
O	0.82881003	-2.72173323	1.76124362
O	0.84895859	-1.86462627	-2.35367600
C	-0.69091658	-0.07945992	-2.59271291
C	-0.19659385	-1.38341254	-3.25274416
C	-0.76723514	-1.24171138	2.67083475

C	-0.25509416	-2.69200575	2.73301243
N	-0.25281737	3.05266430	-0.79178367
N	-0.61469861	2.63071231	2.23607423
C	-0.40979628	2.77443271	3.69396876
H	0.34688416	3.53304798	3.89700382
H	-1.76152435	-0.09420294	-2.37574827
H	-0.61801647	-0.70471839	3.61313919
C	-0.38181813	4.15892471	-1.69530672
H	0.57277986	4.33072112	-2.21940467
H	-1.12032199	3.94022628	-2.48174352
C	-0.78520925	5.47306958	-1.00106660
C	-1.81430817	3.12372579	4.28049513
C	-2.80831383	2.88364072	3.11223192
H	-3.10277898	3.82961392	2.64553166
H	-0.04275061	1.82462456	4.08712499
C	-2.00447574	2.04540331	2.10338673
H	-1.91162272	1.03810212	2.51466542
H	-3.72184797	2.37789505	3.43074119
C	-2.38100464	1.94776096	0.63232783
H	-3.08826582	2.73745934	0.34896432
H	-0.66402701	3.56987528	1.83976089
H	-2.85688299	0.99274444	0.39932926
C	2.78105717	-3.67522190	-0.54246271
H	1.74034589	-3.97205697	-0.61930267
C	4.46179632	-2.01896327	-0.16700826
H	4.75176523	-0.99631917	0.05238732
C	3.76532623	-4.64193330	-0.72982764
H	3.48254393	-5.66681096	-0.94946343
C	5.45783297	-2.97857153	-0.35203575
H	6.50277109	-2.69469808	-0.27536012
C	5.11299196	-4.29677309	-0.63523988
H	5.88292227	-5.04729513	-0.78080904
C	-0.84883758	6.68428223	-1.95213931

H	0.12168120	6.82111178	-2.44215701
H	-1.02298994	7.58441102	-1.34827519
C	-1.92986649	6.58808186	-2.99263917
H	-2.94071674	6.44783500	-2.60946169
C	-1.74871879	6.66815043	-4.30791767
H	-0.76092480	6.80681002	-4.73755447
H	-2.57846220	6.60223092	-5.00280030
H	0.25395999	-1.24017101	-4.23460767
H	-0.48570749	0.80835311	-3.19501743
H	-0.95938107	-2.16046437	-3.31502238
H	-1.00717134	-3.41370881	2.41517221
H	0.15692622	-2.98086399	3.70044474
H	-1.82722083	-1.20940395	2.41238263
H	-2.03951309	2.48455321	5.13670773
H	-1.85093924	4.15609618	4.63424586
H	-1.75863203	5.33919034	-0.51314223
H	-0.05966702	5.68104466	-0.20678049
H	-1.38072125	2.53829672	-0.27710184
N	-2.61923220	-2.45618854	0.12161077
H	-1.93288475	-1.75290806	-0.13581944
H	-3.53520263	-2.04012306	-0.02011147
C	-2.47329260	-3.66015984	-0.70828757
H	-2.65482299	-3.47659828	-1.78080601
H	-1.43690705	-4.00075654	-0.62000655
C	-3.41308960	-4.76712795	-0.23113872
H	-4.45098579	-4.41708287	-0.29165069
H	-3.21334595	-4.96226134	0.82783663
C	-3.27401087	-6.06621747	-1.04345748
H	-2.22846561	-6.39893824	-0.99368173
H	-3.49133972	-5.87216256	-2.09956417
C	-4.16488986	-7.16722566	-0.54092754
C	-5.12438929	-7.76184118	-1.24337258
H	-5.32940669	-7.48500816	-2.27350793

H -5.73687788 -8.54918191 -0.81869099

H -3.99589854 -7.47894253 0.48924247

MP2 Electronic Energy(Ha): 1740.412828718211

B3LYP Electronic Energy(Ha): 1744.911294256515

M06-L Electronic Energy(Ha): 1744.680063990482

Zero point energy correction(kcal/mol): 471.626

Enthalpy correction(kcal/mol): 494.981

Entropy correction(cal/mol): 221.906

Imaginary Frequencies: -1601.49 -56.39 -55.82 -52.47 -50.49 -45.55 -44.82 -37.33 -33.01

Deuterated zero point energy correction(kcal/mol): 463.826

Deuterated enthalpy correction(kcal/mol): 487.481

Deuterated entropy correction(cal/mol): 223.746

Deuterated imaginary Frequencies: -1164.41 -56.34 -55.78 -52.40 -50.12 -45.51 -44.55 -36.49 -32.69

Product geometry

Zr -0.64298339 0.16392573 0.66845728

C -1.05777060 2.62291983 0.86043809

C -2.33929253 2.01105811 0.63974179

H -2.91561915 2.06868713 -0.27239921

C -0.71382626 2.29329025 2.19696740

H 0.20415687 2.58204906 2.68846128

C -1.70391590 1.44245075 2.75423974

H -1.71857172 1.04118602 3.75885429

C -2.72597941 1.27988766 1.78577529

H -3.64160603 0.72128618 1.91216624

B -0.03235620 3.17067639 -0.29922562

C 0.06047595 4.77077183 -0.49260126

C 1.42594473 2.42112595 -0.04213778

C -0.49105578 2.32023707 -1.63532409

N -0.67965608 1.04128599 -1.54630147

N 1.54408505 1.18670477 0.34536631

O 2.57817525 3.02262553 -0.39053137

O -0.72471747 2.85421621 -2.84473374

C	-1.19933789	0.53768136	-2.82749004
C	-1.06129667	1.76240847	-3.75315961
C	2.95820324	0.77632306	0.23030459
C	3.66674752	2.07532810	-0.19972237
N	-1.41424366	-1.45128715	0.07345356
N	0.57117629	-0.93546175	2.56146452
C	1.40858917	-0.06135413	3.46061274
H	0.79729691	0.26272290	4.30385668
H	-0.62461884	-0.32339786	-3.17409549
H	3.33303898	0.40151438	1.18578778
C	-2.26805608	-2.50104668	-0.39600126
H	-2.27659385	-2.52865965	-1.50058502
H	-1.89084899	-3.49121429	-0.08852191
C	-3.72392476	-2.37363583	0.08546551
C	2.62587282	-0.89936495	3.91332384
C	2.24047591	-2.34141983	3.57022742
H	1.65210114	-2.78798524	4.38032626
H	1.71164725	0.82860437	2.91423665
C	1.35812210	-2.20152850	2.32187493
H	1.98830278	-2.02508878	1.44454291
H	3.10334153	-2.98743249	3.39516326
C	0.45691802	-3.39768336	2.06047377
H	-0.18511345	-3.59523521	2.92673242
H	-0.24762361	-1.21984376	3.09667751
H	1.06410383	-4.28926489	1.88622980
C	0.81294013	5.36226366	-1.52228618
H	1.35412225	4.72982337	-2.21786420
C	-0.61753683	5.64359190	0.37141213
H	-1.21539574	5.22794225	1.17623134
C	0.88685186	6.74367813	-1.67997996
H	1.47685606	7.16496610	-2.48804923
C	-0.55014987	7.02956585	0.22464759
H	-1.08945289	7.67282036	0.91295780

C	0.20420770	7.58659522	-0.80375320
H	0.25919930	8.66354227	-0.92406933
C	-4.65820478	-3.48543758	-0.43112883
H	-4.63736020	-3.51307047	-1.52676228
H	-5.68670233	-3.22717270	-0.14638922
C	-4.34235472	-4.85083634	0.11307341
H	-4.32898803	-4.93010636	1.20029225
C	-4.09508148	-5.93956998	-0.61027247
H	-4.09635021	-5.91209201	-1.69606409
H	-3.88613152	-6.89718969	-0.14643930
H	-1.97568266	2.03586271	-4.27812695
H	-2.23635970	0.21254139	-2.70405923
H	-0.24486906	1.67080968	-4.47273219
H	4.20756904	1.99509864	-1.14309553
H	4.33291994	2.48420481	0.56187459
H	3.04451671	-0.03363582	-0.49855124
H	3.51795841	-0.60380797	3.35481966
H	2.84817763	-0.75767552	4.97249617
H	-3.72936997	-2.36413489	1.18193770
H	-4.10988545	-1.39995241	-0.23368707
H	-0.17697499	-3.21901941	1.19416614
N	1.59731523	-1.96730871	-1.71345065
H	1.49302655	-1.15425972	-2.31240300
H	0.70292158	-2.07086471	-1.23250155
C	1.90608219	-3.15587836	-2.52124016
H	1.08567633	-3.44379073	-3.19850170
H	2.76713564	-2.91857401	-3.15601723
C	2.25736121	-4.34900838	-1.63253299
H	1.41980229	-4.55900652	-0.95800103
H	3.10822226	-4.07346875	-0.99985429
C	2.58608910	-5.62022541	-2.43448310
H	3.40056360	-5.39219262	-3.13578217
H	1.72206001	-5.91167406	-3.04130485

C	2.99894107	-6.77140699	-1.56107670
C	2.35752171	-7.93187437	-1.46203699
H	1.45970887	-8.13571726	-2.03816973
H	2.70583978	-8.72139941	-0.80564503
H	3.89520376	-6.61285046	-0.96201428

MP2 Electronic Energy(Ha): 1740.470607735891

B3LYP Electronic Energy(Ha): 1744.970456841576

M06-L Electronic Energy(Ha): 1744.738619503421

Zero point energy correction(kcal/mol): 476.993

Enthalpy correction(kcal/mol): 505.751

Entropy correction(cal/mol): 265.699

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.931

Deuterated enthalpy correction(kcal/mol): 497.112

Deuterated entropy correction(cal/mol): 269.300

Deuterated imaginary Frequencies: -0.00

Axial Reaction C1

Reactant geometry

Zr	0.26280249	0.66566684	0.28967863
C	-0.55210280	-1.16387800	-1.16962685
C	-1.67138645	-0.27919789	-1.14460700
H	-2.60589370	-0.47045874	-0.63513277
C	0.45158077	-0.48021815	-1.92818108
H	1.43954128	-0.85870696	-2.14398787
C	-0.00596696	0.81066249	-2.27455143
H	0.54112475	1.55832910	-2.82979357
C	-1.33507781	0.93122886	-1.78573472
H	-1.97174182	1.79421732	-1.90834400
B	-0.32908792	-2.47859559	-0.22000077
C	-0.84066237	-3.89364121	-0.80208521
C	1.25961794	-2.41137692	0.19794077

C	-0.98283357	-2.04409039	1.23325515
N	-0.77850101	-0.85906291	1.72549766
N	1.84441967	-1.29165781	0.48395025
O	2.01097463	-3.51899811	0.33744186
O	-1.70569520	-2.86332566	2.00802568
C	-1.45258340	-0.74197018	3.02938706
C	-2.01936415	-2.16007283	3.24760146
C	3.23887082	-1.57622906	0.87639208
C	3.31655939	-3.11527297	0.83482986
N	1.91968535	1.83584459	0.84896545
H	-0.74090345	-0.45149224	3.80611996
C	3.36525928	1.79338874	1.05296837
H	3.59453926	1.47561368	2.08236467
H	3.80649199	1.03689781	0.39723108
C	4.09499437	3.12627665	0.81462538
C	4.38478769	3.50311874	-0.65060219
H	5.02769323	4.39423161	-0.63359949
H	4.97774479	2.71040827	-1.12104414
C	3.19312831	3.81411846	-1.51228654
H	2.46518572	4.50435371	-1.08812839
C	3.00324984	3.36125570	-2.74865606
H	3.70200897	2.67413526	-3.21692096
C	-1.45574314	-3.97880154	-2.05992106
H	-1.58132795	-3.07501042	-2.64773605
C	-0.70350752	-5.09457865	-0.08448538
H	-0.23118673	-5.08141408	0.89200673
C	-1.15439150	-6.31023625	-0.59189931
H	-1.03111377	-7.21830208	-0.00995080
C	-1.91193529	-5.19093621	-2.57900142
H	-2.38373659	-5.21708018	-3.55625011
C	-1.76313563	-6.36409362	-1.84521475
H	-2.11624327	-7.30966831	-2.24321953
H	3.45169930	-1.16859011	1.86692632

H	3.93289272	-1.11228378	0.17101029
H	3.45505106	-3.57317029	1.81589265
H	4.07074140	-3.50148135	0.14883644
H	-2.22807417	0.02617740	2.98025488
H	-1.53720506	-2.70155053	4.06285226
H	-3.10016734	-2.19200497	3.38221795
H	3.53130626	3.93392250	1.30114303
H	5.05749441	3.08128022	1.33733114
H	1.59907091	2.78748941	1.00863617
H	2.14664056	3.66418941	-3.34011304
N	-0.96020057	2.18620589	1.05857791
H	-0.52676899	2.62207403	1.87151907
C	-2.26732885	2.79560339	0.84281792
H	-2.86283435	2.14326157	0.19769212
H	-2.82260038	2.87140935	1.79015755
C	-2.19019641	4.19202580	0.20335136
H	-1.63616272	4.10976839	-0.73841026
H	-1.60364925	4.85694541	0.84795546
C	-3.57165908	4.82025256	-0.05482583
H	-4.10247480	4.96252318	0.89291557
H	-4.17125072	4.11518673	-0.64720195
C	-3.48880274	6.12801425	-0.79015118
H	-3.02984034	6.08422557	-1.77743795
C	-3.91070573	7.30234234	-0.33088229
H	-4.37426472	7.39754967	0.64673166
H	-3.81249582	8.21044600	-0.91508724

MP2 Electronic Energy(Ha): 1489.146765825905

B3LYP Electronic Energy(Ha): 1493.005588029720

M06-L Electronic Energy(Ha): 1492.809099917538

Zero point energy correction(kcal/mol): 376.928

Enthalpy correction(kcal/mol): 400.536

Entropy correction(cal/mol): 226.151

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.821

Deuterated enthalpy correction(kcal/mol): 396.657

Deuterated entropy correction(cal/mol): 227.566

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.33462088	0.82717445	-0.13043743
C	-1.22934611	-0.96885444	-0.77838392
C	-2.08526408	0.02456867	-0.21231778
H	-2.57445742	-0.04278119	0.74845757
C	-0.81426156	-0.43497889	-2.03736955
H	-0.14909519	-0.92093184	-2.73559366
C	-1.36114198	0.85245008	-2.21506243
H	-1.20880264	1.50279256	-3.06432685
C	-2.15697692	1.13521464	-1.08331763
H	-2.72820056	2.03679570	-0.93092547
B	-0.61984629	-2.29768836	-0.04823152
C	-1.47316760	-3.66046232	-0.19804353
C	0.91355220	-2.36818865	-0.63872840
C	-0.33728958	-1.81716320	1.49035960
N	0.03039169	-0.60157936	1.73875320
N	1.65385604	-1.31081468	-0.76730459
O	1.45681731	-3.52150796	-1.07430801
O	-0.36745693	-2.63708494	2.55514219
C	0.36069901	-0.47043128	3.16626279
C	-0.03604689	-1.84768324	3.73563473
C	2.88596599	-1.70206037	-1.48301300
C	2.81840341	-3.23809826	-1.49169384
N	2.24976496	1.35146935	0.96213966
H	1.42514000	-0.25185032	3.28384705
C	3.52512645	0.70226441	1.21595855
H	3.73930309	0.64680001	2.29144290
H	3.48508534	-0.32656625	0.85317824

C	4.63516074	1.48229493	0.48881507
C	4.11247437	1.77150880	-0.92063744
H	4.73315994	2.52592813	-1.41869737
H	4.15725402	0.87230484	-1.54013806
C	2.69862335	2.29880439	-0.90775731
H	2.58339453	3.27726340	-0.45034227
C	1.73932800	1.93494915	-1.86314588
H	2.00196026	1.18405835	-2.60240636
C	-2.67896362	-3.68961315	-0.91396537
H	-3.03908072	-2.77705821	-1.37843054
C	-1.05485998	-4.87055279	0.38225165
H	-0.12917863	-4.89833314	0.94737064
C	-1.79638164	-6.04223463	0.25583545
H	-1.44241251	-6.95881396	0.71752034
C	-3.43105715	-4.85741198	-1.04766243
H	-4.35987252	-4.84097149	-1.60934096
C	-2.99186594	-6.04105505	-0.46197820
H	-3.57238365	-6.95224981	-0.56220536
H	3.78038154	-1.33326931	-0.97955494
H	2.87618459	-1.27921618	-2.49399902
H	3.49310216	-3.69937300	-0.76618540
H	2.97468741	-3.69220769	-2.46949892
H	-0.20233790	0.35057971	3.61557788
H	0.76619050	-2.36109538	4.26536211
H	-0.92394568	-1.81455796	4.36937884
H	4.82049795	2.42532453	1.01680631
H	5.58354257	0.93575850	0.46347280
H	2.16245765	2.14814791	1.58503148
H	1.02677297	2.68668257	-2.18492923
N	-0.24507048	2.63337722	0.78278811
H	0.55213573	3.09531981	1.21222937
C	-1.40874415	3.47782797	1.03693241
H	-2.31896610	2.88267412	0.93546432

H	-1.39762522	3.82775454	2.08006576
C	-1.49821718	4.70317220	0.11287216
H	-1.53142967	4.35739821	-0.92644271
H	-0.58265315	5.29812617	0.21015661
C	-2.71750219	5.59471719	0.40952417
H	-2.67015560	5.95882681	1.44182449
H	-3.62650929	4.98198098	0.33507239
C	-2.83297301	6.76038014	-0.53129490
H	-2.94865266	6.50720383	-1.58470910
C	-2.79037475	8.04227150	-0.18022447
H	-2.67625449	8.34382470	0.85702190
H	-2.87171390	8.83695456	-0.91331115

MP2 Electronic Energy(Ha): 1489.144195458380

B3LYP Electronic Energy(Ha): 1492.981782927893

M06-L Electronic Energy(Ha): 1492.802366721918

Zero point energy correction(kcal/mol): 377.652

Enthalpy correction(kcal/mol): 399.992

Entropy correction(cal/mol): 212.001

Imaginary Frequencies: -290.35

Deuterated zero point energy correction(kcal/mol): 373.479

Deuterated enthalpy correction(kcal/mol): 396.040

Deuterated entropy correction(cal/mol): 213.347

Deuterated imaginary Frequencies: -288.67

Product geometry

Zr	0.29368444	0.82321968	-0.25025623
C	-1.23176804	-1.00162254	-0.87700304
C	-2.10127675	0.02025297	-0.38675592
H	-2.62857717	-0.00637198	0.55664599
C	-0.75569404	-0.51675767	-2.13540918
H	-0.05939969	-1.02953394	-2.78226691
C	-1.26478223	0.77577209	-2.37715281
H	-1.05999414	1.39534319	-3.23790292

C	-2.10953166	1.10746294	-1.29074264
H	-2.66817088	2.02452897	-1.18925060
B	-0.62852795	-2.28365374	-0.05063929
C	-1.45900904	-3.66436647	-0.14770254
C	0.91931175	-2.36764977	-0.59930056
C	-0.39360325	-1.72258407	1.47473214
N	0.08116847	-0.53511158	1.68499249
N	1.66288159	-1.31269523	-0.71321055
O	1.46176555	-3.51912795	-1.04296280
O	-0.62957630	-2.44916020	2.58024179
C	0.22832294	-0.31371435	3.13214672
C	-0.28802693	-1.63542890	3.73924531
C	2.89217446	-1.69665301	-1.43569323
C	2.82896645	-3.23265559	-1.44293366
N	2.41555644	1.54218366	0.75271649
H	1.27478216	-0.12061561	3.38547551
C	3.54186163	0.72701195	1.27642027
H	3.51618630	0.70984844	2.36802398
H	3.42846680	-0.29928636	0.92760171
C	4.80554676	1.38039517	0.69948354
C	4.35426495	1.79414043	-0.70907156
H	4.95453670	2.60254209	-1.13094531
H	4.42937080	0.94508367	-1.39340291
C	2.87172707	2.21071811	-0.56560931
H	2.81021884	3.28912602	-0.39234368
C	1.89478115	1.79004480	-1.65734424
H	2.34672607	1.09351096	-2.36882836
C	-2.64455962	-3.75325803	-0.89156778
H	-3.00848474	-2.87256965	-1.41127129
C	-1.03333589	-4.83574200	0.50223091
H	-0.12089454	-4.81819465	1.08967024
C	-1.74808246	-6.02733199	0.41569965
H	-1.38829596	-6.91293874	0.93029608

C	-3.37007588	-4.94157228	-0.98627092
H	-4.28314639	-4.97225275	-1.57257851
C	-2.92391853	-6.08578460	-0.33163522
H	-3.48336166	-7.01278084	-0.40227307
H	3.78931070	-1.32261966	-0.93960245
H	2.87273462	-1.27178901	-2.44503215
H	3.49504207	-3.69102786	-0.70738044
H	2.99884677	-3.68854678	-2.41753930
H	-0.35724444	0.55497813	3.44242284
H	0.46088113	-2.17787923	4.31720094
H	-1.19112498	-1.51888368	4.33948759
H	5.07748187	2.26023522	1.29268579
H	5.66503553	0.70559658	0.69684658
H	2.23439790	2.27007579	1.43611594
H	1.51420911	2.64512300	-2.22074772
N	-0.30260694	2.59499788	0.73650066
H	0.47859878	3.09271862	1.15633826
C	-1.49386960	3.40398484	0.97847892
H	-2.38405474	2.79373983	0.80739245
H	-1.54125847	3.70963910	2.03517099
C	-1.56661277	4.66475954	0.10184417
H	-1.54132788	4.36012160	-0.95028910
H	-0.66829636	5.27151234	0.26608024
C	-2.81437688	5.52432986	0.37313476
H	-2.82104212	5.85324157	1.41831877
H	-3.70795269	4.90013283	0.23485519
C	-2.90531224	6.71993892	-0.53233507
H	-2.97319653	6.50048958	-1.59739120
C	-2.89123857	7.98990486	-0.13821036
H	-2.82370474	8.25846791	0.91217788
H	-2.94984332	8.80782786	-0.84761115

MP2 Electronic Energy(Ha): 1489.172360030415

B3LYP Electronic Energy(Ha): 1493.005002928279

M06-L Electronic Energy(Ha): 1492.822601627272

Zero point energy correction(kcal/mol): 379.226

Enthalpy correction(kcal/mol): 401.640

Entropy correction(cal/mol): 213.623

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.915

Deuterated enthalpy correction(kcal/mol): 397.519

Deuterated entropy correction(cal/mol): 214.807

Deuterated imaginary Frequencies: -0.00

Axial Reaction C2

Reactant geometry

Zr	0.64320074	-1.23211808	0.38622881
C	0.08487745	0.89494411	1.53683070
C	-0.88709383	-0.02906161	2.03028348
H	-1.93698538	-0.02965964	1.77207594
C	1.31651594	0.49175755	2.14019711
H	2.27493399	0.96663162	1.98260267
C	1.12194351	-0.68630984	2.90291783
H	1.87072367	-1.21392175	3.47650499
C	-0.25878211	-1.01312442	2.83400156
H	-0.74371613	-1.82915535	3.35081199
B	-0.05601456	1.78378165	0.15724127
C	-0.43001645	3.34496392	0.32136221
C	1.35988578	1.50654869	-0.68032414
C	-1.11409642	0.92328851	-0.80289174
N	-1.06655058	-0.37667881	-0.90721442
N	1.91928848	0.32934413	-0.74825914
O	1.97069297	2.45809508	-1.39124141
O	-2.02984413	1.51246154	-1.57632387
C	-2.04314860	-0.82923674	-1.91545683
C	-2.79231406	0.47113111	-2.26305848

C	3.09575251	0.38934301	-1.63478048
C	3.15769077	1.88188457	-2.01780477
N	1.07849247	-3.00186334	-0.03602008
H	-1.51872680	-1.25906320	-2.77314005
H	3.98975162	0.05313979	-1.10554822
C	1.40137939	-4.38945714	-0.20910572
H	2.33903051	-4.47698025	-0.77933069
H	1.59937159	-4.87041481	0.76316470
C	0.32841409	-5.21177259	-0.95411482
C	-0.88813300	-5.66504252	-0.11805048
H	-1.49696030	-6.34530854	-0.72404966
H	-0.51290654	-6.25569969	0.72913091
C	-1.76949691	-4.57180052	0.41822098
H	-1.30470479	-3.89243488	1.12720765
C	-3.05242466	-4.40167924	0.10305892
H	-3.55886887	-5.06056048	-0.59687314
H	-3.64759611	-3.60901848	0.54413724
C	-0.61290808	3.90639299	1.59365322
H	-0.50013486	3.27385772	2.46824886
C	-0.58829431	4.20635021	-0.77817779
H	-0.45831505	3.82012015	-1.78352776
C	-0.91028564	5.55135162	-0.61785454
H	-1.02502603	6.18766943	-1.48973876
C	-0.93565406	5.25263333	1.76684047
H	-1.06966693	5.65183371	2.76717573
C	-1.08577250	6.08211287	0.65948186
H	-1.33678682	7.12975312	0.78786316
H	-0.01144218	-4.63375911	-1.81997041
H	0.80694222	-6.11862703	-1.34421116
H	-2.80138616	0.71500395	-3.32443772
H	-3.81066751	0.50471748	-1.87335824
H	-2.69323006	-1.60130572	-1.50128012
H	3.08849234	2.07027299	-3.08873269

H 4.02569834 2.40299175 -1.61314943

H 2.95058338 -0.26564168 -2.49732777

MP2 Electronic Energy(Ha): 1237.820635186627

B3LYP Electronic Energy(Ha): 1241.007842741381

M06-L Electronic Energy(Ha): 1240.849816502672

Zero point energy correction(kcal/mol): 279.593

Enthalpy correction(kcal/mol): 297.485

Entropy correction(cal/mol): 182.777

Imaginary Frequencies: -0.00

Transition State geometry

Zr 0.58724971 1.48545107 0.20978382

C 1.50561392 -0.86405779 0.24615151

C 2.32512448 -0.28113123 -0.77326603

H 2.24038238 -0.48244403 -1.83286648

C 1.97677887 -0.30288133 1.46952624

H 1.60116017 -0.53351659 2.45465350

C 2.99650219 0.64476421 1.19958969

H 3.56017376 1.20549431 1.93311469

C 3.22576381 0.63264808 -0.19970200

H 3.94919935 1.23276169 -0.73338521

B 0.12609247 -1.70114271 -0.00168934

C 0.23600408 -3.30675704 -0.13713277

C -0.87824946 -1.18054144 1.19392365

C -0.58995682 -0.93150202 -1.28354925

N -0.50549260 0.36357796 -1.46210850

N -0.81264669 0.03989030 1.61057244

O -1.86137941 -1.92669926 1.73293244

O -1.41480890 -1.55164525 -2.13173197

C -1.45578555 0.77057554 -2.51643529

C -1.89335051 -0.57969297 -3.10721074

C -1.88319481 0.28330110 2.58752260

C -2.55770398 -1.09991666 2.71275876

N	-0.73729612	2.81032701	0.64941476
H	-2.28533393	1.32579958	-2.06889255
H	-1.46324640	0.63164093	3.53474491
C	-1.72996121	3.82980833	0.70118360
H	-2.73822200	3.40100653	0.80425422
H	-1.58702931	4.48624196	1.57621523
C	-1.65747656	4.66980227	-0.58718169
C	-0.17582446	4.99659211	-0.89050973
H	0.04181574	4.87078496	-1.95390131
H	0.03239484	6.04674489	-0.65375076
C	0.81165626	4.17990959	-0.08264994
H	0.92622577	4.50590554	0.94664704
C	1.86913262	3.46852056	-0.64364741
H	1.96498408	3.40649353	-1.72436728
H	2.78698663	3.35140864	-0.08047300
C	1.47221938	-3.95711538	-0.00847476
H	2.36369168	-3.36197572	0.16168449
C	-0.88825105	-4.12362400	-0.35072272
H	-1.86744188	-3.66801425	-0.44910635
C	-0.78516929	-5.51003814	-0.43059605
H	-1.67542775	-6.10981415	-0.59283862
C	1.58744693	-5.34558344	-0.08522398
H	2.56057052	-5.81416915	0.02344790
C	0.45677709	-6.12937019	-0.29673103
H	0.53974810	-7.20972517	-0.35426925
H	-2.06759863	4.07711930	-1.41024969
H	-2.26176209	5.57925086	-0.51216264
H	-2.97072164	-0.70530355	-3.20232729
H	-1.41286613	-0.80874964	-4.06019503
H	-0.97383325	1.41332000	-3.25492099
H	-3.61757153	-1.10263365	2.45648039
H	-2.42277325	-1.56336975	3.69102183
H	-2.55497744	1.06134198	2.21804549

MP2 Electronic Energy(Ha): 1237.799245788107

B3LYP Electronic Energy(Ha): 1240.973626117792

M06-L Electronic Energy(Ha): 1240.826494943223

Zero point energy correction(kcal/mol): 279.061

Enthalpy correction(kcal/mol): 295.747

Entropy correction(cal/mol): 171.476

Imaginary Frequencies: -206.00 -69.94

Product geometry

Zr	0.42135250	1.42052970	0.35180672
C	0.85245671	-0.85447243	1.22058819
C	2.17168519	-0.33333776	1.05907115
H	2.87651821	-0.64290485	0.30041636
C	0.29280031	-0.11987793	2.31440904
H	-0.70526297	-0.24968524	2.70896837
C	1.20329707	0.87520756	2.74176187
H	1.05402239	1.58034753	3.54689311
C	2.37896341	0.74168604	1.95014905
H	3.27655970	1.33604722	2.04040584
B	0.02633263	-1.73930124	0.10572311
C	0.02798842	-3.34078627	0.28863116
C	-1.47103718	-1.04233463	0.04815129
C	0.61897563	-1.19571773	-1.34224804
N	0.79505963	0.07204013	-1.56416903
N	-1.61203778	0.24897867	0.06268084
O	-2.60762360	-1.73766310	-0.09235384
O	0.92936012	-2.00347603	-2.36503134
C	1.33623828	0.26266622	-2.92068782
C	1.36174942	-1.17317852	-3.48484446
C	-3.03323690	0.59139930	-0.11895683
C	-3.71762167	-0.79146286	-0.13220388
N	-0.46597296	3.25575743	0.54555840
H	0.69527459	0.93059211	-3.50083602

H	-3.38512562	1.22640877	0.69677991
C	-1.49603081	4.22499041	0.85732771
H	-2.48057200	3.75144031	0.89961396
H	-1.31474706	4.68151329	1.84264283
C	-1.39905186	5.31905900	-0.25242914
C	-0.05885694	5.03045687	-0.97331334
H	-0.23522168	4.54729765	-1.93879751
H	0.53148844	5.93215556	-1.15552178
C	0.67780118	4.04081996	-0.04893984
H	1.16131756	4.60961048	0.76174680
C	1.67800447	3.05080516	-0.66803724
H	1.60207622	3.04576880	-1.75967764
H	2.71260180	3.25132253	-0.38854116
C	0.68612556	-3.94676905	1.36874229
H	1.20404543	-3.32099453	2.08863693
C	-0.62539318	-4.19730937	-0.61424633
H	-1.14859283	-3.77632305	-1.46659946
C	-0.62303887	-5.57973362	-0.44928269
H	-1.13804789	-6.21117041	-1.16646105
C	0.69553862	-5.33083250	1.54484790
H	1.21578179	-5.76432703	2.39309540
C	0.03957561	-6.15438061	0.63466620
H	0.04361871	-7.23128880	0.76626673
H	-2.24238787	5.25543520	-0.94367993
H	-1.41768566	6.31908566	0.18721682
H	0.65883575	-1.33408647	-4.30335056
H	2.35158286	-1.51472620	-3.78657598
H	2.32890247	0.71597055	-2.86748521
H	-4.29394271	-0.99453517	-1.03438886
H	-4.33962114	-0.97805893	0.74425972
H	-3.17201095	1.14071898	-1.05425956

MP2 Electronic Energy(Ha): 1237.844207883629

B3LYP Electronic Energy(Ha): 1241.018847084336

M06-L Electronic Energy(Ha): 1240.869848701324

Zero point energy correction(kcal/mol): 280.292

Enthalpy correction(kcal/mol): 297.516

Entropy correction(cal/mol): 176.680

Imaginary Frequencies:

Axial Reaction H4

Reactant geometry

Zr	-0.35519619	0.63163900	-0.14292852
C	0.80558241	-1.26248726	-1.28832326
C	-0.36229697	-1.09684056	-2.08920298
H	-1.22179797	-1.75137478	-2.09143622
C	1.65035535	-0.15427966	-1.60925518
H	2.62939391	0.02580069	-1.19174734
C	1.00510003	0.67043376	-2.55057701
H	1.40852869	1.56852485	-2.99964333
C	-0.24989422	0.09027989	-2.84415116
H	-0.97258061	0.48064166	-3.54347396
B	1.05657195	-2.36369190	-0.11631625
C	1.66087120	-3.78742295	-0.58774940
C	1.96691353	-1.55251285	0.97847231
C	-0.37770099	-2.44466302	0.66683002
N	-1.11120431	-1.38704818	0.83391987
N	1.72844458	-0.32279876	1.29897940
O	3.01734038	-2.13570853	1.59791840
O	-0.84720785	-3.56355473	1.24402085
C	-2.25851928	-1.72915906	1.69260781
C	-2.15042661	-3.25905608	1.81795897
C	2.70678510	0.07550706	2.33225200
C	3.67833032	-1.11700831	2.39189500
N	-0.82065156	1.69236102	1.70629499
H	-2.16570325	-1.22623275	2.65752502

H	3.20676338	1.00878931	2.05964620
C	-1.64615523	2.90327676	1.79851038
H	-1.04584758	3.79201600	2.06349432
H	-2.13585113	3.13852893	0.84977211
C	-2.67541613	2.64030416	2.93202682
C	-2.04059446	1.49105374	3.75482583
H	-1.97845965	1.72377997	4.82136549
H	-2.63417448	0.58039264	3.65724991
C	-0.63869972	1.30149318	3.11186718
H	-0.30949414	0.26062554	3.15943881
C	0.38942195	2.17787589	3.86320562
H	0.58969700	1.77138485	4.86023320
H	1.33259984	2.23654677	3.31945891
C	1.96379066	-4.04153599	-1.93369379
H	1.78483966	-3.26444427	-2.67007072
C	1.91279269	-4.82988978	0.32135964
H	1.69639256	-4.68223353	1.37406939
C	2.43547339	-6.05392994	-0.08762740
H	2.61695283	-6.83580111	0.64347372
C	2.48886348	-5.26373050	-2.35605956
H	2.71100512	-5.42244675	-3.40684949
C	2.72713547	-6.27747867	-1.43280385
H	3.13480268	-7.23011831	-1.75498637
H	-2.16024272	-3.62675983	2.84353180
H	-2.90142115	-3.79609070	1.23467956
H	-3.19531955	-1.40693928	1.23584744
H	3.83577383	-1.51495082	3.39441779
H	4.64757866	-0.91061420	1.93121585
H	2.20162469	0.23722626	3.28647101
H	-2.85534259	3.53646144	3.53136062
H	-3.63887103	2.33500815	2.51603163
N	-2.27281195	1.16593935	-0.78464304
H	-2.78748131	1.52302394	0.01574137

C	-3.14725652	1.22278443	-1.95694581
H	-2.91054255	0.39788570	-2.63249054
H	-2.96572391	2.14904570	-2.52476149
C	-4.64579818	1.17070962	-1.62338061
H	-4.86974917	1.93384618	-0.86726582
H	-5.21232546	1.45685503	-2.51799210
C	-5.15059921	-0.19965588	-1.12847899
H	-4.52758016	-0.54341059	-0.29817213
H	-6.16603190	-0.07104612	-0.73246247
C	-5.18371116	-1.24459775	-2.20875950
H	-5.81853267	-1.01429889	-3.06442110
C	-4.51521355	-2.39454569	-2.20060776
H	-3.86420135	-2.66764760	-1.37586742
H	-4.59168801	-3.10512318	-3.01582839
N	0.50479847	2.92444761	-0.59155054
C	1.87244972	3.27188966	-0.13969561
H	-0.16497358	3.50571859	-0.09385078
H	0.39616301	3.13154874	-1.58033319
H	1.93731895	2.97751805	0.90936583
H	2.57234359	2.64258035	-0.69580098
C	2.25348460	4.74949296	-0.28703608
H	1.53982247	5.36507006	0.27494081
H	3.22771145	4.89915793	0.19069172
C	2.33430562	5.24539632	-1.74232664
H	1.35958499	5.10765841	-2.22987046
H	3.05507256	4.63625185	-2.29895932
C	2.71648038	6.69613088	-1.84045482
H	2.03565528	7.39880503	-1.36156520
C	3.80404009	7.16272957	-2.44571249
H	4.51096120	6.50022259	-2.93634295
H	4.02633657	8.22318492	-2.47726767
H	0.02155147	3.19874724	3.99982191

MP2 Electronic Energy(Ha): 1740.492284349692

B3LYP Electronic Energy(Ha): 1744.984385583118

M06-L Electronic Energy(Ha): 1744.766741570203

Zero point energy correction(kcal/mol): 477.207

Enthalpy correction(kcal/mol): 505.583

Entropy correction(cal/mol): 262.288

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.655

Deuterated enthalpy correction(kcal/mol): 497.413

Deuterated entropy correction(cal/mol): 264.684

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.42785576	0.50589226	-0.44719600
C	0.56055434	-1.53761024	-1.38741683
C	-0.76390809	-1.52909993	-1.92129508
H	-1.56766148	-2.18709722	-1.62688405
C	1.24933359	-0.48670961	-2.06552665
H	2.27600883	-0.20187774	-1.89677391
C	0.36582364	0.17120722	-2.94702271
H	0.60025054	1.01367950	-3.58115768
C	-0.88316220	-0.48249785	-2.86390400
H	-1.76048676	-0.22672287	-3.43543100
B	1.10018209	-2.35280192	-0.08150349
C	1.72065055	-3.81741545	-0.35737760
C	2.11625151	-1.28494695	0.64473388
C	-0.15557968	-2.30382341	0.97282537
N	-0.88461165	-1.23618334	1.09322453
N	1.82919184	-0.02680812	0.76237712
O	3.28888277	-1.67500827	1.18252302
O	-0.45218046	-3.29781975	1.82480449
C	-1.80917237	-1.41267213	2.22734195
C	-1.62912034	-2.89785197	2.58590306
C	2.90402557	0.61221186	1.55303969

C	3.98159879	-0.48062030	1.63517044
N	-0.58228381	2.17884849	1.35365464
H	-1.52055559	-0.75008985	3.04693686
H	3.26546185	1.52231220	1.07113648
C	-1.67077535	3.17123239	1.45515673
H	-1.27138380	4.17958109	1.64788292
H	-2.24342990	3.24541707	0.52833272
C	-2.50606850	2.71836531	2.66233388
C	-1.44487856	2.13222293	3.62218601
H	-1.27142032	2.79249916	4.47601638
H	-1.76323631	1.17074144	4.02974482
C	-0.14862193	1.99822987	2.75915784
H	0.28874631	1.00345630	2.87184526
C	0.89358592	3.04570510	3.19568933
H	1.22332032	2.86053254	4.22361443
H	1.77195759	3.03034713	2.54820407
C	1.80558747	-4.33748157	-1.65749914
H	1.44290744	-3.74196245	-2.48937279
C	2.20571386	-4.63243246	0.68022851
H	2.16294990	-4.27498106	1.70358957
C	2.74436684	-5.89278911	0.43529264
H	3.10983440	-6.49442071	1.26167712
C	2.34403873	-5.59867521	-1.91579293
H	2.39382938	-5.96662659	-2.93584500
C	2.81660040	-6.38322681	-0.86801064
H	3.23645506	-7.36465356	-1.06231898
H	-1.42678904	-3.08521223	3.63963825
H	-2.46145625	-3.52469549	2.25917977
H	-2.83232591	-1.16701150	1.94088666
H	4.35798722	-0.66641261	2.64050147
H	4.82346739	-0.30868734	0.95999235
H	2.52715743	0.88733508	2.54056205
H	-3.08091828	3.53352190	3.10919821

H	-3.21746607	1.94416497	2.35953725
N	-2.44787389	0.95996589	-0.70258190
H	-2.74380902	1.47971723	0.11936439
C	-3.60114190	0.85472421	-1.59469910
H	-3.43061469	0.05695298	-2.31909316
H	-3.71505705	1.78290298	-2.17606613
C	-4.93283795	0.58919452	-0.87274531
H	-5.04657327	1.31568411	-0.05874356
H	-5.75414600	0.78985376	-1.57177343
C	-5.09406251	-0.83625020	-0.31013927
H	-4.21811524	-1.09765847	0.28963773
H	-5.95880790	-0.84346156	0.36624411
C	-5.31033181	-1.87967424	-1.37127452
H	-6.13662874	-1.68845732	-2.05598740
C	-4.59876279	-2.99317026	-1.52404074
H	-3.76787661	-3.23229144	-0.86719075
H	-4.82264330	-3.71121871	-2.30477134
N	0.56138606	2.59125444	-0.83593118
C	1.91314006	2.86957669	-1.32965498
H	0.23770837	2.62430166	0.40078607
H	-0.10772803	3.18639961	-1.31960509
H	2.58291263	2.10284056	-0.93357780
H	1.95328581	2.76606168	-2.42358262
C	2.46911389	4.24945689	-0.94310440
H	2.45499199	4.34855898	0.14869978
H	3.52001559	4.30046838	-1.25179491
C	1.71369401	5.43255356	-1.57354097
H	0.66396041	5.39566188	-1.25481902
H	1.72050476	5.33336521	-2.66519528
C	2.29244733	6.76357597	-1.18439178
H	2.27538166	6.99291528	-0.11939326
C	2.82525851	7.64714766	-2.02314736
H	2.86758261	7.46190406	-3.09253284

H 3.23666651 8.58761369 -1.67432544

H 0.47466063 4.05541130 3.16370958

MP2 Electronic Energy(Ha): 1740.478513113473

B3LYP Electronic Energy(Ha): 1744.967048309119

M06-L Electronic Energy(Ha): 1744.746743851206

Zero point energy correction(kcal/mol): 474.403

Enthalpy correction(kcal/mol): 502.192

Entropy correction(cal/mol): 255.539

Imaginary Frequencies: -1337.67

Deuterated zero point energy correction(kcal/mol): 466.835

Deuterated enthalpy correction(kcal/mol): 494.966

Deuterated entropy correction(cal/mol): 257.590

Deuterated imaginary Frequencies: -959.46

Product geometry

Zr -0.35400894 0.53845145 -0.48324014

C 0.19464714 -1.68510329 -1.41257632

C -1.19880276 -1.55143058 -1.67492853

H -1.98641958 -2.08280178 -1.16171584

C 0.83441162 -0.76651478 -2.30555897

H 1.89969781 -0.60148513 -2.37503539

C -0.13893490 -0.06628122 -3.04858994

H 0.04639942 0.70541845 -3.78086596

C -1.40679798 -0.54996618 -2.65261626

H -2.35969021 -0.23599164 -3.04839937

B 0.88642870 -2.45281511 -0.13889901

C 1.36779346 -3.97348216 -0.38572499

C 2.07962566 -1.41760108 0.30847229

C -0.21074710 -2.26378531 1.06648146

N -0.80658899 -1.13023539 1.26455638

N 1.88404667 -0.13570206 0.35123053

O 3.33838921 -1.81918463 0.56666830

O -0.58951377 -3.26724204 1.87957774

C	-1.83627639	-1.31292454	2.30333616
C	-1.53973290	-2.72500868	2.83937446
C	3.19419877	0.52187841	0.52569462
C	4.10029966	-0.64089108	0.95177424
N	0.00530923	2.05888056	1.77305643
H	-1.76107999	-0.54859621	3.07749498
H	3.50834139	0.96820089	-0.42318254
C	-0.84362415	3.25972299	1.96935642
H	-0.24893652	4.12563852	2.28958350
H	-1.35052458	3.52718464	1.04167978
C	-1.79319290	2.83254914	3.08897755
C	-0.88738590	2.00468123	4.02166470
H	-0.52161843	2.62350310	4.84511755
H	-1.41885852	1.16505076	4.47309559
C	0.31151580	1.53835623	3.14536842
H	0.35929088	0.45069584	3.08063945
C	1.63976418	2.05620565	3.70796303
H	1.78288995	1.69170788	4.72938262
H	2.49143568	1.71462915	3.11749351
C	1.20375375	-4.59830445	-1.63051701
H	0.74396988	-4.04383489	-2.44249550
C	1.96888046	-4.73747805	0.62923753
H	2.11711055	-4.29828225	1.61079790
C	2.38204093	-6.04984526	0.41642340
H	2.84208135	-6.61049743	1.22424849
C	1.61387769	-5.91281258	-1.85674749
H	1.47040616	-6.36329167	-2.83391025
C	2.20563339	-6.64542467	-0.83206857
H	2.52604308	-7.66804389	-1.00195068
H	-1.05589481	-2.72119981	3.81902991
H	-2.40418013	-3.38730732	2.86696210
H	-2.82979414	-1.23191226	1.85312980
H	4.25734119	-0.68522379	2.03311827

H	5.06218055	-0.67919125	0.44306992
H	3.15815697	1.32135005	1.26497003
H	-2.25505727	3.68445854	3.59108214
H	-2.59936005	2.21258104	2.68779149
N	-2.30226839	1.30380517	-0.25688981
H	-2.38727981	1.71893565	0.66730429
C	-3.49868684	1.65711313	-1.01361915
H	-3.49590708	1.11834547	-1.96325873
H	-3.48189522	2.72780145	-1.27641937
C	-4.82205005	1.38102745	-0.27779856
H	-4.76187970	1.81943525	0.72630166
H	-5.63009383	1.91678121	-0.79202839
C	-5.20392214	-0.10719723	-0.16192185
H	-4.34648509	-0.67964107	0.20362271
H	-5.99748986	-0.20336560	0.59091105
C	-5.70223061	-0.69668707	-1.45273386
H	-6.53502364	-0.16809352	-1.91698414
C	-5.22807452	-1.78771641	-2.04778245
H	-4.40232515	-2.35336534	-1.62791797
H	-5.65255614	-2.16204613	-2.97263784
N	0.58719944	2.36886041	-1.10190360
C	1.60617880	2.70829247	-2.08417408
H	0.85012998	2.32284398	1.26942528
H	-0.04440489	3.15691152	-0.98906629
H	2.22457196	1.82423935	-2.26704404
H	1.16110562	2.96621202	-3.06176749
C	2.54293054	3.86135748	-1.67723355
H	3.03368622	3.60528456	-0.73024755
H	3.33396669	3.95814625	-2.43102796
C	1.83367576	5.21891315	-1.53217584
H	1.04427417	5.12529527	-0.77475227
H	1.33980818	5.47833956	-2.47568371
C	2.76311269	6.32725244	-1.12681055

H 3.27394594 6.19063311 -0.17374860

C 3.01272422 7.42507467 -1.83469664

H 2.53224359 7.60496064 -2.79199270

H 3.70398201 8.18392124 -1.48549250

H 1.65938812 3.15001666 3.74005787

MP2 Electronic Energy(Ha): 1740.493298675923

B3LYP Electronic Energy(Ha): 1744.987463452245

M06-L Electronic Energy(Ha): 1744.769399646426

Zero point energy correction(kcal/mol): 476.949

Enthalpy correction(kcal/mol): 505.145

Entropy correction(cal/mol): 257.147

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.561

Deuterated enthalpy correction(kcal/mol): 497.150

Deuterated entropy correction(cal/mol): 259.629

Deuterated imaginary Frequencies: -0.00

Axial Reaction H6

Reactant geometry

Zr -0.93466033 -0.08407289 0.20347078

C -0.47300386 2.00750140 1.44563533

C -1.83361061 1.70558678 1.76464219

H -2.69594941 2.24787746 1.40240118

C 0.29537893 1.02297115 2.13977055

H 1.37318230 0.94102681 2.11753950

C -0.56568493 0.10168608 2.78719366

H -0.26879468 -0.74202324 3.39363136

C -1.89932963 0.53005203 2.55340633

H -2.79230046 0.06875222 2.95019679

B 0.03229542 2.86016747 0.13126458

C 0.48739933 4.38867731 0.37763070

C 1.19916202 1.90605122 -0.58407011

C	-1.18619608	2.68201482	-0.99363933
N	-1.80507466	1.54886518	-1.18440992
N	1.08720120	0.60911016	-0.68752048
O	2.28524503	2.42172856	-1.16469985
O	-1.55639488	3.66735666	-1.81499962
C	-2.76008512	1.68627867	-2.29939479
C	-2.61659928	3.17155384	-2.68955779
C	2.22048155	0.07599212	-1.46680540
C	3.08624329	1.32807267	-1.70887944
N	-1.45732691	-1.81862209	-0.27773072
N	1.50454163	-4.11227790	-0.04837017
C	1.84873729	-4.61167566	-1.38055201
H	2.12982349	-3.80111886	-2.07630434
H	-2.49240857	1.00514415	-3.11065508
H	2.74583927	-0.69553641	-0.90074033
C	-1.99607849	-3.14448063	-0.40970831
H	-2.98857440	-3.10521950	-0.88654176
H	-1.36910592	-3.74525494	-1.08423237
C	-2.12649717	-3.88387983	0.93196808
C	3.07304800	-5.51317145	-1.11056442
C	3.66666367	-4.97026100	0.21823239
H	4.71660962	-4.68312763	0.12809971
H	1.00865972	-5.15133234	-1.82301765
C	2.77844202	-3.76223359	0.58584424
H	3.22168345	-2.85960457	0.11840851
H	3.59964430	-5.72549596	1.00546102
C	2.63152645	-3.50827564	2.08119972
H	3.60094599	-3.28606485	2.53674004
H	0.84751256	-3.33669619	-0.07678994
H	2.20799025	-4.38828853	2.57198789
C	0.93631057	5.22464321	-0.65951423
H	0.98517195	4.84103787	-1.67298212
C	0.44797155	4.94577026	1.66435266

H	0.10682871	4.33274611	2.49229550
C	1.32398455	6.54140235	-0.42633959
H	1.66549744	7.15874794	-1.25123436
C	0.83390770	6.26371876	1.91016862
H	0.78989318	6.66030065	2.91948637
C	1.27436134	7.06834339	0.86359057
H	1.57576677	8.09398482	1.04856391
C	-2.64579934	-5.32795543	0.80080224
H	-3.63273677	-5.33733789	0.32354698
H	-2.78714794	-5.72897558	1.81332985
C	-1.70945331	-6.23833783	0.05364936
H	-0.67062003	-6.20734160	0.38011901
C	-2.05117354	-7.04568320	-0.94743480
H	-3.07188743	-7.09656643	-1.31606848
H	-1.32548373	-7.68989560	-1.43183359
H	-3.50829196	3.76631836	-2.49067243
H	-3.76990826	1.43363887	-1.96943889
H	-2.29550749	3.33235301	-3.71829838
H	3.27177657	1.54709464	-2.75975072
H	4.03281217	1.31693254	-1.16761271
H	1.85810544	-0.37620106	-2.39354233
H	2.76510015	-6.55394491	-0.99533014
H	3.78750866	-5.47491458	-1.93543457
H	-1.14584345	-3.89550089	1.41879444
H	-2.79657439	-3.31207214	1.58278492
H	1.96888756	-2.65974362	2.27599569

MP2 Electronic Energy(Ha): 1489.137733423341

B3LYP Electronic Energy(Ha): 1492.987782209962

M06-L Electronic Energy(Ha): 1492.786966691619

Zero point energy correction(kcal/mol): 378.590

Enthalpy correction(kcal/mol): 401.754

Entropy correction(cal/mol): 225.173

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.373

Deuterated enthalpy correction(kcal/mol): 397.705

Deuterated entropy correction(cal/mol): 226.284

Deuterated imaginary Frequencies:

Transition State geometry

Zr	-0.34956089	-0.36382069	0.41926511
C	-0.53621645	1.91106534	1.37997258
C	-1.80175492	1.27779020	1.61213534
H	-2.72516669	1.51885922	1.10496346
C	0.36923281	1.26920276	2.27262716
H	1.42723934	1.47918011	2.34610874
C	-0.29360068	0.22695773	2.96588828
H	0.14637339	-0.44042557	3.69348068
C	-1.65357135	0.23890554	2.56226379
H	-2.43392528	-0.40947006	2.93290027
B	-0.12179769	2.80301575	0.06196075
C	-0.11094605	4.40578908	0.23599492
C	1.30997030	2.14676161	-0.45554190
C	-1.10554213	2.23050455	-1.13408096
N	-1.30443568	0.95452690	-1.26180231
N	1.50912271	0.86325434	-0.50876650
O	2.32040590	2.90246640	-0.90935457
O	-1.71012412	2.99622676	-2.05083972
C	-2.18253524	0.70037495	-2.41578812
C	-2.44468051	2.12096940	-2.96108753
C	2.83785580	0.60274461	-1.09334405
C	3.40383335	2.01922554	-1.32060201
N	-1.13930910	-2.05260157	-0.08072660
N	1.58554609	-4.17820208	-0.37861086
C	2.59749128	-5.04435977	-0.98771707
H	2.91572311	-4.68590990	-1.98266805
H	-1.68276305	0.05383887	-3.14073651

H	3.45089179	0.01142850	-0.41007058
C	-1.85688008	-3.28721919	-0.27931690
H	-2.88966347	-3.04894957	-0.57169544
H	-1.43633858	-3.85511728	-1.12241166
C	-1.89070982	-4.19585425	0.95992780
C	3.77703592	-4.94864205	-0.00060721
C	3.59409288	-3.56399400	0.67691836
H	4.44916125	-2.90192154	0.52048257
H	2.22149071	-6.06352466	-1.10643225
C	2.30464569	-2.96724712	0.05586412
H	2.60221189	-2.36460831	-0.82315284
H	3.46160191	-3.67549005	1.75534945
C	1.47743711	-2.09092295	0.99703366
H	2.08887563	-1.23053991	1.29285111
H	0.83889267	-3.95506326	-1.02853396
H	1.27149370	-2.64507489	1.91983688
C	0.19485336	5.27316592	-0.82702330
H	0.43432313	4.86034470	-1.80147548
C	-0.41294676	5.00222562	1.46903147
H	-0.65646727	4.36824260	2.31570339
C	0.19996809	6.65644026	-0.66928705
H	0.44056035	7.29622752	-1.51254841
C	-0.41069278	6.38700082	1.63963528
H	-0.64967159	6.81257372	2.60910885
C	-0.10347370	7.22127048	0.56889902
H	-0.10052087	8.29880284	0.69532765
C	-2.71046701	-5.48385042	0.75041262
H	-3.73858449	-5.23423410	0.46348698
H	-2.77346717	-6.00546001	1.71411704
C	-2.11535744	-6.42184252	-0.26324436
H	-1.08332462	-6.71737353	-0.07660875
C	-2.73960800	-6.90311087	-1.33490196
H	-3.76681156	-6.63362151	-1.56326052

H	-2.25116684	-7.58741013	-2.01981684
H	-3.49247203	2.41971226	-2.93007410
H	-3.09564025	0.19446454	-2.09344920
H	-2.05128645	2.28637368	-3.96444062
H	3.63619571	2.24150182	-2.36217780
H	4.27091739	2.24941601	-0.70042378
H	2.73721177	0.03674376	-2.02362422
H	3.71591665	-5.74681222	0.74157946
H	4.73743043	-5.04864019	-0.51041917
H	-0.86296956	-4.45760528	1.23187817
H	-2.31251163	-3.62930809	1.79657030
H	0.12434002	-2.25189708	0.39639333

MP2 Electronic Energy(Ha): 1489.100724528162

B3LYP Electronic Energy(Ha): 1492.938403844744

M06-L Electronic Energy(Ha): 1492.746329675635

Zero point energy correction(kcal/mol): 375.945

Enthalpy correction(kcal/mol): 398.447

Entropy correction(cal/mol): 218.107

Imaginary Frequencies: -1547.42

Deuterated zero point energy correction(kcal/mol): 372.483

Deuterated enthalpy correction(kcal/mol): 395.128

Deuterated entropy correction(cal/mol): 218.899

Deuterated imaginary Frequencies: -1132.80

Product geometry

Zr	-0.92708156	-0.09638200	0.22655707
C	-0.44299261	1.99841171	1.45695042
C	-1.79527927	1.69313005	1.80680837
H	-2.66702628	2.23286820	1.46378548
C	0.34352509	1.01671328	2.13459883
H	1.42077925	0.93761856	2.08823682
C	-0.50019625	0.09347835	2.80166154
H	-0.18742161	-0.74827531	3.40285983

C	-1.84008419	0.51797503	2.59750823
H	-2.72257649	0.05485571	3.01510746
B	0.03033638	2.85110971	0.13060139
C	0.48538231	4.38171840	0.36333563
C	1.18390228	1.89923808	-0.60878155
C	-1.21220462	2.66762478	-0.96689249
N	-1.83230477	1.53254830	-1.14151426
N	1.07251940	0.60192965	-0.70793434
O	2.25608095	2.41628212	-1.21350062
O	-1.60233190	3.64982833	-1.78270172
C	-2.81068193	1.66436736	-2.23666627
C	-2.68042535	3.14934860	-2.63243367
C	2.18950165	0.07000598	-1.51110918
C	3.04780970	1.32327744	-1.77252224
N	-1.45336866	-1.82949054	-0.25614068
N	1.50399699	-4.06415570	-0.04208236
C	1.86524710	-4.51007412	-1.38828335
H	2.14440840	-3.67159628	-2.05118044
H	-2.55736385	0.98252438	-3.05193757
H	2.72805067	-0.70034882	-0.95597098
C	-1.98924675	-3.15460504	-0.40551117
H	-2.98181310	-3.11079448	-0.88180327
H	-1.36076103	-3.74445551	-1.08814162
C	-2.11820678	-3.91397839	0.92502228
C	3.09616161	-5.40835359	-1.14015881
C	3.67573737	-4.90419411	0.20995420
H	4.72142878	-4.59785304	0.13482887
H	1.03485949	-5.04121075	-1.85853134
C	2.76787092	-3.72319268	0.61659280
H	3.20297653	-2.79688476	0.18961712
H	3.61770217	-5.68811428	0.96933950
C	2.60505225	-3.53037802	2.11946513
H	3.56751904	-3.31362911	2.59202098

H	0.83705311	-3.29636156	-0.04783772
H	2.18923601	-4.43456080	2.57141094
C	0.91027455	5.21559855	-0.68556161
H	0.94035095	4.82851276	-1.69843544
C	0.46946862	4.94330761	1.64857787
H	0.14731779	4.33200051	2.48536393
C	1.29736046	6.53466704	-0.46494172
H	1.61996234	7.15024315	-1.29872676
C	0.85497474	6.26368256	1.88184992
H	0.82946342	6.66386197	2.89038011
C	1.27128023	7.06616764	0.82380451
H	1.57218782	8.09366725	0.99900827
C	-2.62795918	-5.35913672	0.76965808
H	-3.61419679	-5.36714344	0.29093102
H	-2.76779982	-5.77792156	1.77515478
C	-1.68460046	-6.25032043	0.00823793
H	-0.64663625	-6.21900993	0.33737293
C	-2.01908156	-7.04089899	-1.00852625
H	-3.03862005	-7.09108227	-1.38047525
H	-1.28830724	-7.67130977	-1.50332341
H	-3.56922640	3.74176053	-2.41446583
H	-3.81254372	1.40886543	-1.88538760
H	-2.38302105	3.30936127	-3.66837698
H	3.21147006	1.54121761	-2.82723003
H	4.00522898	1.31453883	-1.25062301
H	1.80778356	-0.38339128	-2.42945071
H	2.79664456	-6.45493180	-1.06104271
H	3.81559830	-5.33684581	-1.95848793
H	-1.13869295	-3.92725588	1.41392177
H	-2.79344402	-3.35650444	1.58287350
H	1.92957729	-2.69887178	2.34142116

MP2 Electronic Energy(Ha): 1489.137995175677

B3LYP Electronic Energy(Ha): 1492.987810154406

M06-L Electronic Energy(Ha): 1492.787164781128

Zero point energy correction(kcal/mol): 378.589

Enthalpy correction(kcal/mol): 401.753

Entropy correction(cal/mol): 225.138

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.371

Deuterated enthalpy correction(kcal/mol): 397.702

Deuterated entropy correction(cal/mol): 226.247

Deuterated imaginary Frequencies:

Axial Reaction H7

Reactant geometry

Zr	-0.77259078	0.12947864	0.06812235
C	0.82575645	1.65913299	-1.05561737
C	1.53459908	0.42877679	-0.88071450
H	2.33190635	0.26123678	-0.17232586
C	-0.12664937	1.40240184	-2.08762772
H	-0.84758489	2.11563391	-2.46249959
C	-0.05995184	0.04660929	-2.46840014
H	-0.66548996	-0.44710794	-3.21277155
C	0.97504931	-0.56700070	-1.71261949
H	1.30353370	-1.59234262	-1.80535174
B	0.84955729	2.94339129	-0.04201057
C	1.71040515	4.22568443	-0.50854531
C	-0.73823608	3.24703592	0.28077716
C	1.27714780	2.29292787	1.40669064
N	0.78741808	1.16995821	1.82617541
N	-1.58030986	2.27477964	0.46954862
O	-1.24208777	4.47448890	0.45868548
O	2.12592430	2.91756873	2.24336378
C	1.33161924	0.89917368	3.17287700
C	2.27945092	2.08855074	3.42751665

C	-2.88607280	2.82303165	0.87420790
C	-2.65726085	4.34579291	0.78994087
N	2.27289502	-4.43712062	-0.88937419
H	0.52262881	0.84978380	3.90660984
H	-3.67121542	2.47249732	0.20258648
C	1.44065960	-5.21826154	-1.81014495
H	0.58981903	-5.65919175	-1.28542105
H	1.04649866	-4.60976763	-2.64145200
C	2.42355088	-6.27624740	-2.35616659
C	3.82758133	-5.64058384	-2.16189697
H	4.41643802	-6.22338139	-1.44898249
H	4.39854845	-5.58365073	-3.09085483
C	3.55490669	-4.23711470	-1.58173517
H	3.44046678	-3.53155332	-2.42534683
C	4.63654526	-3.70798811	-0.64834066
H	4.77514392	-4.38988076	0.19471291
H	5.58876387	-3.60469366	-1.17620988
C	2.40424808	4.22984291	-1.72758268
H	2.35891493	3.35135647	-2.36352382
C	1.80522518	5.38894873	0.27507884
H	1.28847157	5.43383291	1.22781602
C	2.54853243	6.49285062	-0.13380748
H	2.59970925	7.37429210	0.49773835
C	3.15267285	5.32988718	-2.14820769
H	3.67665951	5.29596587	-3.09822171
C	3.22763793	6.46840915	-1.35141139
H	3.80785464	7.32697138	-1.67293694
H	2.00954038	2.69052845	4.29587061
H	3.32981571	1.80296362	3.50110395
H	1.85677872	-0.05859252	3.18961549
H	-2.82682023	4.87318591	1.72833227
H	-3.22576069	4.82992839	-0.00512246
H	-3.13671409	2.49204511	1.88630611

H	2.34083198	-7.20464261	-1.78842416
H	2.21200057	-6.51302260	-3.40061022
H	1.83716222	-3.56025190	-0.62195673
N	-2.61197864	-0.45371116	-0.74401621
H	-3.18968104	-0.85469111	-0.00706647
C	-3.37259141	-0.46482553	-1.98781259
H	-2.75467661	-0.04127015	-2.78132845
H	-3.59870250	-1.49955058	-2.28559779
C	-4.69258542	0.32589785	-1.94819305
H	-4.47204126	1.37730844	-1.73397553
H	-5.13593005	0.29823186	-2.95181059
C	-5.73185060	-0.18456957	-0.93029043
H	-5.33427761	-0.11273449	0.08788579
H	-6.59930184	0.48697602	-0.96702258
C	-6.19667963	-1.59008485	-1.19387989
H	-6.61257492	-1.77165939	-2.18464992
C	-6.14083856	-2.59857671	-0.32822442
H	-5.73860381	-2.46779940	0.67239926
H	-6.50273923	-3.58864328	-0.58167051
N	-1.01350275	-1.45071315	1.44194128
C	-0.59300609	-1.96584087	2.74035732
H	4.37104441	-2.72342866	-0.25138913
H	-1.62636031	-2.13896852	1.00984843
H	-0.07305215	-1.17627292	3.27999305
H	-1.47622145	-2.21613928	3.34933265
C	0.32002551	-3.20331127	2.68707433
H	1.20097108	-2.97016032	2.07818682
H	0.68154138	-3.41732181	3.70028334
C	-0.36874682	-4.46432760	2.13614639
H	-0.74969553	-4.24871625	1.12913358
H	-1.23699852	-4.70848823	2.75986972
C	0.55498319	-5.64776734	2.05849391
H	1.40545318	-5.53196128	1.38755969

C 0.40276545 -6.78025936 2.73993962

H -0.43466186 -6.93267203 3.41540716

H 1.10874922 -7.59826585 2.64747869

MP2 Electronic Energy(Ha): 1740.463216692815

B3LYP Electronic Energy(Ha): 1744.985171192098

M06-L Electronic Energy(Ha): 1744.744481179492

Zero point energy correction(kcal/mol): 476.596

Enthalpy correction(kcal/mol): 505.217

Entropy correction(cal/mol): 266.044

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.234

Deuterated enthalpy correction(kcal/mol): 497.252

Deuterated entropy correction(cal/mol): 268.524

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr -0.55672692 -0.03176335 -0.62492005

C -0.54730761 2.34676096 -1.24621199

C 0.01205594 1.69979211 -2.39199082

H 1.05238168 1.72190015 -2.68078574

C -1.93907975 2.02743547 -1.27583407

H -2.67089012 2.34530609 -0.54753064

C -2.20891261 1.18475416 -2.37415830

H -3.17248805 0.79090351 -2.65513252

C -0.99476360 0.97496849 -3.06720490

H -0.87012695 0.38675421 -3.96513531

B 0.27115625 3.03556824 -0.00655476

C 0.42405222 4.64110295 -0.04499337

C -0.47450562 2.42728707 1.32446108

C 1.68791281 2.20475130 0.01625470

N 1.72066183 0.92388010 -0.17799966

N -0.88955373 1.19776225 1.34152152

O -0.66998947 3.11088823 2.46013358

O	2.88139238	2.79761033	0.19812700
C	3.13469525	0.50307651	-0.26023711
C	3.88890196	1.74634641	0.23652682
C	-1.49790635	0.89966141	2.64879959
C	-1.33165198	2.22855142	3.41526763
N	1.79194930	-3.98983046	-1.33806042
H	3.32959193	-0.38069555	0.34694229
H	-2.54482984	0.61509892	2.51887185
C	1.80001990	-5.34482022	-1.89612339
H	2.65637435	-5.91609024	-1.52851653
H	0.88600360	-5.91039517	-1.64351225
C	1.85084138	-5.09564681	-3.41749757
C	1.23223934	-3.68257358	-3.59223594
H	1.96831637	-2.98792642	-4.00393834
H	0.36680453	-3.67788991	-4.25892910
C	0.83951056	-3.22673629	-2.16537939
H	-0.19712281	-3.56471266	-1.97591408
C	0.90995468	-1.71419147	-1.92195423
H	1.93547582	-1.37636875	-2.10747221
H	0.30376249	-1.25592197	-2.71545528
C	-0.05010438	5.39149091	-1.13099511
H	-0.53730309	4.87917573	-1.95465879
C	1.04659463	5.35574593	0.99288827
H	1.42888317	4.81967036	1.85527791
C	1.18767364	6.74026676	0.95042314
H	1.67361808	7.25978088	1.77034013
C	0.08713291	6.77893885	-1.18585448
H	-0.29079990	7.32613617	-2.04374377
C	0.70769042	7.46024593	-0.14293982
H	0.81711792	8.53903829	-0.17979560
H	4.23169726	1.65458727	1.27027210
H	4.72099578	2.05404148	-0.39488874
H	3.38244238	0.25189741	-1.29626179

H	-0.69053929	2.15256742	4.29395109
H	-2.27547379	2.69619707	3.69638548
H	-0.98127692	0.06825426	3.13202386
H	2.88334717	-5.10890525	-3.77191206
H	1.30684039	-5.86670302	-3.96675755
H	1.52051884	-3.98528147	-0.36183933
N	-2.22352992	-1.28650298	-0.45114308
H	-2.02169846	-1.98927189	0.25489004
C	-3.57869724	-1.53793155	-0.93242633
H	-3.75546042	-0.95352204	-1.83517951
H	-3.68157267	-2.59219037	-1.22415724
C	-4.67973863	-1.19916404	0.08903431
H	-4.60798945	-0.13668658	0.34487713
H	-5.65495097	-1.34384665	-0.39339496
C	-4.63592597	-2.02858510	1.38800525
H	-3.68959513	-1.85812019	1.91220063
H	-5.42694774	-1.65927023	2.05331375
C	-4.83668655	-3.50261364	1.17020774
H	-5.74802245	-3.78143744	0.64173793
C	-4.00802502	-4.46515984	1.56631896
H	-3.09028949	-4.24093072	2.10292437
H	-4.21972190	-5.51233373	1.38211703
N	0.36993121	-1.65753620	0.77000186
C	1.22714499	-1.48883074	1.94643917
H	0.79442393	-1.71541680	-0.46743061
H	-0.19631926	-2.49482534	0.86662201
H	1.67764718	-0.49711608	1.89246555
H	0.61574711	-1.49086634	2.86219807
C	2.33851711	-2.54073007	2.10686531
H	2.90447007	-2.60783612	1.17119250
H	3.03918182	-2.20204881	2.87927326
C	1.82939256	-3.94033982	2.49788986
H	1.06131260	-4.26206691	1.78045106

H	1.33813390	-3.89380054	3.47643329
C	2.92413481	-4.96964283	2.52540629
H	3.44274826	-5.12915163	1.58091905
C	3.30350060	-5.66371391	3.59405631
H	2.81923322	-5.53604612	4.55782721
H	4.11024807	-6.38631979	3.54523801

MP2 Electronic Energy(Ha): 1740.427026307388

B3LYP Electronic Energy(Ha): 1744.923552766800

M06-L Electronic Energy(Ha): 1744.699653202410

Zero point energy correction(kcal/mol): 474.017

Enthalpy correction(kcal/mol): 501.958

Entropy correction(cal/mol): 260.221

Imaginary Frequencies: -1479.71

Deuterated zero point energy correction(kcal/mol): 466.302

Deuterated enthalpy correction(kcal/mol): 494.595

Deuterated entropy correction(cal/mol): 262.268

Deuterated imaginary Frequencies: -1077.89

Product geometry

Zr	-0.88545606	0.14919686	0.21347337
C	-1.38985003	-2.25545993	-0.01055292
C	-2.15823647	-1.84657375	1.12273789
H	-1.93638130	-2.09005392	2.15100391
C	-2.04230685	-1.67429017	-1.13782607
H	-1.71819911	-1.76580265	-2.16444100
C	-3.14607086	-0.90745698	-0.70069350
H	-3.83291746	-0.36367849	-1.32878556
C	-3.21405655	-1.00728725	0.70778117
H	-3.94529154	-0.53279183	1.34566483
B	0.08935928	-2.95549408	0.02099579
C	0.13368147	-4.55562117	-0.18824658
C	0.97486073	-2.09302675	-1.05803820
C	0.71504297	-2.41833442	1.44018115

N	0.61981152	-1.17675951	1.79502522
N	0.86187190	-0.80455569	-1.14826926
O	1.89466411	-2.64812246	-1.86649634
O	1.28671702	-3.24537710	2.33670711
C	1.10771809	-1.05456857	3.18357267
C	1.71710215	-2.43939603	3.46732490
C	1.82417619	-0.30295972	-2.14371164
C	2.48110199	-1.59259019	-2.67784147
N	-1.43962405	3.57091847	1.35632921
H	1.84484698	-0.25651227	3.28075734
H	1.30866183	0.25952885	-2.92559526
C	-1.92176360	4.89428700	1.77153652
H	-1.33592477	5.69293107	1.30847416
H	-2.97746339	5.04904188	1.49425103
C	-1.78692038	4.85650093	3.30292146
C	-1.96893005	3.35772271	3.65991500
H	-1.11850928	2.98917093	4.23844305
H	-2.86586623	3.17789833	4.25690545
C	-2.05118896	2.59860600	2.30437080
H	-3.11908247	2.47976145	2.05174040
C	-1.38135119	1.22468623	2.26800448
H	-0.40893535	1.32063921	2.77395162
H	-1.96835488	0.54543111	2.89832972
C	-1.03524275	-5.29336215	-0.42569413
H	-1.98776420	-4.77441526	-0.46510865
C	1.33778130	-5.27935627	-0.14392690
H	2.26947482	-4.75369042	0.03893076
C	1.37485634	-6.65901993	-0.32687379
H	2.32351217	-7.18518739	-0.28511437
C	-1.01143122	-6.67631699	-0.61065181
H	-1.93722858	-7.21353364	-0.79152884
C	0.19627260	-7.36618703	-0.56219283
H	0.22106535	-8.44153344	-0.70472632

H	2.80965154	-2.43478147	3.47652677
H	1.35182457	-2.91388788	4.37767587
H	0.27221524	-0.81584886	3.84822170
H	3.56240237	-1.62800999	-2.54363106
H	2.24074206	-1.80299729	-3.72103280
H	2.55269325	0.36521532	-1.67276820
H	-0.79398561	5.20256010	3.60033893
H	-2.51686100	5.50666020	3.78984134
H	-1.75079763	3.33725949	0.41671215
N	-1.43786605	1.64780501	-1.20225898
H	-0.72384515	2.36541819	-1.29291782
C	-2.48782122	1.98603146	-2.16590060
H	-3.42333885	1.51832178	-1.85807241
H	-2.67635159	3.06914333	-2.14704939
C	-2.19623889	1.57230818	-3.61943114
H	-2.03544336	0.49008570	-3.65320542
H	-3.08893129	1.77906118	-4.22433317
C	-0.98488014	2.27596477	-4.26081375
H	-0.07816041	2.05348912	-3.68858628
H	-0.83278240	1.84962623	-5.26080764
C	-1.14634095	3.76494157	-4.39121163
H	-2.03832638	4.09816332	-4.92131231
C	-0.30090616	4.68094528	-3.92593990
H	0.60647508	4.40112838	-3.39764046
H	-0.47350498	5.74204452	-4.06622924
N	0.88607742	1.88227737	0.41171673
C	2.10847407	1.76727710	1.23496147
H	0.31172053	2.66275182	0.77287822
H	1.15567167	2.12231247	-0.53913070
H	1.78339629	1.58896787	2.25943793
H	2.65694967	0.87687870	0.91457668
C	3.01878921	3.00240624	1.21199478
H	2.44212394	3.87709739	1.53470850

H 3.80741966 2.85953188 1.95883531

C 3.67912625 3.29065108 -0.14844658

H 2.90063363 3.43533681 -0.91030341

H 4.27328151 2.42463353 -0.46169916

C 4.54908706 4.51649902 -0.12190836

H 4.04403733 5.44835637 0.12889457

C 5.85602849 4.53583937 -0.36364626

H 6.40214561 3.63153771 -0.61568302

H 6.42842808 5.45537602 -0.32132356

MP2 Electronic Energy(Ha): 1740.473269771673

B3LYP Electronic Energy(Ha): 1744.967447157475

M06-L Electronic Energy(Ha): 1744.745729009920

Zero point energy correction(kcal/mol): 477.887

Enthalpy correction(kcal/mol): 505.928

Entropy correction(cal/mol): 260.185

Imaginary Frequencies:

Deuterated zero point energy correction(kcal/mol): 469.051

Deuterated enthalpy correction(kcal/mol): 497.452

Deuterated entropy correction(cal/mol): 262.261

Deuterated imaginary Frequencies: -0.00

Axial Reaction C1-S

Reactant geometry

Zr 0.29924511 -0.30025993 -0.15463732

C -0.40268172 -2.42099319 -1.22727915

C -1.49058569 -1.54660544 -1.53071256

H -2.47935203 -1.60837202 -1.09726682

C 0.69492808 -1.94182083 -2.01018839

H 1.68879853 -2.36451959 -2.01507487

C 0.31804613 -0.76384583 -2.69310022

H 0.94401207 -0.16360753 -3.33667833

C -1.05046562 -0.52131936 -2.39296301

H	-1.64130635	0.29759904	-2.77547392
B	-0.32644684	-3.47687441	0.02034008
C	-0.77005735	-4.99865779	-0.28104695
C	1.18309065	-3.28826096	0.64218833
C	-1.16843274	-2.72085799	1.22571086
N	-0.96918295	-1.46353586	1.48187384
N	1.76123627	-2.13018321	0.70657838
O	1.83322127	-4.29961256	1.24858950
O	-2.07649215	-3.32597502	2.00549149
C	-1.86455123	-1.03742189	2.57014096
C	-2.55033313	-2.35531575	2.98568673
C	2.98295501	-2.26110251	1.52469874
C	3.09742748	-3.78049689	1.74579377
N	2.00044089	0.91323096	0.11541129
H	-1.29321871	-0.58850883	3.38650887
C	3.45459712	0.81446396	0.18198817
H	3.78533207	0.66922025	1.22339753
H	3.78490547	-0.07759174	-0.36368181
C	4.22614821	2.02889665	-0.36042626
C	4.29028575	2.19976525	-1.88967329
H	5.04356246	2.97391675	-2.09287670
H	4.67089616	1.28055724	-2.34928043
C	3.01746681	2.61700794	-2.57359600
H	2.44739270	3.40315359	-2.08018341
C	2.58508036	2.15133082	-3.74221709
H	3.12135757	1.37348021	-4.27819699
C	-1.15112131	-5.39882332	-1.57045030
H	-1.14800759	-4.66656225	-2.37165906
C	-0.79446262	-5.98675527	0.71857374
H	-0.50608482	-5.72741361	1.73167762
C	-1.17651550	-7.29805591	0.44788613
H	-1.18348280	-8.03491325	1.24510934
C	-1.53541777	-6.70978151	-1.85430910

H	-1.82388268	-6.98179749	-2.86484200
C	-1.54993651	-7.66685290	-0.84394760
H	-1.84839733	-8.68777937	-1.05826673
H	2.86293806	-1.70620911	2.46110834
H	3.85028548	-1.85247818	1.00679527
H	3.19628950	-4.07817647	2.78950507
H	3.89773660	-4.24040614	1.16220986
H	-2.56743300	-0.28637975	2.20187659
H	-2.24885462	-2.71081629	3.97241285
H	-3.63830431	-2.32989831	2.92848393
H	3.81541368	2.94212391	0.09216450
H	5.25686373	1.95462454	0.00602532
H	1.72627556	1.89196255	0.10391253
H	1.68288484	2.53191099	-4.20729329
N	-0.93282430	1.34564375	0.16807558
H	-0.53800669	1.98069915	0.87104740
C	-2.25038693	1.83506010	-0.20871828
H	-2.76186423	1.07501482	-0.80758485
H	-2.87850414	1.98975197	0.68399414
C	-2.21290718	3.15238828	-1.00095789
H	-1.61848060	2.99856233	-1.90859355
H	-1.68775482	3.91021571	-0.40970810
C	-3.61344490	3.67505205	-1.36779841
H	-4.20313109	3.82859279	-0.45712815
H	-4.13444747	2.90431046	-1.95242536
C	-3.57469450	4.94989548	-2.16160845
H	-3.05703867	4.89544623	-3.11883461
C	-4.10277212	6.11114300	-1.78350115
H	-4.63043469	6.21415990	-0.83967022
H	-4.03487510	6.99750590	-2.40430710
N	0.36428056	3.34798803	2.49125166
H	1.32751679	3.02333040	2.50983982
H	-0.07910046	2.97234626	3.32420894

C	0.31732586	4.81983298	2.51048812
H	-0.73346009	5.12070023	2.54074305
H	0.79638732	5.25446956	3.40248747
C	0.97751985	5.39915493	1.26032640
H	0.50592317	4.95779309	0.37596411
H	2.03141053	5.09505727	1.23754182
C	0.90394390	6.93601693	1.17930624
H	1.36249151	7.38165808	2.06925621
H	1.50783662	7.25956536	0.32243657
C	-0.49523451	7.46227500	1.01106993
H	-1.04077059	7.08525442	0.14647348
C	-1.09380461	8.33332179	1.81841953
H	-0.59153835	8.73793587	2.69243472
H	-2.10389093	8.68014846	1.63151881

MP2 Electronic Energy(Ha): 1740.440482402094

B3LYP Electronic Energy(Ha): 1744.968908877737

M06-L Electronic Energy(Ha): 1744.726407821124

Zero point energy correction(kcal/mol): 472.883

Enthalpy correction(kcal/mol): 497.740

Entropy correction(cal/mol): 235.997

Imaginary Frequencies: -49.73 -47.82 -46.23 -45.31 -39.01 -35.89 -32.79 -7.40

Deuterated zero point energy correction(kcal/mol): 464.455

Deuterated enthalpy correction(kcal/mol): 489.703

Deuterated entropy correction(cal/mol): 238.559

Deuterated imaginary Frequencies: -49.69 -47.78 -46.21 -45.28 -38.87 -35.83 -32.56 -7.34

Transition State geometry

Zr	-0.01012829	0.16794712	0.47352366
C	-1.34832619	2.24803670	0.56005562
C	-2.24313217	1.31134115	-0.04053621
H	-2.53091077	1.29740593	-1.08170309
C	-1.26384726	1.86157690	1.93322519
H	-0.66389308	2.35045865	2.68626758

C	-2.04811957	0.71081736	2.15513271
H	-2.16571293	0.18580106	3.09217061
C	-2.66185409	0.37286181	0.92975621
H	-3.34276967	-0.44906951	0.77751249
B	-0.41000638	3.35505261	-0.18908361
C	-1.05031049	4.82414758	-0.39470201
C	0.97826372	3.31787414	0.69077010
C	0.07626583	2.61140974	-1.56278911
N	0.27558303	1.33365468	-1.58120477
N	1.50967257	2.20755330	1.09680814
O	1.60220781	4.44731315	1.08317927
O	0.39270925	3.25924580	-2.69913917
C	0.84336541	0.94364183	-2.88002476
C	0.82713545	2.26661876	-3.67347877
C	2.63709429	2.54261078	1.99077476
C	2.79995118	4.06089197	1.80637629
N	1.95034333	-0.76869622	-0.12039039
H	1.84998602	0.54160393	-2.74055233
C	3.33347265	-0.33544882	-0.18452118
H	3.75886600	-0.49731605	-1.18538230
H	3.38996590	0.73842155	0.00545181
C	4.15194122	-1.10731252	0.86791819
C	3.33253898	-1.09182324	2.16090338
H	3.72770787	-1.82039192	2.87920681
H	3.39312421	-0.11364762	2.64421849
C	1.88425124	-1.44220073	1.92328140
H	1.71150920	-2.45601488	1.57510837
C	0.82890161	-0.82087203	2.60257724
H	1.05356989	0.00278060	3.27369056
C	-2.34459695	5.12371931	0.05538443
H	-2.92065935	4.35166175	0.55556999
C	-0.35005017	5.86132631	-1.03513941
H	0.65408135	5.67800077	-1.40262881

C	-0.90854329	7.12377649	-1.21711431
H	-0.33811490	7.90060864	-1.71697678
C	-2.91511938	6.38504668	-0.12060785
H	-3.92004827	6.57911567	0.24137158
C	-2.19803227	7.39242024	-0.75935503
H	-2.63655355	8.37495638	-0.89992946
H	3.54175893	1.99645417	1.72003718
H	2.38365646	2.27363652	3.02244127
H	3.66305698	4.32671740	1.19091210
H	2.83232071	4.62770560	2.73633852
H	0.23170991	0.16645565	-3.34480785
H	1.80355551	2.57346218	-4.04904239
H	0.10759001	2.27192539	-4.49399018
H	4.28918210	-2.14175843	0.53139872
H	5.14982854	-0.68148601	1.01735152
H	1.86456786	-1.66818725	-0.58946121
H	-0.04114081	-1.41612304	2.85701143
N	-0.70715232	-1.64714155	-0.31404972
H	0.07136231	-2.24076138	-0.59304422
C	-1.93078405	-2.37463792	-0.63043756
H	-2.75128665	-1.67041879	-0.78867605
H	-1.81308516	-2.91114787	-1.58449562
C	-2.34102233	-3.39117644	0.44829157
H	-2.47277717	-2.85923561	1.39719287
H	-1.52104296	-4.10118922	0.60428037
C	-3.62569244	-4.16212827	0.09649969
H	-3.49136276	-4.70113006	-0.84789651
H	-4.43490419	-3.43734567	-0.06881740
C	-4.04359113	-5.12551954	1.17069068
H	-4.23571040	-4.68686206	2.14943586
C	-4.18156697	-6.43985245	1.01874892
H	-4.00500289	-6.92112279	0.06114625
H	-4.48289350	-7.08065940	1.83982376

N	1.68218863	-3.57471176	-2.01810379
H	2.67745884	-3.49784849	-2.21219406
H	1.20748251	-3.12005679	-2.79278926
C	1.29780156	-4.99701753	-1.95346679
H	0.20990119	-5.04650538	-1.86135424
H	1.56258702	-5.55000176	-2.86813882
C	1.94602017	-5.68153519	-0.75135036
H	1.63794315	-5.16092751	0.16182224
H	3.03542694	-5.57239041	-0.81987367
C	1.60618560	-7.18028259	-0.64113781
H	1.92384716	-7.70285281	-1.55036881
H	2.19555510	-7.60173607	0.18253324
C	0.14937074	-7.45257103	-0.38405762
H	-0.26952648	-6.98942105	0.50872286
C	-0.64056513	-8.20335287	-1.14641040
H	-0.27156751	-8.68771938	-2.04590569
H	-1.68169276	-8.36839299	-0.89379624

MP2 Electronic Energy(Ha): 1740.438251626199

B3LYP Electronic Energy(Ha): 1744.945669230568

M06-L Electronic Energy(Ha): 1744.721280178398

Zero point energy correction(kcal/mol): 474.372

Enthalpy correction(kcal/mol): 499.363

Entropy correction(cal/mol): 232.424

Imaginary Frequencies: -289.31 -37.26 -33.61 -29.76 -26.68 -13.67

Deuterated zero point energy correction(kcal/mol): 465.778

Deuterated enthalpy correction(kcal/mol): 491.150

Deuterated entropy correction(cal/mol): 234.846

Deuterated imaginary Frequencies: -288.29 -37.21 -33.46 -29.72 -26.64 -13.57

Product geometry

Zr	-0.05151496	0.13940466	0.57103671
C	-1.29941820	2.25654140	0.76148459
C	-2.27014677	1.32652071	0.27886499

H	-2.67050296	1.30466655	-0.72521310
C	-1.06501844	1.88245970	2.12138341
H	-0.36924969	2.36274739	2.79309771
C	-1.81856406	0.73433110	2.44139394
H	-1.82603400	0.21569633	3.38883630
C	-2.57534932	0.39222406	1.29564163
H	-3.26929411	-0.43066994	1.22696864
B	-0.39481156	3.30436026	-0.11666884
C	-0.99063979	4.79346417	-0.30499166
C	1.06861262	3.23174680	0.62848733
C	-0.07474313	2.50948173	-1.51726405
N	0.21726334	1.24745881	-1.51933187
N	1.60697414	2.10497864	0.96999012
O	1.74141306	4.34177714	0.99781865
O	-0.05373213	3.10502676	-2.72355292
C	0.48261801	0.80738802	-2.89708325
C	0.30993805	2.10426664	-3.71613353
C	2.79555306	2.39800553	1.79513081
C	2.98497361	3.91339474	1.61435067
N	2.00585507	-1.04137974	-0.01122699
H	1.49121801	0.39276567	-2.97999210
C	3.29629330	-0.47296189	-0.47165501
H	3.40934669	-0.63209733	-1.54700488
H	3.30431523	0.60314685	-0.29638443
C	4.36837181	-1.18537671	0.36687275
C	3.68658562	-1.31951880	1.73650531
H	4.10042731	-2.12683326	2.34437747
H	3.80219845	-0.39439464	2.30727529
C	2.18852039	-1.55282989	1.42958951
H	1.98715148	-2.62800667	1.39264697
C	1.15833256	-0.84909804	2.30833416
H	1.61911689	-0.12944372	2.99132370
C	-2.23052127	5.15839191	0.23943080

H	-2.79656304	4.42195418	0.80103329
C	-0.29961650	5.78701972	-1.01992925
H	0.66483648	5.55373039	-1.45959819
C	-0.81502770	7.06986801	-1.18407654
H	-0.25268839	7.81187669	-1.74256981
C	-2.75806241	6.44079373	0.08234798
H	-3.72119763	6.68634086	0.51892583
C	-2.05125713	7.40371387	-0.63189477
H	-2.45631676	8.40250664	-0.75739961
H	3.66748076	1.83059933	1.46545236
H	2.59721286	2.12167199	2.83624631
H	3.80061889	4.16334793	0.93078287
H	3.11092048	4.46799499	2.54362011
H	-0.22708253	0.02654005	-3.18326805
H	1.22564669	2.43899584	-4.20565324
H	-0.49418571	2.05713629	-4.45125386
H	4.57898738	-2.17360125	-0.05579664
H	5.31122795	-0.63363525	0.40494670
H	1.81325618	-1.84542740	-0.61360266
H	0.57461162	-1.55233123	2.90740057
N	-0.84415778	-1.60399891	-0.31064378
H	-0.11174595	-2.23951440	-0.61653427
C	-2.12583076	-2.21344087	-0.64417913
H	-2.90242287	-1.44399906	-0.65301060
H	-2.10363478	-2.62186783	-1.66748100
C	-2.54828805	-3.33833786	0.31615607
H	-2.57763684	-2.93367529	1.33387402
H	-1.78134268	-4.12114404	0.31877510
C	-3.90970611	-3.95971007	-0.04391586
H	-3.87561337	-4.37558418	-1.05713690
H	-4.66506891	-3.16165447	-0.05889542
C	-4.34491644	-5.02424856	0.92250878
H	-4.44213979	-4.70736911	1.96046723

C	-4.60486637	-6.29155491	0.61203211
H	-4.52480281	-6.65375886	-0.40885534
H	-4.91493154	-7.01009757	1.36259076
N	1.66469260	-3.43807749	-2.13218940
H	2.60667639	-3.42183214	-2.51595117
H	1.06638250	-3.01789827	-2.83828365
C	1.25281243	-4.83685898	-1.89661593
H	0.21108913	-4.82758315	-1.56701816
H	1.28970843	-5.44468385	-2.81328845
C	2.12384155	-5.49185992	-0.82658564
H	2.07008759	-4.89479340	0.09025996
H	3.17156903	-5.47183466	-1.15129319
C	1.72572449	-6.94974208	-0.52409762
H	1.78521427	-7.55083485	-1.43830417
H	2.46477211	-7.36545057	0.17159187
C	0.35493586	-7.08109694	0.08117279
H	0.19599289	-6.53832244	1.01244775
C	-0.64930147	-7.78996335	-0.42664686
H	-0.53953915	-8.34862977	-1.35188934
H	-1.61429171	-7.83811518	0.06458969

MP2 Electronic Energy(Ha): 1740.470453882787

B3LYP Electronic Energy(Ha): 1744.971738414957

M06-L Electronic Energy(Ha): 1744.744828605455

Zero point energy correction(kcal/mol): 476.984

Enthalpy correction(kcal/mol): 505.383

Entropy correction(cal/mol): 262.592

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.264

Deuterated enthalpy correction(kcal/mol): 497.019

Deuterated entropy correction(cal/mol): 264.909

Deuterated imaginary Frequencies: -0.00

Axial Reaction H6-S

Reactant geometry

Zr	1.29002629	0.92823525	-0.64993762
C	2.94207830	-0.69361241	0.22678065
C	3.56908980	-0.15187019	-0.93909296
H	3.71908852	-0.67915222	-1.87106572
C	2.96869010	0.36560791	1.18472919
H	2.56549694	0.31192541	2.18645023
C	3.50877267	1.53803765	0.59877407
H	3.65916091	2.49149761	1.08478141
C	3.88766663	1.21302567	-0.73091673
H	4.37517554	1.87577911	-1.43140506
B	1.89964565	-1.96932540	0.24958792
C	2.47933499	-3.38155787	0.77355549
C	0.56127063	-1.42556464	1.08410180
C	1.26542138	-2.02788278	-1.29135590
N	0.91318825	-0.95391374	-1.94424116
N	0.07696430	-0.22042542	0.93881929
O	-0.13298654	-2.21256275	1.90442006
O	1.03409461	-3.17502682	-1.93595024
C	0.34673625	-1.33020799	-3.25202392
C	0.48337635	-2.86657123	-3.25328769
C	-1.12254481	-0.06563685	1.78549349
C	-1.30311723	-1.47195764	2.38211434
N	0.44424835	2.44919740	-1.34942781
N	-1.31386497	4.33305555	1.36221445
C	-2.75982002	4.23067217	1.15993891
H	-3.12212927	3.18896802	1.22019751
H	-0.69082045	-0.99481728	-3.32826787
H	-0.94696630	0.70168896	2.54389390
C	0.04934541	3.69817940	-1.94082931
H	0.02789787	3.60896872	-3.03899464
H	-0.97912754	3.95136619	-1.64554825

C	0.97126211	4.86930372	-1.56384163
C	-3.33645741	5.05034888	2.33457549
C	-2.21579793	5.02466522	3.41004328
H	-2.55729637	4.62857203	4.36888658
H	-3.04485223	4.62524650	0.18207871
C	-1.10018957	4.14831308	2.80082144
H	-1.29035083	3.09831840	3.09939787
H	-1.83265095	6.03252056	3.58922348
C	0.31353536	4.52356875	3.22831990
H	0.43844227	4.40872871	4.30900839
H	-0.79113005	3.67047309	0.79491094
H	0.52475690	5.56198016	2.96028609
C	1.69275457	-4.54400144	0.84983253
H	0.64955225	-4.50439676	0.55519344
C	3.81844192	-3.49934555	1.17401911
H	4.45871491	-2.62420070	1.13087674
C	2.21215865	-5.75513544	1.29900336
H	1.57535420	-6.63297871	1.34527845
C	4.35026695	-4.70744414	1.62585492
H	5.39147523	-4.76017308	1.92758517
C	3.54766278	-5.84255241	1.68990356
H	3.95552617	-6.78474126	2.04052453
C	0.52455995	6.22493819	-2.14262279
H	0.49542847	6.18217429	-3.23773692
H	1.28717868	6.97084235	-1.88173562
C	-0.80384076	6.69568106	-1.61556042
H	-0.91747088	6.65237742	-0.53306133
C	-1.81602554	7.13845790	-2.35733893
H	-1.75258154	7.18233260	-3.44107539
H	-2.74313813	7.47910405	-1.90931336
H	1.18547364	-3.24389135	-3.99689863
H	0.90791772	-0.85694182	-4.06049368
H	-0.46356335	-3.39751078	-3.34692830

H	-2.18632801	-1.97525212	1.99172424
H	-1.28851150	-1.50734691	3.47068296
H	-1.98111329	0.22786845	1.18118170
H	-3.54324456	6.07537588	2.02157529
H	-4.27480219	4.62510946	2.69655982
H	1.01467635	4.93929377	-0.47211907
H	1.98590155	4.64133669	-1.90739364
H	1.05709318	3.88880521	2.73705658
N	-3.14942630	-1.48426928	-0.63739626
H	-2.39960238	-1.02408019	-1.14524471
H	-3.98318356	-0.92392410	-0.79321477
C	-3.35981025	-2.84628092	-1.15376165
H	-3.61001766	-2.86898832	-2.22715588
H	-2.42020053	-3.39632174	-1.03474155
C	-4.46307000	-3.55953701	-0.37306753
H	-5.39775548	-2.99251852	-0.46216596
H	-4.19936324	-3.55914648	0.68985620
C	-4.70420499	-5.00089978	-0.85393976
H	-3.76013409	-5.55714759	-0.77860752
H	-4.98485088	-4.99923854	-1.91285997
C	-5.75958787	-5.71339964	-0.05542583
C	-6.89760104	-6.19629804	-0.54434434
H	-7.14506418	-6.11158948	-1.59852822
H	-7.62160521	-6.69774918	0.08779395
H	-5.55451311	-5.82238629	1.00886587

MP2 Electronic Energy(Ha): 1740.426208404227

B3LYP Electronic Energy(Ha): 1744.948606537377

M06-L Electronic Energy(Ha): 1744.700095650011

Zero point energy correction(kcal/mol): 475.739

Enthalpy correction(kcal/mol): 505.212

Entropy correction(cal/mol): 278.665

Imaginary Frequencies:

Deuterated zero point energy correction(kcal/mol): 467.263

Deuterated enthalpy correction(kcal/mol): 497.075

Deuterated entropy correction(cal/mol): 281.110

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	1.04901858	1.30962481	0.03926914
C	2.84955278	-0.35676141	0.36727885
C	3.31815867	0.53909925	-0.65019503
H	3.41725759	0.29918836	-1.69967934
C	2.89991619	0.39522945	1.57554923
H	2.58673855	0.03710811	2.54637707
C	3.30304482	1.72491751	1.30020016
H	3.41324951	2.52363172	2.02017715
C	3.57676974	1.81273774	-0.08902042
H	3.93892217	2.68487738	-0.61332355
B	1.98668586	-1.73837590	0.12952362
C	2.79358205	-3.13019325	0.23991592
C	0.68268386	-1.59408263	1.14140371
C	1.23943027	-1.48663784	-1.32127189
N	0.65966998	-0.35151751	-1.57228160
N	0.02024818	-0.48206223	1.27103445
O	0.21428777	-2.62628067	1.85327983
O	1.17805947	-2.38754949	-2.31011440
C	0.13067711	-0.35864486	-2.94691332
C	0.41574319	-1.80280814	-3.41054999
C	-1.08563115	-0.68715529	2.22858738
C	-0.98460956	-2.18563342	2.56303705
N	0.31243684	2.79448886	-0.95139009
N	-2.07788658	4.06005439	1.18613525
C	-3.39349041	4.39908003	1.73353341
H	-4.14315339	3.60956602	1.54837270
H	-0.93328887	-0.11227763	-2.95484210
H	-0.95134071	-0.04601093	3.10366643

C	-0.01011594	3.97059741	-1.72123472
H	0.38859213	3.84366693	-2.73818595
H	-1.09853221	4.07437827	-1.84236824
C	0.54713745	5.27651005	-1.13202508
C	-3.12350925	4.51200891	3.24706185
C	-1.88945942	3.60011521	3.48317962
H	-2.08948616	2.79524289	4.19438463
H	-3.77297688	5.32646021	1.29733587
C	-1.52267270	3.03403015	2.08781659
H	-2.06577950	2.07930687	1.95897010
H	-1.04974222	4.17937183	3.87362385
C	-0.03163131	2.78699952	1.85647415
H	0.30878530	2.02834653	2.57045746
H	-2.14092788	3.72044210	0.23188159
H	0.53033928	3.69722547	2.09460499
C	2.16337237	-4.37688038	0.08495211
H	1.09429693	-4.41603369	-0.09732054
C	4.17521862	-3.14892298	0.48085474
H	4.70081858	-2.20781016	0.60762851
C	2.86988750	-5.57389132	0.16451707
H	2.35012155	-6.51878416	0.04050154
C	4.89459761	-4.34162756	0.56220271
H	5.96343115	-4.31644397	0.74938228
C	4.24350467	-5.56135499	0.40356224
H	4.79754147	-6.49206675	0.46572253
C	0.29105169	6.50681773	-2.02391840
H	0.74695462	6.35799675	-3.00961623
H	0.80226540	7.36556048	-1.57000093
C	-1.16431932	6.84772868	-2.18761376
H	-1.71597614	7.00381346	-1.26097306
C	-1.80445641	6.97280546	-3.34710665
H	-1.29599967	6.82448201	-4.29549858
H	-2.85611946	7.23320255	-3.39305833

H	1.02850692	-1.86965136	-4.30884536
H	0.64731120	0.39119576	-3.55157198
H	-0.48450269	-2.40498990	-3.54204653
H	-1.82575711	-2.75488390	2.16978187
H	-0.83850628	-2.40239134	3.62099864
H	-2.04259263	-0.44731249	1.76325074
H	-2.89176785	5.54442762	3.51547915
H	-3.99326269	4.20898722	3.83352975
H	0.09852517	5.43734652	-0.14634513
H	1.62534235	5.15893660	-0.98139855
H	0.04254370	2.94110054	0.37981886
N	-2.87952219	-1.97809701	-0.37030783
H	-2.04519845	-1.51074712	-0.71273616
H	-3.66881399	-1.38857388	-0.61937123
C	-3.02489908	-3.30501176	-0.98814422
H	-3.14952371	-3.26475904	-2.08293581
H	-2.10254762	-3.86280982	-0.79700669
C	-4.20708910	-4.06011239	-0.38100277
H	-5.12916898	-3.48869721	-0.54379951
H	-4.06566143	-4.11735403	0.70348165
C	-4.38305096	-5.47269421	-0.96457211
H	-3.44596676	-6.02795309	-0.82322991
H	-4.55242034	-5.41298924	-2.04522416
C	-5.50704752	-6.23446236	-0.32017828
C	-6.58185693	-6.69955611	-0.94938543
H	-6.72000030	-6.56087496	-2.01774685
H	-7.36056943	-7.23977469	-0.42294616
H	-5.41247139	-6.39868718	0.75263667

MP2 Electronic Energy(Ha): 1740.389942389490

B3LYP Electronic Energy(Ha): 1744.898860420873

M06-L Electronic Energy(Ha): 1744.659668191243

Zero point energy correction(kcal/mol): 473.818

Enthalpy correction(kcal/mol): 502.080

Entropy correction(cal/mol): 259.135

Imaginary Frequencies: -1549.21

Deuterated zero point energy correction(kcal/mol): 466.089

Deuterated enthalpy correction(kcal/mol): 494.673

Deuterated entropy correction(cal/mol): 261.256

Deuterated imaginary Frequencies: -1134.50

Product geometry

Zr	1.27732220	0.91861706	-0.66508860
C	2.94202454	-0.69885043	0.19604220
C	3.55236363	-0.16267422	-0.98120786
H	3.68938547	-0.69450754	-1.91261310
C	2.98197636	0.36501013	1.14836641
H	2.59303486	0.31615866	2.15594638
C	3.51336888	1.53468553	0.54911926
H	3.67050351	2.49048098	1.02838374
C	3.87345806	1.20329012	-0.78424201
H	4.35088264	1.86269477	-1.49477347
B	1.90017140	-1.97452500	0.23964640
C	2.48699197	-3.38427001	0.76234527
C	0.57330173	-1.42689702	1.08980415
C	1.24489734	-2.04060290	-1.29218254
N	0.88246271	-0.96984031	-1.94482175
N	0.08734115	-0.22225409	0.94625462
O	-0.11043749	-2.21057292	1.92220150
O	1.00683291	-3.19071781	-1.92886237
C	0.29934570	-1.35247326	-3.24342816
C	0.43869588	-2.88857530	-3.24026244
C	-1.10038980	-0.06353608	1.80870226
C	-1.27481689	-1.46820241	2.41091028
N	0.41949710	2.43504129	-1.35982010
N	-1.27388255	4.32915673	1.38149502
C	-2.72435051	4.20365356	1.23049233

H	-3.06809905	3.15680828	1.30748788
H	-0.73978309	-1.01934230	-3.30721786
H	-0.91307291	0.70515919	2.56292840
C	0.01200654	3.67931644	-1.95254863
H	-0.03279668	3.58139328	-3.04925748
H	-1.00992980	3.93499823	-1.63743392
C	0.94159555	4.85332210	-1.60460444
C	-3.27332040	5.01971924	2.42108597
C	-2.11341084	5.02367428	3.45427448
H	-2.41261359	4.63324289	4.42943421
H	-3.04951403	4.58920197	0.26157238
C	-1.00730017	4.15860369	2.81305081
H	-1.17160691	3.10833796	3.12579204
H	-1.73999909	6.03937422	3.60797391
C	0.41473106	4.55761654	3.18821491
H	0.57856805	4.45353107	4.26477624
H	-0.76152399	3.66974622	0.80112102
H	0.60124008	5.59674864	2.90504662
C	1.70143981	-4.54625163	0.85468359
H	0.65430349	-4.50785868	0.57416242
C	3.83142850	-3.50035024	1.14506353
H	4.47111888	-2.62549555	1.08914212
C	2.22688030	-5.75538233	1.30222083
H	1.59072142	-6.63293630	1.36112875
C	4.36929149	-4.70643190	1.59514811
H	5.41450505	-4.75790140	1.88292567
C	3.56758775	-5.84115410	1.67526892
H	3.98016085	-6.78178699	2.02455276
C	0.48207182	6.20446541	-2.18379642
H	0.43074405	6.15391539	-3.27776460
H	1.24918207	6.95277534	-1.94377400
C	-0.83590937	6.67775509	-1.63327104
H	-0.92831644	6.64057518	-0.54851760

C	-1.86269754	7.11586354	-2.35750588
H	-1.82054637	7.15362843	-3.44250481
H	-2.78105599	7.45852695	-1.89330385
H	1.13191904	-3.26767346	-3.99126667
H	0.84882306	-0.88153795	-4.06122953
H	-0.50842031	-3.42149426	-3.31958372
H	-2.16264941	-1.97241576	2.03215401
H	-1.24836771	-1.50088273	3.49932564
H	-1.96661920	0.22969697	1.21540211
H	-3.51309123	6.03822396	2.11038598
H	-4.18843550	4.57755468	2.82036577
H	1.00870291	4.93165973	-0.51464066
H	1.94863127	4.62286259	-1.96826461
H	1.15006187	3.92961787	2.67639619
N	-3.15355015	-1.45072262	-0.60506829
H	-2.40189993	-0.99441333	-1.11370902
H	-3.98326241	-0.88286178	-0.75516960
C	-3.37705915	-2.80859142	-1.12651598
H	-3.63020801	-2.82476104	-2.19938110
H	-2.44195228	-3.36730389	-1.01212393
C	-4.48453048	-3.51555427	-0.34609871
H	-5.41454431	-2.94026102	-0.43090912
H	-4.21848015	-3.52145453	0.71622472
C	-4.73889837	-4.95286346	-0.83220243
H	-3.79955114	-5.51756072	-0.76059907
H	-5.02117498	-4.94454914	-1.89066100
C	-5.79916432	-5.65945363	-0.03493158
C	-6.94169130	-6.13116900	-0.52423369
H	-7.18964697	-6.04057856	-1.57781189
H	-7.66909018	-6.62892085	0.10692817
H	-5.59372954	-5.77396660	1.02870702

MP2 Electronic Energy(Ha): 1740.426294524385

B3LYP Electronic Energy(Ha): 1744.948626031205

M06-L Electronic Energy(Ha): 1744.700187819691

Zero point energy correction(kcal/mol): 475.738

Enthalpy correction(kcal/mol): 505.213

Entropy correction(cal/mol): 278.671

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.262

Deuterated enthalpy correction(kcal/mol): 497.075

Deuterated entropy correction(cal/mol): 281.115

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction C1

Reactant geometry

Zr	1.11100620	0.63183704	-0.16614800
C	1.40230074	-1.83695086	-0.16841817
C	2.07727665	-1.50138057	-1.38364905
H	1.69493436	-1.67175109	-2.37989611
C	2.27994855	-1.41273092	0.87878995
H	2.09783511	-1.52987176	1.93676821
C	3.41198931	-0.78250456	0.32125205
H	4.24790045	-0.36598567	0.86548751
C	3.28562535	-0.84796720	-1.08842239
H	3.99696802	-0.46432969	-1.80714876
B	-0.14556913	-2.34074901	-0.02116917
C	-0.41125032	-3.93268379	-0.07196424
C	-0.65125174	-1.59620042	1.35421608
C	-0.93295864	-1.47553980	-1.17842610
N	-0.56568912	-0.26369602	-1.47194170
N	-0.28665784	-0.38456112	1.63084712
O	-1.43469532	-2.19184028	2.27256707
O	-2.00726569	-1.91626981	-1.84563331
C	-1.47460827	0.30130386	-2.48261775
C	-2.42181625	-0.87805469	-2.78359518

C	-0.78669034	-0.03476152	2.97291954
C	-1.71745838	-1.21322345	3.31317638
N	2.14961423	1.95801732	-1.43536740
H	-1.99332650	1.17181916	-2.07756187
C	2.15848126	3.39550863	-1.66762835
H	2.35666116	3.61135933	-2.72681740
H	1.16395029	3.80656878	-1.46692398
C	3.20057602	4.15017180	-0.82108011
C	2.99818282	4.03530858	0.70158953
H	3.70376071	4.72647960	1.18239001
H	1.99828509	4.38237975	0.98419129
C	3.25023283	2.67484808	1.28915106
H	4.15973773	2.18197469	0.95293810
C	2.50838381	2.07879811	2.23221249
H	1.60496719	2.53855461	2.61566091
C	0.64620443	-4.84085576	-0.22705797
H	1.65898860	-4.46018145	-0.31347800
C	-1.70195323	-4.47872579	0.03675752
H	-2.55257752	-3.81656983	0.15995065
C	-1.92557851	-5.85234150	-0.00774015
H	-2.93621202	-6.23897779	0.07972272
C	0.43479021	-6.21939997	-0.27264325
H	1.27822407	-6.89203922	-0.39337418
C	-0.85469661	-6.73170587	-0.16334822
H	-1.02527888	-7.80267389	-0.19823363
H	-1.30525010	0.92340946	2.96561709
H	0.05473715	0.04519702	3.66985227
H	-2.77710162	-0.95614552	3.24636003
H	-1.51937661	-1.68082559	4.27692695
H	-0.91015605	0.62533368	-3.35967016
H	-3.47356976	-0.66257508	-2.59557308
H	-2.31007257	-1.28247864	-3.79031308
H	4.20323793	3.78611120	-1.07852309

H	3.17754736	5.21091567	-1.09774707
H	2.97272792	1.56088185	-1.87327445
H	2.81876066	1.14370655	2.68372962
N	-0.18047753	2.25103865	0.26198641
H	0.22001324	3.15935382	0.05075067
C	-1.55068300	2.43886644	0.70959511
H	-2.07192574	1.47606747	0.66916220
H	-1.59402969	2.76321513	1.76509991
C	-2.33788431	3.47203658	-0.11218779
H	-2.33000768	3.17852952	-1.16795876
H	-1.82423820	4.44003101	-0.06046102
C	-3.78835445	3.65031682	0.37145501
H	-3.79338729	3.95263307	1.42444139
H	-4.29564167	2.67684191	0.32240598
C	-4.56189649	4.64956746	-0.44148987
H	-4.66844618	4.41731500	-1.50076709
C	-5.09797858	5.77322014	0.02560918
H	-5.01747449	6.04816810	1.07331398
H	-5.63900425	6.45759224	-0.61815507

MP2 Electronic Energy(Ha): 1489.156003713187

B3LYP Electronic Energy(Ha): 1492.999980507281

M06-L Electronic Energy(Ha): 1492.817728129331

Zero point energy correction(kcal/mol): 377.270

Enthalpy correction(kcal/mol): 400.565

Entropy correction(cal/mol): 221.394

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.130

Deuterated enthalpy correction(kcal/mol): 396.653

Deuterated entropy correction(cal/mol): 222.817

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-1.13779598	-0.62789339	-0.12046258

C	-1.33864502	1.84514856	-0.40264692
C	-1.79722507	1.35336543	-1.66851926
H	-1.25119702	1.40635263	-2.59922755
C	-2.39653201	1.57378089	0.51216294
H	-2.38189652	1.80172392	1.56798532
C	-3.43655745	0.89019889	-0.15182300
H	-4.36217397	0.54915653	0.29144431
C	-3.06610479	0.76685278	-1.51387865
H	-3.65696984	0.31732302	-2.30077636
B	0.17167619	2.35825574	-0.04088972
C	0.43789381	3.94927746	-0.08678791
C	0.49704524	1.63675287	1.39853016
C	1.10179759	1.46379186	-1.05578047
N	0.81280356	0.21991773	-1.26955351
N	0.08672512	0.43427737	1.65010362
O	1.22608048	2.21248048	2.37073301
O	2.16769465	1.93167200	-1.72659171
C	1.72017594	-0.31737828	-2.29782751
C	2.74650242	0.81855374	-2.46927005
C	0.51781598	0.04649346	3.00327678
C	1.38261647	1.24357782	3.44742379
N	-2.49533212	-2.18617349	-0.98757927
H	2.17201221	-1.25462454	-1.97529918
C	-2.34009184	-3.58088363	-1.40444258
H	-2.63777512	-3.69264405	-2.45186263
H	-1.28607104	-3.85937120	-1.34221638
C	-3.19058479	-4.46041025	-0.47670516
C	-2.97441483	-3.88805490	0.92462561
H	-3.70646135	-4.28055177	1.63797057
H	-1.98585392	-4.16062195	1.30778616
C	-3.11173505	-2.37995427	0.90332261
H	-4.11707677	-2.03986576	0.67111904
C	-2.36091031	-1.54281976	1.78288399

H	-1.62953562	-2.03639065	2.41493409
C	-0.59154282	4.85277887	-0.38857538
H	-1.58568733	4.46908257	-0.59519456
C	1.70581303	4.49951061	0.16899787
H	2.53453646	3.84092304	0.40741077
C	1.93441589	5.87229106	0.12547968
H	2.92818568	6.26205709	0.32284029
C	-0.37568962	6.23073429	-0.43186667
H	-1.19719660	6.89972985	-0.66853811
C	0.89087268	6.74712674	-0.17434755
H	1.06524342	7.81757520	-0.20708118
H	1.07713457	-0.89006748	2.97756553
H	-0.35508445	-0.10168906	3.64546266
H	2.44504112	1.00578739	3.52654410
H	1.04969856	1.71528518	4.37179340
H	1.16056549	-0.51778934	-3.21782573
H	3.71680442	0.59254543	-2.02173183
H	2.89045724	1.14300183	-3.49906320
H	-4.24819666	-4.37787355	-0.75252727
H	-2.91596541	-5.51646894	-0.54274850
H	-3.32935179	-1.80306715	-1.41344950
H	-2.89222268	-0.72353070	2.25390212
N	0.18254765	-2.28470153	0.09041730
H	-0.27735298	-3.17759819	0.24192451
C	1.56939194	-2.41890277	0.50652919
H	2.08757397	-1.47469238	0.31116063
H	1.65630657	-2.58513106	1.59572466
C	2.31477589	-3.56815177	-0.19164313
H	2.26562642	-3.42258142	-1.27692869
H	1.79262090	-4.51112098	0.01239267
C	3.78098635	-3.70192412	0.25736526
H	3.82383397	-3.86203343	1.34032797
H	4.29586005	-2.75097681	0.06173816

C	4.51296874	-4.81088739	-0.44394759
H	4.58417817	-4.71983951	-1.52749012
C	5.05077378	-5.87401922	0.14669418
H	5.00443750	-6.00963420	1.22339868
H	5.55912718	-6.64547680	-0.42074181

MP2 Electronic Energy(Ha): 1489.146387810158

B3LYP Electronic Energy(Ha): 1492.979176340977

M06-L Electronic Energy(Ha): 1492.798783774173

Zero point energy correction(kcal/mol): 377.991

Enthalpy correction(kcal/mol): 400.217

Entropy correction(cal/mol): 211.563

Imaginary Frequencies: -356.42

Deuterated zero point energy correction(kcal/mol): 373.728

Deuterated enthalpy correction(kcal/mol): 396.168

Deuterated entropy correction(cal/mol): 212.802

Deuterated imaginary Frequencies: -355.05

Product geometry

Zr	1.02165634	-0.62459422	0.17312722
C	1.20596994	1.82199159	0.68950614
C	1.35776334	1.17536360	1.95961878
H	0.62804767	1.17109048	2.75625698
C	2.43002869	1.58964480	-0.00072109
H	2.64925042	1.91634805	-1.00707576
C	3.27207189	0.77550774	0.78049068
H	4.25606446	0.42516856	0.50058177
C	2.60514120	0.52144924	2.00944143
H	2.99793900	-0.03219644	2.85237830
B	-0.17534517	2.42912486	0.05531755
C	-0.36309945	4.03130547	0.09497092
C	-0.26164400	1.75303754	-1.43831672
C	-1.32845260	1.56508255	0.84048906
N	-1.20115704	0.28612206	0.98475793

N	0.13885334	0.53750762	-1.64901998
O	-0.81441469	2.36271826	-2.49884015
O	-2.39993263	2.11916742	1.44022056
C	-2.25475704	-0.18601075	1.90287823
C	-3.18443304	1.03515467	2.01301765
C	-0.13578313	0.16080201	-3.04509729
C	-0.79878600	1.42985221	-3.61911628
N	2.64720949	-2.36574058	0.77555832
H	-2.76351653	-1.06737639	1.51370514
C	2.45758733	-3.76017405	1.27061345
H	2.78773939	-3.83671315	2.30857823
H	1.39542121	-4.01246424	1.25116285
C	3.25666327	-4.64859320	0.30528971
C	3.10972841	-3.90772952	-1.02905325
H	3.86280087	-4.18704992	-1.76824317
H	2.12808603	-4.11099567	-1.47014684
C	3.21259719	-2.41653603	-0.66730170
H	4.26991403	-2.14170031	-0.59279348
C	2.43596184	-1.42518376	-1.52216221
H	1.85718096	-1.93388606	-2.29701539
C	0.63002674	4.87119652	0.61973326
H	1.54295851	4.43003386	1.00728160
C	-1.52533094	4.65570579	-0.39018275
H	-2.32272646	4.04823305	-0.80577887
C	-1.68769991	6.03807421	-0.35509596
H	-2.59948668	6.48566952	-0.73833276
C	0.47933303	6.25791578	0.66037065
H	1.26996748	6.87587031	1.07454812
C	-0.68254902	6.84826002	0.17191067
H	-0.80572633	7.92590305	0.20123649
H	-0.79278448	-0.71150669	-3.08076690
H	0.79376527	-0.09798050	-3.55593656
H	-1.83058383	1.28017149	-3.93934111

H	-0.23413298	1.89417821	-4.42817873
H	-1.80947250	-0.46039407	2.86614892
H	-4.09461901	0.93300206	1.41670285
H	-3.44958907	1.31309500	3.03233234
H	4.30890360	-4.68767962	0.60569395
H	2.88054473	-5.67366567	0.27753803
H	3.33336929	-1.91273558	1.36524059
H	3.08304141	-0.68717450	-1.99808126
N	-0.21633998	-2.32528582	-0.04986319
H	0.30811552	-3.18748925	-0.16901661
C	-1.56586508	-2.55812404	-0.54704573
H	-2.12839688	-1.62274608	-0.48501414
H	-1.55029791	-2.82698243	-1.61752726
C	-2.31912026	-3.66728875	0.20440845
H	-2.36306303	-3.41104788	1.26918171
H	-1.74603190	-4.60017531	0.13822168
C	-3.73798544	-3.91232974	-0.33989858
H	-3.68711775	-4.17921380	-1.40126087
H	-4.30387751	-2.97201474	-0.28175609
C	-4.48088554	-4.98021880	0.41196460
H	-4.63895133	-4.78905179	1.47302124
C	-4.93229089	-6.11746571	-0.10883873
H	-4.79778948	-6.35329028	-1.16056030
H	-5.45479924	-6.85253376	0.49302367

MP2 Electronic Energy(Ha): 1489.161892564942

B3LYP Electronic Energy(Ha): 1492.994294633727

M06-L Electronic Energy(Ha): 1492.811719496656

Zero point energy correction(kcal/mol): 379.305

Enthalpy correction(kcal/mol): 401.692

Entropy correction(cal/mol): 214.173

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.940

Deuterated enthalpy correction(kcal/mol): 397.522

Deuterated entropy correction(cal/mol): 215.306

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction C2

Reactant geometry

Zr	-0.25648530	-1.47731531	0.24391037
C	-0.25897539	0.71307876	1.43313602
C	-1.48750681	0.06615093	1.79615581
H	-2.47320854	0.35726198	1.46268283
C	0.75698135	-0.01020094	2.11530158
H	1.81729080	0.19292964	2.05263129
C	0.18103107	-1.10226271	2.82135848
H	0.70850463	-1.82026101	3.43317063
C	-1.21822934	-1.04614366	2.63143594
H	-1.94798331	-1.71723845	3.06032250
B	-0.03953255	1.70199333	0.13857184
C	0.03505454	3.28658655	0.43462895
C	1.27601856	1.09510435	-0.67559426
C	-1.22049531	1.23752852	-0.91989197
N	-1.46164335	-0.02161132	-1.11672355
N	1.46023759	-0.17465256	-0.89143285
O	2.18311465	1.90700116	-1.24315992
O	-1.96638915	2.08073639	-1.64601078
C	-2.54982721	-0.17408138	-2.09552106
C	-2.85480082	1.28644453	-2.49166200
C	2.62191197	-0.34445973	-1.78535409
C	3.19234860	1.08213521	-1.88991196
N	-1.11128881	-3.08899584	-0.21483796
H	-2.22252854	-0.78386182	-2.94024298
H	3.34345527	-1.05165115	-1.36955178
C	-1.43963604	-4.47580848	-0.22080249
H	-2.34747770	-4.67865687	0.36954530

H	-1.65080059	-4.83645979	-1.24181784
C	-0.28135894	-5.29918118	0.36798933
C	1.04273228	-5.04420422	-0.37729625
H	1.81052092	-5.70962624	0.03384547
H	0.91129217	-5.33327376	-1.42443838
C	1.59417479	-3.63376042	-0.33908572
H	1.73966845	-3.16715729	-1.31087956
C	2.08454906	-2.99059602	0.74165651
H	2.03036888	-3.42787909	1.73265521
H	2.64229715	-2.06757977	0.64781555
C	0.00186882	3.77768257	1.74814651
H	-0.08087923	3.07443514	2.57067580
C	0.13716035	4.24040310	-0.59288659
H	0.16293739	3.91117316	-1.62638815
C	0.20439144	5.60523816	-0.32607648
H	0.28178112	6.31347752	-1.14513532
C	0.06967046	5.14282750	2.02842150
H	0.04114283	5.48528091	3.05805990
C	0.17180103	6.06405983	0.99022981
H	0.22385757	7.12694732	1.20180443
H	-0.16580526	-5.04111315	1.42621909
H	-0.51046115	-6.37037127	0.31965156
H	-2.61296954	1.51862384	-3.52963757
H	-3.87698712	1.59973886	-2.28039188
H	-3.40177483	-0.67819652	-1.63317672
H	3.31586344	1.44161809	-2.91086774
H	4.12812002	1.21497764	-1.34373814
H	2.29272124	-0.73482208	-2.75402638

MP2 Electronic Energy(Ha): 1237.834519971642

B3LYP Electronic Energy(Ha): 1241.006667378887

M06-L Electronic Energy(Ha): 1240.862528550063

Zero point energy correction(kcal/mol): 279.380

Enthalpy correction(kcal/mol): 297.256

Entropy correction(cal/mol): 184.391

Imaginary Frequencies: -0.00

Transition State geometry

Zr	0.03897584	1.50596543	-0.11414767
C	0.02241826	-0.63287859	-1.37825371
C	-1.07463156	0.14118978	-1.87971105
H	-2.11883102	-0.06059220	-1.69399498
C	1.19053735	0.00747028	-1.88149122
H	2.20707628	-0.29700688	-1.67595705
C	0.82725673	1.16963874	-2.60475497
H	1.50316362	1.85621966	-3.09432339
C	-0.58737604	1.24968704	-2.61246141
H	-1.18316740	2.00253011	-3.10764537
B	-0.03285345	-1.71403399	-0.14169357
C	-0.07290458	-3.27708930	-0.53898027
C	1.22045122	-1.27962414	0.84878184
C	-1.28454255	-1.19017603	0.79356596
N	-1.42319621	0.07307483	1.04584782
N	1.45390043	-0.04398725	1.16883904
O	2.04605722	-2.18495618	1.40329641
O	-2.18710424	-1.99273682	1.37753413
C	-2.57762162	0.27946112	1.93378532
C	-3.10467948	-1.15642926	2.14543052
C	2.63365570	0.00778819	2.05058073
C	2.95014725	-1.48000057	2.29974470
N	-0.95411458	3.10900796	0.28381818
H	-2.26060132	0.75460554	2.86568582
H	3.45582191	0.52979385	1.55170683
C	-1.57823736	4.39134695	0.29644714
H	-2.63975637	4.29884212	0.03797149
H	-1.53871762	4.84920803	1.29999559
C	-0.85690664	5.30985769	-0.71181883

C	0.66469658	5.01532363	-0.64122899
H	1.05272625	4.73145445	-1.62218714
H	1.21717997	5.91152829	-0.33610639
C	1.00886907	3.93176237	0.35770191
H	0.81423278	4.19813920	1.39220344
C	1.99844552	2.96102663	0.13141943
H	2.52229749	2.95964541	-0.81841332
H	2.56469163	2.59716501	0.98023378
C	-0.01702957	-3.68757125	-1.87909329
H	0.05258906	-2.93480134	-2.65802099
C	-0.16430881	-4.29289323	0.42837979
H	-0.21242202	-4.02634068	1.47921774
C	-0.19741736	-5.64044585	0.07979674
H	-0.26900323	-6.39807489	0.85400076
C	-0.04863734	-5.03474686	-2.24115632
H	-0.00317252	-5.31409662	-3.28912194
C	-0.13901235	-6.01871433	-1.26104675
H	-0.16444731	-7.06789783	-1.53636500
H	-1.22208314	5.08973167	-1.71784036
H	-1.07734773	6.36294404	-0.51247302
H	-3.06698471	-1.49127018	3.18241443
H	-4.10766075	-1.31953806	1.74988943
H	-3.30941353	0.93664637	1.45867498
H	2.72758937	-1.80528288	3.31785745
H	3.96921159	-1.76874741	2.04377553
H	2.40547650	0.54772506	2.97319317

MP2 Electronic Energy(Ha): 1237.834547994893

B3LYP Electronic Energy(Ha): 1241.003703074780

M06-L Electronic Energy(Ha): 1240.857593767239

Zero point energy correction(kcal/mol): 279.435

Enthalpy correction(kcal/mol): 296.637

Entropy correction(cal/mol): 177.910

Imaginary Frequencies: -169.61

Product geometry

Zr	-0.17327936	-1.43208153	-0.22775962
C	-0.07893800	0.72383285	-1.42348316
C	0.97546888	-0.06374680	-1.98580768
H	2.03122626	0.09119960	-1.81174392
C	-1.28395297	0.13999408	-1.92153482
H	-2.28423276	0.47070976	-1.67972392
C	-0.98514144	-1.01361887	-2.67858210
H	-1.69761912	-1.66478998	-3.16369327
C	0.43148966	-1.14232343	-2.72212449
H	0.98520228	-1.90152538	-3.25568234
B	0.03531020	1.74562801	-0.13764977
C	0.13341653	3.32253218	-0.45720698
C	-1.23403880	1.30405939	0.83073417
C	1.27728516	1.13482287	0.76536069
N	1.39865687	-0.14437673	0.95799797
N	-1.50069554	0.05497468	1.06819590
O	-2.04587192	2.18595867	1.43027041
O	2.17820883	1.89350781	1.40313562
C	2.51287899	-0.40054934	1.88675924
C	3.10350014	1.00807410	2.10379431
C	-2.69290762	-0.03595770	1.92810928
C	-2.99571838	1.44144382	2.25093491
N	0.67666584	-3.25296070	0.16902560
H	2.13703636	-0.84820925	2.81102399
H	-3.50573397	-0.52789657	1.38818890
C	1.73064908	-4.24696849	0.02788717
H	2.43229447	-3.95037147	-0.75787140
H	2.31253611	-4.33528736	0.95680581
C	1.02396602	-5.60297937	-0.28906190
C	-0.47520531	-5.25297691	-0.36219976
H	-0.76919429	-5.02040850	-1.39054616

H	-1.12093409	-6.05809774	-0.00199494
C	-0.60771892	-3.98001917	0.49010800
H	-0.59946394	-4.26465321	1.55466791
C	-1.77926261	-3.03118310	0.18222406
H	-2.35012768	-3.37066850	-0.68546139
H	-2.46519078	-2.91146770	1.02301451
C	0.13422396	3.79664565	-1.77714162
H	0.06481599	3.08419948	-2.59303474
C	0.22360622	4.28762290	0.56074342
H	0.22616615	3.97083213	1.59866033
C	0.31066047	5.64820260	0.27864078
H	0.37893340	6.36587281	1.09018036
C	0.22079623	5.15751856	-2.07256999
H	0.21827341	5.48745298	-3.10661781
C	0.30983409	6.09050567	-1.04371090
H	0.37750499	7.14999308	-1.26728905
H	1.39017168	-6.04539289	-1.21799130
H	1.21474173	-6.32541907	0.50878914
H	3.13697345	1.32208315	3.14657123
H	4.08826815	1.14123366	1.65373443
H	3.22994142	-1.09676437	1.44739270
H	-2.80763749	1.70706418	3.29243627
H	-3.99843250	1.76323171	1.97156338
H	-2.48132942	-0.62658092	2.82223461

MP2 Electronic Energy(Ha): 1237.844690229003

B3LYP Electronic Energy(Ha): 1241.019447208439

M06-L Electronic Energy(Ha): 1240.870405003531

Zero point energy correction(kcal/mol): 279.833

Enthalpy correction(kcal/mol): 297.343

Entropy correction(cal/mol): 183.989

Imaginary Frequencies: -0.00

Equatorial Reaction C3

Reactant geometry

Zr	0.35794061	-0.74134832	-0.26274688
C	0.46028977	1.24189155	1.20158015
C	-0.31517584	0.28046473	1.92508719
H	-1.38269699	0.33212796	2.08149081
C	1.80062569	0.74982224	1.24237807
H	2.65381879	1.22100008	0.77426987
C	1.82911820	-0.50585454	1.88665230
H	2.69369536	-1.13192052	2.04922251
C	0.50623471	-0.80015359	2.31631869
H	0.19747461	-1.67521326	2.86932407
B	-0.11661980	2.41517519	0.21414192
C	-0.19681636	3.90819264	0.81793004
C	0.79488225	2.25247848	-1.15803956
C	-1.52356597	1.81221108	-0.38640283
N	-1.65772605	0.55274579	-0.66927849
N	0.98987305	1.08359672	-1.68876531
O	1.38221693	3.27659523	-1.79431215
O	-2.53508969	2.60304244	-0.78361050
C	-2.88159325	0.38007176	-1.47666230
C	-3.57437675	1.74504228	-1.33749747
C	1.88255033	1.22154638	-2.85233674
C	2.03502997	2.75004308	-2.98772176
N	-0.89324742	-2.40728073	-0.54497665
N	1.98324746	-1.77971934	-1.08202743
C	3.42454726	-1.94623042	-0.93824054
H	3.71989699	-1.58865027	0.05124961
H	-2.60775033	0.15094305	-2.51214842
H	2.83124430	0.71530952	-2.65599886
C	-2.24975629	-2.80380436	-0.18495802
H	-2.75568198	-1.94763459	0.27307866
H	-2.83753038	-3.06962468	-1.07604992

C	-2.29735037	-3.97819322	0.80328980
C	3.90247339	-3.39705935	-1.12260963
C	3.40815012	-4.38366301	-0.04859667
H	3.63551966	-5.40218948	-0.38956796
H	3.97084298	-1.32280127	-1.66500390
H	1.70303338	-2.18680990	-1.97762119
C	4.04840039	-4.17961172	1.29642994
H	5.13857221	-4.18448430	1.30515715
H	2.32055958	-4.31339260	0.04273668
C	3.40063726	-4.01506291	2.44686351
H	3.92842676	-3.89364963	3.38632169
H	-0.36204546	-3.23469831	-0.80590663
H	2.31570351	-4.00622558	2.48912609
C	0.17328600	4.17443362	2.14450031
H	0.52297507	3.35800791	2.76847929
C	-0.63972406	5.00247943	0.05465002
H	-0.93944185	4.84732238	-0.97633921
C	0.10656774	5.45835789	2.68662737
H	0.40143525	5.62580966	3.71776603
C	-0.71036522	6.28819007	0.58430011
H	-1.05741171	7.10974971	-0.03457835
C	-0.33648538	6.52269517	1.90694509
H	-0.39021683	7.52340012	2.32275152
C	-3.72303057	-4.38445582	1.22606945
H	-4.23651907	-3.52749941	1.67680707
H	-3.64049133	-5.14538001	2.01278767
C	-4.55777361	-4.94224727	0.10666323
H	-4.12798822	-5.79458731	-0.41970214
C	-5.75208412	-4.49363308	-0.26970383
H	-6.22385978	-3.64960838	0.22508752
H	-6.30546859	-4.95631469	-1.07921201
H	3.57577239	-3.74993479	-2.10894034
H	4.99965527	-3.40458043	-1.14563717

H	-1.79215005	-4.84415481	0.35519923
H	-1.71913836	-3.71031845	1.69353172
H	-3.90666418	2.18404276	-2.27718897
H	-4.40487161	1.73288578	-0.62801801
H	-3.49369453	-0.44118851	-1.10652597
H	1.51605733	3.16232125	-3.85489019
H	3.06681202	3.09985972	-2.98424584
H	1.43738162	0.76593271	-3.74002571

MP2 Electronic Energy(Ha): 1489.155251172080

B3LYP Electronic Energy(Ha): 1493.010723316320

M06-L Electronic Energy(Ha): 1492.815552855435

Zero point energy correction(kcal/mol): 376.741

Enthalpy correction(kcal/mol): 400.376

Entropy correction(cal/mol): 228.835

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.667

Deuterated enthalpy correction(kcal/mol): 396.531

Deuterated entropy correction(cal/mol): 230.260

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.39597199	-0.65531310	0.25529161
C	0.24111060	1.59232799	1.29969226
C	-0.53614035	0.71152815	2.12321133
H	-1.61414294	0.69757292	2.18736317
C	1.59681089	1.24890618	1.55722635
H	2.45550085	1.69898246	1.07886176
C	1.65096857	0.14244678	2.43725146
H	2.54364706	-0.34404891	2.80416589
C	0.31904565	-0.18955888	2.79891490
H	0.01964520	-0.96452252	3.48981709
B	-0.30997696	2.49051474	0.03906115
C	-0.49223258	4.06132549	0.35340584

C	0.66922211	2.10028701	-1.23638538
C	-1.64955016	1.67237436	-0.46545002
N	-1.62903727	0.37986183	-0.55269062
N	1.07694432	0.88260377	-1.44241398
O	0.97045922	2.97089515	-2.21473339
O	-2.78658698	2.26140864	-0.87118768
C	-2.90917332	-0.09055707	-1.10858367
C	-3.72086950	1.21255169	-1.26316122
C	1.69999335	0.80124451	-2.77599933
C	1.77610941	2.27634613	-3.20932841
N	-0.42751322	-2.43944718	-0.00285427
N	2.35954321	-1.71829643	-0.15539874
C	3.73368464	-1.19671049	-0.15202912
H	3.91381829	-0.74274801	0.82474680
H	-2.74455916	-0.59912775	-2.06245500
H	2.68284397	0.32836133	-2.72562697
C	-1.52743934	-3.32601908	-0.33602005
H	-2.17068200	-2.85509623	-1.09064903
H	-1.13596881	-4.23991625	-0.80372708
C	-2.39603772	-3.72884614	0.86597738
C	4.69869348	-2.38084588	-0.38648720
C	3.95060101	-3.65562170	0.06928358
H	4.56263320	-4.26335425	0.74146638
H	3.86849281	-0.40670830	-0.89613241
H	2.18444812	-2.13695017	-1.07223994
C	2.65590953	-3.29384945	0.78783451
H	2.83978506	-2.80505204	1.74488016
H	3.70463200	-4.29254709	-0.78555651
C	1.53782124	-4.17999048	0.76780238
H	1.09559440	-4.42445048	1.73031165
H	0.44590363	-3.21542550	0.32495659
H	1.59491957	-5.02341147	0.08253880
C	0.53098621	4.99480726	0.12066437

H	1.44625582	4.67506684	-0.36562373
C	-1.65298624	4.54862970	0.97778697
H	-2.47671110	3.87114360	1.17632167
C	0.40662783	6.33479744	0.48460494
H	1.21982732	7.02575642	0.28551404
C	-1.78932251	5.88544882	1.34571448
H	-2.70308273	6.22313017	1.82452049
C	-0.75694156	6.78810575	1.10052234
H	-0.85865833	7.83010298	1.38470826
C	-3.54558122	-4.68670236	0.49203125
H	-4.16989344	-4.23450110	-0.28790172
H	-4.18911427	-4.81287390	1.37218802
C	-3.08051918	-6.04307240	0.03835146
H	-2.45696399	-6.58621041	0.74818240
C	-3.36540457	-6.61233616	-1.12957694
H	-3.97863435	-6.11047474	-1.87256213
H	-2.99810616	-7.59969793	-1.38659113
H	4.96373821	-2.45372638	-1.44518379
H	5.63234863	-2.23115668	0.16086986
H	-1.75835340	-4.19428875	1.62554339
H	-2.81019855	-2.82364051	1.32381373
H	-4.04153405	1.41845596	-2.28427135
H	-4.58224320	1.27142223	-0.59613674
H	-3.38290517	-0.80283706	-0.43023846
H	1.34664414	2.48021114	-4.18919144
H	2.78634246	2.68801152	-3.16290405
H	1.07288138	0.20091209	-3.44340387

MP2 Electronic Energy(Ha): 1489.100914462199

B3LYP Electronic Energy(Ha): 1492.941766817454

M06-L Electronic Energy(Ha): 1492.752493288006

Zero point energy correction(kcal/mol): 374.575

Enthalpy correction(kcal/mol): 397.348

Entropy correction(cal/mol): 225.430

Imaginary Frequencies: -1065.59

Deuterated zero point energy correction(kcal/mol): 371.120

Deuterated enthalpy correction(kcal/mol): 394.060

Deuterated entropy correction(cal/mol): 226.299

Deuterated imaginary Frequencies: -884.93

Product geometry

Zr	0.11363491	0.72361114	-0.05604277
C	0.06510532	-1.41713088	-1.35993067
C	-0.83715487	-0.52004770	-2.02507186
H	-1.91492352	-0.59408046	-2.01898910
C	1.36475106	-0.93245062	-1.66496379
H	2.28866570	-1.36937094	-1.31118511
C	1.26694447	0.26392878	-2.42137223
H	2.08729012	0.85199758	-2.80806939
C	-0.10843132	0.51356731	-2.65645128
H	-0.51955536	1.32625764	-3.23733678
B	-0.32833588	-2.46585939	-0.16176805
C	-0.43723272	-4.02566143	-0.56468790
C	0.70494531	-2.15247249	1.10037001
C	-1.68609893	-1.80389424	0.50260895
N	-1.72813506	-0.53186138	0.73728276
N	1.05240721	-0.95338227	1.46712978
O	1.11450908	-3.13874906	1.91983144
O	-2.78465958	-2.49143630	0.85490899
C	-3.03613419	-0.17821282	1.30817950
C	-3.72263198	-1.55217698	1.46369491
C	1.72441106	-1.03671877	2.77802560
C	1.93575376	-2.54884944	2.96393403
N	-0.76343331	2.34758403	0.30309495
N	2.31566577	1.74948298	0.48566478
C	3.57360874	0.92469127	0.48562108
H	3.33166501	-0.12690672	0.34659166

H	-2.91297846	0.34502134	2.25875561
H	2.66589777	-0.48348490	2.78338316
C	-1.60724829	3.49877509	0.40596444
H	-2.48668632	3.27767466	1.03636726
H	-1.09201965	4.32854900	0.91789675
C	-2.11413664	4.01035110	-0.95439849
C	4.43787366	1.50460344	-0.63566954
C	4.11340016	2.99931427	-0.56875967
H	4.35826745	3.53887311	-1.48584103
H	4.08780901	1.03499974	1.44642648
H	2.10487192	2.01416375	1.44481945
C	2.60550863	3.03703818	-0.26923794
H	2.04830948	2.98482164	-1.20734079
H	4.66916336	3.46886436	0.25106801
C	2.14362066	4.26074881	0.50822518
H	2.33067677	5.16829783	-0.07159540
H	1.07587049	4.19821221	0.71672323
H	2.68986712	4.35122539	1.45412569
C	-0.87491037	-5.00963453	0.33899253
H	-1.15681634	-4.72116037	1.34595784
C	-0.09414518	-4.46334936	-1.85269033
H	0.24224273	-3.73449848	-2.58313827
C	-0.96305145	-6.35210432	-0.01995184
H	-1.30743780	-7.08407008	0.70410334
C	-0.17678510	-5.80583114	-2.22397399
H	0.09676948	-6.10606560	-3.23069587
C	-0.61214752	-6.75798459	-1.30695268
H	-0.68041933	-7.80319556	-1.59022396
C	-3.03715105	5.24153047	-0.86027118
H	-3.88466087	5.02393943	-0.20000464
H	-3.45914789	5.43020039	-1.85618146
C	-2.34269383	6.49062680	-0.39377886
H	-1.48185849	6.79708576	-0.98850901

C	-2.69305123	7.23305913	0.65295206
H	-3.54173203	6.96945372	1.27735887
H	-2.14870594	8.13127471	0.92302516
H	5.49692985	1.28241986	-0.49184250
H	4.13848777	1.08709289	-1.60008191
H	-1.24880563	4.24267807	-1.58663889
H	-2.64814663	3.19434943	-1.45232661
H	-3.86208362	-1.85487981	2.50293524
H	-4.67040039	-1.63984888	0.93290340
H	-3.57206881	0.49015563	0.62922754
H	1.59384883	-2.93769276	3.92231234
H	2.96794706	-2.86299233	2.79304293
H	1.07831302	-0.60608262	3.55096201

MP2 Electronic Energy(Ha): 1489.176501343367

B3LYP Electronic Energy(Ha): 1493.007312374909

M06-L Electronic Energy(Ha): 1492.821222301796

Zero point energy correction(kcal/mol): 379.117

Enthalpy correction(kcal/mol): 402.000

Entropy correction(cal/mol): 222.832

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.797

Deuterated enthalpy correction(kcal/mol): 397.840

Deuterated entropy correction(cal/mol): 223.852

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H1

Reactant geometry

Zr	-0.01251811	0.48499648	0.95264327
C	0.65711921	-1.89806366	1.35083847
C	1.90084064	-1.22446267	1.48306288
H	2.71673158	-1.28213183	0.77425477
C	-0.10971153	-1.49908247	2.49676153

H	-1.11217085	-1.82973898	2.72786342
C	0.62335633	-0.56429012	3.26485295
H	0.30288663	-0.09687288	4.18460775
C	1.87561003	-0.38385836	2.62615584
H	2.68445556	0.23675200	2.98725045
B	0.06295734	-2.57737922	-0.02071866
C	0.28206068	-4.16693835	-0.20200722
C	-1.50804474	-2.07405051	-0.06619663
C	0.64919930	-1.65960902	-1.27433272
N	0.69396689	-0.36065062	-1.25018442
N	-1.80603953	-0.84373071	0.20899420
O	-2.54687504	-2.85463568	-0.40184939
O	1.01834804	-2.22224377	-2.43949756
C	1.09377816	0.12868323	-2.58315589
C	1.44019185	-1.16567387	-3.34397419
C	-3.26146876	-0.65339760	0.10963074
C	-3.75194576	-2.02995406	-0.38700451
N	1.80513121	1.96693770	0.27899533
N	-1.08126665	1.95344765	1.43891859
C	-1.91378059	2.98621418	1.97633852
H	-2.88842923	2.57578505	2.29391261
H	0.26520315	0.67653060	-3.04395733
H	-3.67050680	-0.38347030	1.08659687
H	1.49385109	2.39294599	-0.59130328
C	2.21439132	3.04354310	1.21994465
H	1.30507420	3.57524596	1.50628626
H	2.58184379	2.54838940	2.12036666
H	2.61920632	1.40732784	0.03314749
C	-2.18724189	4.14683185	0.99734938
H	-1.46495937	3.41578534	2.88720886
C	3.28418419	4.00471185	0.68188744
C	2.78050009	5.14649779	-0.23119101
H	2.14714181	5.81055429	0.36866250

H	3.64706872	5.73748864	-0.54336634
C	2.00884860	4.71932840	-1.45345736
H	0.96390919	4.45175851	-1.29941752
C	2.49703630	4.68476224	-2.69170298
H	3.52115643	4.97522529	-2.90793360
H	1.88707153	4.38335259	-3.53584564
C	-0.24813872	-4.88077123	-1.29086793
H	-0.83022688	-4.35533014	-2.04059781
C	1.01969748	-4.90594614	0.73473039
H	1.44165229	-4.39360138	1.59346386
C	1.22387299	-6.27945792	0.59742764
H	1.80017010	-6.81754961	1.34359621
C	-0.05240800	-6.25134057	-1.43849803
H	-0.47847475	-6.76982467	-2.29187018
C	0.68789138	-6.95923190	-0.49236290
H	0.84206378	-8.02746857	-0.60395537
C	-2.97822447	3.71922372	-0.24929625
H	-3.95553290	3.33817112	0.07947704
H	-2.45960122	2.88668151	-0.73281938
C	-3.18933593	4.83601139	-1.23065412
H	-3.71923734	5.70989471	-0.85163187
C	-2.77468750	4.84144088	-2.49512041
H	-2.95342268	5.68491349	-3.15276821
H	-2.24531575	3.99326526	-2.92046274
H	3.78475156	4.46613835	1.53995609
H	4.05391048	3.42892217	0.15358061
H	-1.22980223	4.58093415	0.68606118
H	-2.73612693	4.93708783	1.52630925
H	-4.14938536	-2.01144318	-1.40309723
H	-4.47340919	-2.51071734	0.27334684
H	-3.49749181	0.15673026	-0.58319737
H	0.90011648	-1.29018024	-4.28218843
H	2.50977427	-1.28939522	-3.52442622

H 1.94612070 0.81116720 -2.52048780

MP2 Electronic Energy(Ha): 1489.145326877354

B3LYP Electronic Energy(Ha): 1492.992110066169

M06-L Electronic Energy(Ha): 1492.796493651333

Zero point energy correction(kcal/mol): 377.464

Enthalpy correction(kcal/mol): 401.228

Entropy correction(cal/mol): 231.849

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.035

Deuterated enthalpy correction(kcal/mol): 396.973

Deuterated entropy correction(cal/mol): 232.964

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.32223565	-0.41855581	0.70285855
C	-0.84358445	1.93992322	1.21729271
C	-2.13685481	1.34879493	1.12748808
H	-2.84240140	1.50887076	0.32389723
C	-0.27020194	1.40107284	2.41600705
H	0.71401615	1.63263186	2.79747500
C	-1.15116154	0.45531258	2.99008652
H	-0.98656402	-0.11149887	3.89478424
C	-2.31534438	0.41624763	2.17683269
H	-3.19121916	-0.19176062	2.35177540
B	-0.02877425	2.66951874	-0.01123133
C	-0.08378632	4.27944105	-0.07407674
C	1.48700380	2.02336295	0.07188010
C	-0.56937264	1.89783138	-1.37673632
N	-0.69021300	0.60442678	-1.43774535
N	1.65663624	0.75948424	0.32002580
O	2.60848946	2.71155263	-0.16886233
O	-0.89406864	2.55562248	-2.49837944
C	-1.20975610	0.22807312	-2.76494747

C	-1.25284106	1.57464538	-3.51525831
C	3.08998698	0.42782466	0.24332339
C	3.74146842	1.79993629	-0.02808139
N	-1.62435321	-2.14523983	-0.21608571
N	0.48039890	-2.13190071	1.22311877
C	1.15870829	-3.13372758	2.00972724
H	1.87144585	-2.65438212	2.69861415
H	-0.55072332	-0.49802675	-3.24730968
H	3.42853737	-0.02463141	1.17727625
H	-0.52856340	-2.52068787	0.45633935
C	-2.92680029	-2.59537504	0.28055530
H	-2.83502105	-2.74541902	1.36392924
H	-3.69600960	-1.81824754	0.14826894
H	-1.59715662	-2.20333910	-1.23018815
C	1.92291546	-4.18737819	1.18528537
H	0.43995997	-3.67030071	2.64836522
C	-3.46998220	-3.88701080	-0.35073217
C	-2.64329985	-5.17247974	-0.11635720
H	-2.29476933	-5.17605557	0.92512511
H	-3.30279212	-6.03970466	-0.22538052
C	-1.46657834	-5.35064220	-1.03705728
H	-0.68356306	-4.60149511	-0.96529036
C	-1.33390183	-6.34294920	-1.91376741
H	-2.09090377	-7.11522551	-2.01921719
H	-0.46110190	-6.42488401	-2.55202939
C	0.57898553	5.01378048	-1.07263960
H	1.14682813	4.48900082	-1.83396642
C	-0.79861673	5.01673533	0.88119319
H	-1.32433728	4.48785379	1.66984658
C	-0.85346641	6.41049519	0.84809712
H	-1.41670111	6.94742820	1.60476245
C	0.53184572	6.40454723	-1.11607291
H	1.05632079	6.93943372	-1.90160751

C	-0.18699328	7.11125108	-0.15272026
H	-0.22561048	8.19504255	-0.18336943
C	3.05600478	-3.60078126	0.32796560
H	3.74233787	-3.05384177	0.99023871
H	2.63890575	-2.87007356	-0.37034531
C	3.82757895	-4.64811016	-0.42324813
H	4.33222414	-5.39590254	0.18823844
C	3.92272924	-4.73598073	-1.74710787
H	4.48934932	-5.52564924	-2.22791718
H	3.43372907	-4.01828150	-2.39979435
H	-4.47384033	-4.04598205	0.06115184
H	-3.60647324	-3.73744885	-1.42920438
H	1.22153795	-4.72388342	0.53781463
H	2.33808195	-4.92975869	1.87899462
H	4.31678286	1.84377286	-0.95249051
H	4.35394716	2.16491291	0.79707505
H	3.27013206	-0.29223327	-0.55831733
H	-0.51814895	1.64934537	-4.31838221
H	-2.23711485	1.83947770	-3.90008290
H	-2.19858320	-0.22825494	-2.66611297

MP2 Electronic Energy(Ha): 1489.107369309520

B3LYP Electronic Energy(Ha): 1492.959685948660

M06-L Electronic Energy(Ha): 1492.759239582332

Zero point energy correction(kcal/mol): 373.550

Enthalpy correction(kcal/mol): 397.219

Entropy correction(cal/mol): 236.606

Imaginary Frequencies: -1649.03

Deuterated zero point energy correction(kcal/mol): 370.203

Deuterated enthalpy correction(kcal/mol): 394.022

Deuterated entropy correction(cal/mol): 237.451

Deuterated imaginary Frequencies: -1184.59

Product geometry

Zr	-0.26207616	-0.57496559	0.94039628
C	0.37495872	1.76377322	1.43699785
C	-0.62239276	1.42654740	2.40623010
H	-1.63844933	1.79309724	2.41262510
C	1.54118828	1.03909872	1.83130839
H	2.48592290	1.04498350	1.30552615
C	1.24321987	0.22363506	2.94216448
H	1.91978465	-0.44928335	3.44705098
C	-0.11169201	0.46063425	3.30306737
H	-0.63687012	0.01394963	4.13539422
B	0.12355633	2.49008758	-0.01159202
C	0.49978089	4.05441978	-0.12120098
C	0.88963663	1.50408045	-1.09270904
C	-1.43367750	2.11005779	-0.39235103
N	-1.90453797	0.92313888	-0.17970653
N	0.81822054	0.21051277	-0.98745921
O	1.56369273	1.95088353	-2.15970490
O	-2.27458144	2.97320778	-0.98876479
C	-3.29610326	0.86513302	-0.66286146
C	-3.52323880	2.27243770	-1.25397681
C	1.53022002	-0.41680721	-2.11483600
C	2.03249857	0.79827778	-2.92204901
N	-1.99491061	-1.77552708	0.95021040
N	0.90119711	-2.30564887	1.07562252
C	2.13354280	-2.79105724	1.69477365
H	2.85256131	-1.96652841	1.74986072
H	-3.41430047	0.07254961	-1.40617583
H	2.34229622	-1.04532661	-1.74594191
H	0.40682352	-3.09253505	0.65746049
C	-2.35054341	-3.05005751	1.57200737
H	-1.42730111	-3.59009938	1.80940137
H	-2.85459810	-2.88476177	2.53757921
H	-2.84729943	-1.31923625	0.63961636

C	2.78803246	-3.97539486	0.96907369
H	1.94519931	-3.10379494	2.73352792
C	-3.26321242	-3.96121979	0.73300225
C	-2.66199909	-4.52482477	-0.57461435
H	-1.64563062	-4.88351083	-0.36063299
H	-3.23956149	-5.40420060	-0.87863554
C	-2.61636752	-3.55913098	-1.72775298
H	-2.01851213	-2.66602313	-1.57240956
C	-3.25953446	-3.72521686	-2.88127092
H	-3.87487021	-4.60039258	-3.07062858
H	-3.19306507	-2.99570415	-3.68124983
C	0.34641586	4.77991852	-1.31542895
H	-0.03539475	4.27917145	-2.19887125
C	0.99628202	4.75971859	0.98489461
H	1.12978614	4.23719143	1.92684176
C	1.32360267	6.11406327	0.91108978
H	1.70496211	6.62669786	1.78857777
C	0.67006337	6.13132156	-1.40161223
H	0.53864547	6.66010568	-2.34048294
C	1.16164026	6.80666454	-0.28514553
H	1.41457658	7.85981041	-0.34885265
C	3.27037053	-3.66578811	-0.45846431
H	3.95523135	-2.80745868	-0.41158828
H	2.42209361	-3.36148664	-1.07725606
C	3.97545500	-4.82690184	-1.10086548
H	4.87969382	-5.16987946	-0.59880240
C	3.57402540	-5.45780435	-2.20053097
H	4.12417454	-6.29793620	-2.60925048
H	2.67734865	-5.15528651	-2.73385519
H	-3.54367154	-4.80947095	1.36915971
H	-4.19704118	-3.43318380	0.50267562
H	2.08139865	-4.81429059	0.93507054
H	3.63773440	-4.31859472	1.57181977

H	1.60539909	0.86936299	-3.92274505
H	3.11854763	0.86573632	-2.98745993
H	0.85115753	-1.05105708	-2.69080604
H	-3.68094875	2.27201081	-2.33347299
H	-4.32740495	2.82955371	-0.77308963
H	-3.97886018	0.65047745	0.16557909

MP2 Electronic Energy(Ha): 1489.153251138089

B3LYP Electronic Energy(Ha): 1493.010816135724

M06-L Electronic Energy(Ha): 1492.814479505254

Zero point energy correction(kcal/mol): 376.754

Enthalpy correction(kcal/mol): 400.509

Entropy correction(cal/mol): 231.124

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.627

Deuterated enthalpy correction(kcal/mol): 396.613

Deuterated entropy correction(cal/mol): 232.519

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H2

Reactant geometry

Zr	0.94031876	-0.84794896	0.70719356
C	-0.04353710	1.28779929	1.48780058
C	-1.04786080	0.34814699	1.86365251
H	-2.00660134	0.24164084	1.37742694
C	1.04069930	1.06015681	2.39727647
H	1.97381012	1.60357718	2.40935892
C	0.73413923	-0.02828097	3.23987156
H	1.36819204	-0.44314636	4.00944149
C	-0.56999344	-0.47182489	2.90908593
H	-1.09957482	-1.28152634	3.39171014
B	-0.00375819	2.17496742	0.11734077
C	-0.59298889	3.67622688	0.19404884

C	1.56401351	2.04799109	-0.37095612
C	-0.69277887	1.21525446	-1.04248015
N	-0.52436346	-0.07381539	-1.07830801
N	2.21195476	0.93958429	-0.19251867
O	2.22510834	2.99365107	-1.05678640
O	-1.35299723	1.73415626	-2.09238295
C	-1.05137228	-0.58468921	-2.35796022
C	-1.78888086	0.63400361	-2.93904830
C	3.51711635	1.02181564	-0.87000899
C	3.57416407	2.49730117	-1.31163802
N	-0.72025346	-2.67370419	0.50765320
N	2.08529215	-2.03182059	-0.62570063
C	2.45338380	-2.50159196	-1.94059098
H	3.43864590	-2.10871280	-2.25216698
H	-0.22376698	-0.91703080	-2.99214218
H	4.32721043	0.75678306	-0.18760506
C	-2.19612172	-2.60167990	0.57409567
H	-2.46554903	-2.24578544	1.57065560
H	-2.52749088	-1.83641901	-0.12853898
C	-2.89784522	-3.93304100	0.29022225
C	2.55360258	-4.05991330	-1.81054876
C	2.57564231	-4.32393633	-0.28103217
H	3.36205516	-5.02210982	0.01842114
H	1.73621649	-2.18942862	-2.70662159
C	2.76282705	-2.91782385	0.33384233
H	3.84990007	-2.70448138	0.33717653
H	1.62195998	-4.74683451	0.05440784
C	2.14346472	-2.57804780	1.69826747
H	1.62179568	-3.43032612	2.14856910
H	-0.37227853	-3.32688935	1.20564320
H	2.88729218	-2.24577293	2.43051426
C	-0.54834893	4.56119505	-0.89751357
H	-0.10122511	4.23501624	-1.83010851

C	-1.17985590	4.15989828	1.37300275
H	-1.23033623	3.50997235	2.24082192
C	-1.06087503	5.85354764	-0.81767354
H	-1.00790560	6.51021283	-1.68053919
C	-1.69761981	5.45235665	1.46456644
H	-2.14375449	5.79145913	2.39428833
C	-1.64031635	6.30629768	0.36696233
H	-2.04007260	7.31289882	0.43231250
C	-4.43627871	-3.82231275	0.31390699
H	-4.76172480	-3.38576617	1.26441310
H	-4.85145696	-4.83652362	0.27771124
C	-4.99939442	-3.02658030	-0.83195799
H	-4.78844570	-3.42075009	-1.82604544
C	-5.72279476	-1.91567879	-0.72168350
H	-5.96520367	-1.48729701	0.24624650
H	-6.10974564	-1.39956826	-1.59304323
H	-2.87499334	0.55979009	-2.85314946
H	-1.71809285	-1.43651681	-2.20570142
H	-1.52172346	0.87443812	-3.96731855
H	3.78799738	2.64306492	-2.36992871
H	4.26273490	3.09985253	-0.71642675
H	3.54392421	0.32074916	-1.70746524
H	1.70045501	-4.54994012	-2.28780088
H	3.45315706	-4.43813221	-2.30290174
H	-2.57660657	-4.31595825	-0.68693636
H	-2.58064628	-4.67439348	1.03245486
H	-0.42054918	-3.05673303	-0.38716471

MP2 Electronic Energy(Ha): 1489.159636351034

B3LYP Electronic Energy(Ha): 1492.989839045630

M06-L Electronic Energy(Ha): 1492.806714729907

Zero point energy correction(kcal/mol): 378.452

Enthalpy correction(kcal/mol): 401.242

Entropy correction(cal/mol): 219.594

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.479

Deuterated enthalpy correction(kcal/mol): 396.585

Deuterated entropy correction(cal/mol): 222.616

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.79772218	-0.84811626	0.56167438
C	-0.28294048	1.25526001	1.37737045
C	-1.30378759	0.28916524	1.60988978
H	-2.22184610	0.20567361	1.04588530
C	0.74363748	0.95975450	2.33530131
H	1.66522349	1.50931065	2.45978724
C	0.39569229	-0.19669643	3.06030451
H	0.97381964	-0.66065930	3.84630885
C	-0.88179531	-0.62005194	2.60170277
H	-1.43105941	-1.47116618	2.97567309
B	-0.14218524	2.25058353	0.08421270
C	-0.80369448	3.71573705	0.19625735
C	1.47367113	2.21259177	-0.21098883
C	-0.66055942	1.34052458	-1.18488305
N	-0.36302860	0.08000628	-1.26706127
N	2.10989715	1.08611849	-0.17527939
O	2.22076111	3.29737048	-0.47011116
O	-1.32622922	1.83924561	-2.23590764
C	-0.84630303	-0.45826589	-2.54923742
C	-1.53734751	0.76118166	-3.19450814
C	3.54723980	1.33935646	-0.38192102
C	3.59188413	2.85076641	-0.68661163
N	-0.57871754	-2.60309826	-0.01844985
N	2.51493691	-1.83448671	-0.11957571
C	3.45851759	-1.95654256	-1.21811814
H	4.47597073	-1.67610190	-0.90091456

H	-0.00779799	-0.82863114	-3.14619068
H	4.10762480	1.07249906	0.51897206
C	-2.01633897	-2.79580585	0.16261772
H	-2.24837810	-2.67387182	1.22547661
H	-2.60051350	-2.02357123	-0.35892783
C	-2.49802699	-4.18039365	-0.28756684
C	3.44109882	-3.47100838	-1.60356560
C	2.73609926	-4.17109686	-0.41154249
H	3.27207761	-5.05743966	-0.06183040
H	3.18790364	-1.30813353	-2.05514820
C	2.66146058	-3.06934774	0.66533424
H	3.63584493	-3.05143882	1.18833081
H	1.72628470	-4.48827803	-0.68856652
C	1.49919882	-3.10738783	1.66286214
H	1.19846519	-4.13297092	1.90535000
H	0.27584297	-2.94596440	0.91490394
H	1.77478038	-2.65046576	2.61784257
C	-0.68701004	4.66573168	-0.83316871
H	-0.13126906	4.41431418	-1.73070551
C	-1.53135500	4.10253822	1.33116129
H	-1.64355702	3.39990774	2.15093194
C	-1.26424150	5.92907709	-0.73719022
H	-1.15309873	6.63809282	-1.55163313
C	-2.11499554	5.36536164	1.43892197
H	-2.67127090	5.62945250	2.33280974
C	-1.98374894	6.28535832	0.40283414
H	-2.43498737	7.26892546	0.48110505
C	-3.98349905	-4.45251874	0.02175104
H	-4.15345207	-4.37923183	1.10167217
H	-4.20420919	-5.49042813	-0.25828706
C	-4.94067044	-3.54438796	-0.69988800
H	-4.86828847	-3.55014834	-1.78764391
C	-5.85195586	-2.76672388	-0.12172064

H	-5.96338403	-2.72915579	0.95795970
H	-6.52280048	-2.14390041	-0.70263267
H	-2.61331445	0.63873109	-3.32227460
H	-1.53303908	-1.29001572	-2.38128772
H	-1.09377176	1.06897891	-4.14161885
H	3.85249983	3.07644612	-1.72226506
H	4.23726238	3.42278714	-0.02034487
H	3.93723317	0.73724142	-1.20225995
H	2.89623928	-3.63145630	-2.53687385
H	4.45580647	-3.84693370	-1.75594520
H	-2.32475024	-4.29169611	-1.36674595
H	-1.88638970	-4.94430888	0.20392680
H	-0.26291168	-3.03042922	-0.88455218

MP2 Electronic Energy(Ha): 1489.128556700623

B3LYP Electronic Energy(Ha): 1492.957606834803

M06-L Electronic Energy(Ha): 1492.773423072917

Zero point energy correction(kcal/mol): 375.362

Enthalpy correction(kcal/mol): 397.845

Entropy correction(cal/mol): 218.142

Imaginary Frequencies: -1514.43

Deuterated zero point energy correction(kcal/mol): 371.472

Deuterated enthalpy correction(kcal/mol): 394.224

Deuterated entropy correction(cal/mol): 220.585

Deuterated imaginary Frequencies: -1103.32

Product geometry

Zr	0.54639189	-0.94601838	0.30833480
C	0.25029813	1.26243255	1.37586318
C	-0.71973595	0.42572428	2.01443074
H	-1.78650780	0.47300970	1.85103258
C	1.51344380	0.82088367	1.87308361
H	2.47472274	1.22723146	1.59114261
C	1.32580810	-0.29753575	2.71933365

H	2.09265281	-0.84217373	3.24565510
C	-0.07022714	-0.54070367	2.80903495
H	-0.54397131	-1.31764644	3.39102627
B	-0.01358844	2.23262953	0.08091046
C	-0.29419228	3.79205824	0.37818828
C	1.27244277	1.91808649	-0.90511413
C	-1.17551073	1.45533619	-0.78520429
N	-1.18659589	0.16037861	-0.88324717
N	1.62739187	0.69859508	-1.16371455
O	2.03028023	2.87476485	-1.46560929
O	-2.07788823	2.09283222	-1.54591618
C	-2.16280912	-0.23550650	-1.91479814
C	-2.90391614	1.08243383	-2.19772105
C	2.84607662	0.71918018	-1.99190514
C	3.03932806	2.22024328	-2.28885954
N	-0.75751831	-2.60041352	0.26986810
N	2.22716675	-2.14525852	-0.10475758
C	2.08449997	-2.73837590	-1.44708160
H	2.75489479	-2.23913688	-2.16634209
H	-1.63623788	-0.61784835	-2.79565306
H	3.68159109	0.28476455	-1.43593911
C	-2.15553498	-2.81316888	0.61576167
H	-2.26613501	-3.11863016	1.67074912
H	-2.69144763	-1.86360257	0.52749959
C	-2.84470030	-3.87402709	-0.25609797
C	2.51774269	-4.21334120	-1.28231504
C	3.48857860	-4.16758372	-0.07759306
H	4.48870889	-4.53296917	-0.32488383
H	1.06360899	-2.64757971	-1.83614842
C	3.51818920	-2.67325325	0.34566835
H	4.31696376	-2.18285406	-0.24177197
H	3.11334129	-4.77574889	0.75023347
C	3.83859953	-2.47142454	1.81825418

H	4.78928524	-2.95599167	2.05924567
H	3.06228414	-2.91353876	2.44881643
H	3.93249567	-1.41324586	2.06815469
C	-0.51485584	4.72078928	-0.65363749
H	-0.49788937	4.38593429	-1.68560122
C	-0.33073751	4.28745455	1.68991193
H	-0.16372357	3.60436544	2.51679010
C	-0.75891724	6.06640577	-0.39241608
H	-0.92503671	6.75561441	-1.21448300
C	-0.57420954	5.63364405	1.96444838
H	-0.59478756	5.98059217	2.99277730
C	-0.78983046	6.53034691	0.92213248
H	-0.97948313	7.57833289	1.12936996
C	-4.33087339	-4.09801613	0.09052069
H	-4.43511208	-4.30197787	1.16205211
H	-4.67632886	-4.99769646	-0.43395475
C	-5.22080691	-2.94883469	-0.29487944
H	-5.24250268	-2.70951851	-1.35840639
C	-5.96806244	-2.22878110	0.53780106
H	-5.98475346	-2.43046540	1.60474042
H	-6.59618561	-1.41826228	0.18518852
H	-3.89438894	1.12329030	-1.74004663
H	-2.82423232	-1.02122066	-1.55168949
H	-2.97938766	1.34227446	-3.25267479
H	2.83943148	2.48556517	-3.32863421
H	4.01319199	2.61303372	-1.99770380
H	2.70842149	0.12959093	-2.90094361
H	1.65286634	-4.84444213	-1.06583224
H	2.98414303	-4.59979988	-2.19192283
H	-2.74437771	-3.59333278	-1.31120961
H	-2.30784703	-4.82339573	-0.14076474
H	-0.25877253	-3.48562337	0.30648851

MP2 Electronic Energy(Ha): 1489.185894719979

B3LYP Electronic Energy(Ha): 1493.022596309517

M06-L Electronic Energy(Ha): 1492.837584302749

Zero point energy correction(kcal/mol): 378.303

Enthalpy correction(kcal/mol): 401.223

Entropy correction(cal/mol): 221.649

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.831

Deuterated enthalpy correction(kcal/mol): 397.083

Deuterated entropy correction(cal/mol): 224.962

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H3

Reactant geometry

Zr	0.54975710	0.90951325	-0.43959994
C	0.25493261	-1.33717031	-1.42430244
C	-0.67680210	-0.51703181	-2.13447876
H	-1.74912506	-0.53803555	-2.00548019
C	1.54390334	-0.93749425	-1.89586583
H	2.48685789	-1.34624085	-1.56061945
C	1.40577995	0.14692572	-2.79002816
H	2.20068193	0.66694657	-3.30385339
C	0.01701331	0.41057318	-2.93904663
H	-0.42148407	1.16909180	-3.57094677
B	-0.06999820	-2.24604673	-0.10184849
C	-0.34003924	-3.81785556	-0.34139561
C	1.16412039	-1.88787054	0.93632930
C	-1.26611578	-1.43025758	0.68147511
N	-1.28993687	-0.13237279	0.72203268
N	1.53516305	-0.65938349	1.12733640
O	1.83305011	-2.81050816	1.64397674
O	-2.18150222	-2.04531324	1.44755567
C	-2.29113480	0.29201955	1.71991651

C	-3.03487076	-1.01719013	2.03030462
C	2.64213309	-0.63316927	2.09959000
C	2.81708395	-2.12111688	2.46987772
N	-0.67662918	2.61148436	-0.41076586
N	2.29255500	2.09469238	-0.22362054
C	3.63721398	1.85903006	-0.77661587
H	3.58943911	1.35193660	-1.74087575
H	-1.78359285	0.70472789	2.59835506
H	3.53710673	-0.20261714	1.64456880
C	-2.07390229	2.92077376	-0.68398691
H	-2.21013123	3.24358018	-1.72981329
H	-2.66535565	2.00786930	-0.57952063
C	-2.64699843	4.01586861	0.22860744
C	4.29194696	3.24137234	-0.86159673
C	3.79374635	3.88763092	0.43189085
H	3.82104616	4.97973870	0.42026054
H	4.24121356	1.21762026	-0.11186450
C	2.35295924	3.34660066	0.58682534
H	1.66305881	4.08378770	0.14746924
H	4.40856684	3.55164614	1.27485932
C	1.94986718	3.16826202	2.05481824
H	2.02881812	4.12010171	2.59118973
H	0.91519291	2.82729978	2.14452674
H	2.60412097	2.44409792	2.54816954
C	-0.32476034	-4.36688726	-1.63213879
H	-0.12445689	-3.71796884	-2.47887317
C	-0.60271513	-4.70377100	0.71799995
H	-0.62637249	-4.32706070	1.73503582
C	-0.55843372	-5.72330348	-1.86096094
H	-0.53845587	-6.11198596	-2.87427542
C	-0.83723239	-6.05919061	0.50233171
H	-1.03672836	-6.71423352	1.34468539
C	-0.81617955	-6.57675096	-0.79222615

H	-0.99836309	-7.63250359	-0.96372345
C	-4.12819051	4.34530370	-0.04893954
H	-4.26568764	4.56667758	-1.11328554
H	-4.38663993	5.26132376	0.49675376
C	-5.07779038	3.25657849	0.36838683
H	-5.07506886	3.01472304	1.43147616
C	-5.90256952	2.59139665	-0.43639819
H	-5.94680056	2.79850494	-1.50151492
H	-6.56954584	1.82315551	-0.06117840
H	-4.00899058	-1.08148657	1.54074527
H	-2.95019831	1.06190768	1.32114316
H	-3.14608464	-1.23591361	3.09144482
H	2.58706788	-2.34346806	3.51264811
H	3.79864286	-2.52658901	2.22339834
H	2.37856800	-0.01661172	2.96219157
H	5.38165000	3.19628043	-0.93433627
H	3.91343066	3.78164016	-1.73527844
H	-2.51920413	3.71501735	1.27494434
H	-2.05138827	4.92726548	0.09807120
H	-0.12032089	3.45545038	-0.54263399

MP2 Electronic Energy(Ha): 1489.186696481045

B3LYP Electronic Energy(Ha): 1493.024565157822

M06-L Electronic Energy(Ha): 1492.838892552713

Zero point energy correction(kcal/mol): 378.151

Enthalpy correction(kcal/mol): 401.091

Entropy correction(cal/mol): 222.126

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.110

Deuterated enthalpy correction(kcal/mol): 397.250

Deuterated entropy correction(cal/mol): 223.459

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.35082489	0.62568286	-0.54914469
C	0.45075596	-1.69481594	-1.39364089
C	-0.25435162	-0.93410799	-2.38467342
H	-1.31523767	-0.98757210	-2.58064220
C	1.81142903	-1.29382707	-1.51429937
H	2.62263621	-1.64653335	-0.89276825
C	1.92652492	-0.26556712	-2.47615612
H	2.83466479	0.24412110	-2.76214060
C	0.63650243	-0.04207336	-3.02763213
H	0.39248045	0.65085174	-3.82007495
B	-0.20832506	-2.48803010	-0.11821609
C	-0.30747614	-4.09358920	-0.22395580
C	0.59635869	-1.92018862	1.21658103
C	-1.63789435	-1.70097966	0.13160486
N	-1.67983545	-0.40726677	0.06167101
N	0.94191475	-0.67014384	1.35845489
O	0.78821916	-2.68599176	2.29924204
O	-2.79167687	-2.29502340	0.46219173
C	-3.03360375	0.06377434	0.39188993
C	-3.80583306	-1.25395855	0.61630650
C	1.33952104	-0.44952433	2.76546885
C	1.46452966	-1.88025187	3.30774202
N	-0.49706820	2.39478648	-0.48327607
N	2.03312563	2.22408307	-0.13798330
C	2.81273210	2.84587541	-1.21854332
H	2.16706255	3.06054783	-2.07539394
H	-3.00335725	0.68966235	1.28657193
H	2.27253773	0.10641274	2.83666175
C	-1.46011492	3.46112396	-0.59993096
H	-1.24112777	4.08991701	-1.47832323
H	-2.46361118	3.04887598	-0.77472982
C	-1.52111496	4.37732357	0.63598469
C	3.43104222	4.13002030	-0.59838652

C	3.25757997	3.94607912	0.93235971
H	2.47888536	4.61257726	1.31096708
H	3.61103317	2.18311943	-1.58169504
C	2.79737074	2.47530928	1.08949678
H	2.12674568	2.36912115	1.94966773
H	4.17277775	4.15959471	1.49066090
C	3.99558306	1.52684763	1.26923547
H	4.48249698	1.69282673	2.23572475
H	3.68426952	0.48133661	1.20992801
H	4.74792040	1.68747558	0.49215583
C	0.20208831	-4.77500258	-1.33904284
H	0.66792675	-4.20546233	-2.13690824
C	-0.90531712	-4.87852720	0.77737760
H	-1.31700407	-4.39786501	1.65833105
C	0.12571133	-6.16323929	-1.45438057
H	0.53126934	-6.65566996	-2.33247587
C	-0.98774487	-6.26451615	0.67315579
H	-1.45667895	-6.83937075	1.46559379
C	-0.47037011	-6.91511062	-0.44626462
H	-0.53322564	-7.99492212	-0.53050201
C	-2.56650302	5.50633549	0.52122810
H	-2.39093665	6.08592752	-0.39209571
H	-2.41876850	6.19767717	1.36112988
C	-3.99088807	5.02464303	0.54742239
H	-4.27656719	4.45559199	1.43245080
C	-4.90487653	5.24332149	-0.39421463
H	-4.67090370	5.80577290	-1.29330179
H	-5.92022557	4.87412224	-0.30027893
H	-4.58545399	-1.44212597	-0.12265098
H	-3.44113758	0.66821100	-0.42157455
H	-4.22460750	-1.35092681	1.61746421
H	0.96844463	-2.05018152	4.26196213
H	2.49846270	-2.22727860	3.36658195

H	0.56046168	0.12522424	3.27763105
H	4.48039304	4.24157313	-0.88231613
H	2.90635612	5.02232555	-0.94574412
H	-1.73323299	3.76673123	1.52200285
H	-0.53283573	4.82160279	0.79508754
H	0.75757572	2.67520861	-0.20201992

MP2 Electronic Energy(Ha): 1489.138705343308

B3LYP Electronic Energy(Ha): 1492.973617940826

M06-L Electronic Energy(Ha): 1492.781614943870

Zero point energy correction(kcal/mol): 375.227

Enthalpy correction(kcal/mol): 398.123

Entropy correction(cal/mol): 227.228

Imaginary Frequencies: -1627.49

Deuterated zero point energy correction(kcal/mol): 371.949

Deuterated enthalpy correction(kcal/mol): 394.969

Deuterated entropy correction(cal/mol): 228.023

Deuterated imaginary Frequencies: -1170.02

Product geometry

Zr	-0.14109783	0.70322101	0.42124472
C	-0.21551381	-1.59218342	1.41403212
C	0.58628662	-0.79070487	2.29523082
H	1.65833784	-0.86065695	2.40910193
C	-1.55048899	-1.15653592	1.62432803
H	-2.41734990	-1.53718344	1.10367266
C	-1.56545396	-0.07522156	2.54066598
H	-2.43887563	0.45322156	2.89578154
C	-0.23246946	0.14578622	2.96899315
H	0.09232920	0.87341576	3.69808477
B	0.32424263	-2.46548511	0.13544903
C	0.40338636	-4.06702615	0.32464528
C	-0.56664689	-1.97424765	-1.17770018
C	1.73990128	-1.72356934	-0.27189473

N	1.78712389	-0.43132314	-0.33021436
N	-0.90668259	-0.73817445	-1.40545146
O	-0.84650074	-2.83408750	-2.17395262
O	2.88550495	-2.35553657	-0.57211603
C	3.14927988	-0.00162835	-0.67991286
C	3.87491691	-1.34130591	-0.92801947
C	-1.42275047	-0.63852442	-2.78465333
C	-1.55642383	-2.10917696	-3.21432830
N	0.76504385	2.35379050	0.41020470
N	-2.15337115	2.12500196	-0.12343747
C	-2.54802381	3.03752809	0.98769207
H	-1.65490530	3.49345460	1.41134058
H	3.13582985	0.64378214	-1.56106559
H	-2.37745738	-0.11125557	-2.81743174
C	1.57832734	3.52122844	0.56741762
H	1.54828066	3.88556166	1.60921629
H	2.63595941	3.28571249	0.36930435
C	1.16981573	4.68603552	-0.35366791
C	-3.53131344	4.02077354	0.34524280
C	-4.31379906	3.14162019	-0.65429315
H	-4.52426269	3.67075814	-1.58568212
H	-3.03345358	2.44739405	1.76742343
C	-3.42148048	1.88248210	-0.89559148
H	-3.14547342	1.80444253	-1.94937952
H	-5.27578130	2.83882999	-0.23357068
C	-4.11343818	0.59173538	-0.46625839
H	-5.04001567	0.46148845	-1.03247074
H	-3.47554287	-0.27553558	-0.63495101
H	-4.37619719	0.61852562	0.59459921
C	-0.09423891	-4.68227692	1.48298837
H	-0.52947579	-4.06375079	2.26120592
C	0.96512228	-4.91394913	-0.64669764
H	1.36868500	-4.48597589	-1.55798847

C	-0.04211682	-6.06450806	1.66639852
H	-0.43729496	-6.50414714	2.57673419
C	1.02475195	-6.29434011	-0.47452297
H	1.46818118	-6.91712767	-1.24567843
C	0.51837803	-6.87812743	0.68594935
H	0.56373085	-7.95344666	0.82342594
C	2.05246998	5.94177966	-0.20861321
H	2.05988226	6.27299626	0.83586375
H	1.59524679	6.75343016	-0.79000505
C	3.46494386	5.75036729	-0.68723184
H	3.56880882	5.41649057	-1.71971803
C	4.56470278	5.96061388	0.03069206
H	4.51366977	6.29095175	1.06386280
H	5.55476889	5.81273988	-0.38635872
H	4.75012519	-1.49807983	-0.29797712
H	3.58325323	0.57146080	0.14306420
H	4.14878472	-1.50213848	-1.97212491
H	-1.08817806	-2.34479750	-4.16917482
H	-2.58972472	-2.46303036	-3.22087609
H	-0.71100692	-0.08332111	-3.40536180
H	-4.17905679	4.50900097	1.07684183
H	-2.97725972	4.80595253	-0.17829323
H	1.19282290	4.33428418	-1.39251884
H	0.12953412	4.95779186	-0.13813861
H	-1.53979972	2.68952983	-0.71229683

MP2 Electronic Energy(Ha): 1489.170131657662

B3LYP Electronic Energy(Ha): 1493.003302937521

M06-L Electronic Energy(Ha): 1492.815469738553

Zero point energy correction(kcal/mol): 379.176

Enthalpy correction(kcal/mol): 402.121

Entropy correction(cal/mol): 223.562

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.337

Deuterated enthalpy correction(kcal/mol): 397.531

Deuterated entropy correction(cal/mol): 225.860

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H4

Reactant geometry

Zr	-0.14323785	-0.46469007	-0.65856063
C	1.23790039	1.57803378	-1.02329728
C	2.23347105	0.60440840	-0.71249443
H	2.76519953	0.53777075	0.22507224
C	0.84295043	1.29632071	-2.37045757
H	0.10285741	1.84783721	-2.93284346
C	1.55221336	0.17964092	-2.84534468
H	1.48900821	-0.25174909	-3.83072021
C	2.39996379	-0.27031872	-1.80662278
H	3.09455177	-1.09739319	-1.87012754
B	0.57043264	2.66852084	-0.01164508
C	1.17004683	4.16899185	-0.06865174
C	-1.03924894	2.54886811	-0.32189582
C	0.63971932	1.94914105	1.46147480
N	0.55440454	0.66684458	1.58853307
N	-1.56507919	1.40672916	-0.64141244
O	-1.91063672	3.56205732	-0.19777277
O	0.70234570	2.65184373	2.61451172
C	0.55557014	0.32953952	3.02314999
C	0.66249657	1.70462378	3.71664722
C	-3.02147244	1.55667162	-0.79242386
C	-3.24897019	3.04730784	-0.46682286
N	-1.07156491	-1.62835495	-2.18233938
H	-0.35550882	-0.21103128	3.29172614
H	-3.32112591	1.29847753	-1.81132546
C	-2.33231154	-2.36534817	-1.94981212

H	-2.15193993	-3.45276571	-1.88303629
H	-2.79483426	-2.04041029	-1.02395792
C	-3.18481759	-2.08087867	-3.18823517
C	-2.14965521	-2.17136194	-4.31598879
H	-2.12168899	-3.18689361	-4.72334053
H	-2.36518870	-1.49745812	-5.14835145
C	-0.78940091	-1.82737032	-3.63327378
H	-0.41449556	-0.89123821	-4.04327497
C	0.25401152	-2.92336491	-3.89076256
H	0.40253523	-3.07107379	-4.96618706
H	1.21751466	-2.66490567	-3.44729296
C	2.23914823	4.49174864	-0.91771173
H	2.66358376	3.71701731	-1.54831762
C	0.65870466	5.21056596	0.72534127
H	-0.16689624	5.00973810	1.39915163
C	1.18321160	6.49957827	0.67452125
H	0.76263264	7.27923406	1.30218884
C	2.77359635	5.77947095	-0.97656013
H	3.60140752	5.99111874	-1.64630858
C	2.24646358	6.79112117	-0.17911839
H	2.65736569	7.79455526	-0.22088197
H	-0.19918245	1.95062340	4.33957089
H	1.57423915	1.83197829	4.30188911
H	1.40675812	-0.31698022	3.26366457
H	-3.85314313	3.21701702	0.42557786
H	-3.66333248	3.62096775	-1.29610394
H	-3.54146454	0.87925657	-0.11189314
H	-4.01550603	-2.78206077	-3.30836830
H	-3.60185950	-1.07132640	-3.11986740
N	-1.62747927	-1.13052386	0.76492917
H	-1.90770476	-0.37533600	1.38244361
C	-1.91442111	-2.40777540	1.39304404
H	-1.63243355	-3.21199957	0.70289386

H	-1.31611241	-2.57621118	2.31315986
C	-3.39179090	-2.63732806	1.76945054
H	-4.00236534	-2.55949485	0.86438847
H	-3.50195641	-3.66568346	2.13871220
C	-3.95753214	-1.66940475	2.82591556
H	-3.88935781	-0.63554673	2.47136506
H	-5.02906705	-1.88236250	2.93484674
C	-3.31159735	-1.78802185	4.17816861
H	-3.27515736	-2.79372528	4.59672801
C	-2.81520297	-0.78077964	4.89250268
H	-2.83897291	0.24135412	4.52505031
H	-2.38605115	-0.93564089	5.87623871
N	1.14447931	-2.23840185	0.43543884
C	1.45268594	-3.53512875	-0.21584120
H	0.60047818	-2.40173059	1.28037638
H	2.00322230	-1.78191041	0.73111005
H	0.50577753	-3.95629494	-0.55696818
H	2.03872276	-3.31894883	-1.11156700
C	2.18656306	-4.54590612	0.67198353
H	1.58819103	-4.74301824	1.57053049
H	2.24360695	-5.49522150	0.12889785
C	3.61006118	-4.12120999	1.07708750
H	3.56616556	-3.17504459	1.63354054
H	4.20607426	-3.93044739	0.17785734
C	4.30050824	-5.14674655	1.93258940
H	3.81638876	-5.37673544	2.88091185
C	5.42406939	-5.78029901	1.61170471
H	5.94164248	-5.58343929	0.67751573
H	5.87068683	-6.51526663	2.27147582
H	-0.07451512	-3.87660144	-3.46505323

MP2 Electronic Energy(Ha): 1740.495660788808

B3LYP Electronic Energy(Ha): 1744.988074025137

M06-L Electronic Energy(Ha): 1744.770165106552

Zero point energy correction(kcal/mol): 477.042

Enthalpy correction(kcal/mol): 505.375

Entropy correction(cal/mol): 259.866

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.525

Deuterated enthalpy correction(kcal/mol): 497.242

Deuterated entropy correction(cal/mol): 262.299

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.35512472	0.58622175	-0.35830511
C	0.24507264	-1.65833381	-1.42433079
C	-0.70004010	-0.88874374	-2.17989334
H	-1.77449423	-0.97663069	-2.12286894
C	1.52702366	-1.21766680	-1.86283009
H	2.47341559	-1.57829754	-1.48628965
C	1.37417690	-0.17720982	-2.79924284
H	2.16690973	0.34655045	-3.30813043
C	-0.01504020	0.02201180	-3.00060802
H	-0.46591836	0.71459411	-3.69366979
B	-0.08403103	-2.64518454	-0.16982845
C	-0.16453092	-4.22717167	-0.47637720
C	0.99788104	-2.20160459	0.98018402
C	-1.44934370	-1.97681374	0.45143557
N	-1.56905009	-0.68790609	0.48281671
N	1.43423321	-0.98127521	1.07969452
O	1.38057971	-3.02931939	1.96585739
O	-2.49467750	-2.66595693	0.93721519
C	-2.91458504	-0.34218158	0.97530325
C	-3.45387223	-1.69940548	1.46202267
C	2.18802551	-0.84881645	2.34036153
C	2.29988002	-2.30228256	2.83014499
N	2.33712700	1.90389495	-0.36538660

H	-2.86981714	0.41327121	1.76085603
H	3.16225609	-0.39306783	2.16725137
C	2.86083762	2.38746601	0.93592789
H	2.77250792	3.48315361	1.01612252
H	2.30136286	1.96036436	1.76609443
C	4.34340332	2.01003549	0.95341614
C	4.74593118	2.26657762	-0.49694771
H	4.95062894	3.33336213	-0.63963788
H	5.63643153	1.71736489	-0.81113252
C	3.49623413	1.85816201	-1.31375408
H	3.63318611	0.83073379	-1.66675105
C	3.31871725	2.77064820	-2.53323436
H	4.20107463	2.71570723	-3.17917448
H	2.44891130	2.50106856	-3.13373123
C	0.08666788	-4.73315326	-1.76034883
H	0.34081078	-4.04358000	-2.55919463
C	-0.49339887	-5.16375462	0.51895474
H	-0.69806409	-4.81988295	1.52713620
C	-0.56646492	-6.52780911	0.24906059
H	-0.82465150	-7.22262797	1.04211810
C	0.01701656	-6.09791249	-2.04250603
H	0.21742008	-6.45297301	-3.04852893
C	-0.31047932	-7.00253610	-1.03670361
H	-0.36725518	-8.06476449	-1.25031253
H	-3.45708466	-1.79805479	2.55014156
H	-4.43721055	-1.95825132	1.07250063
H	-3.51135087	0.07295582	0.15602907
H	1.98447939	-2.45775429	3.86125988
H	3.29443254	-2.72951160	2.68683573
H	1.63226066	-0.20700204	3.02990188
H	4.92224763	2.59178261	1.67561393
H	4.46645756	0.95043903	1.19895065
N	-0.25644612	1.58338018	1.42617565

H	-0.77696043	0.94850929	2.01991650
C	-0.29613425	2.91797944	2.00845050
H	0.39250552	3.57193124	1.46523821
H	-1.29695576	3.37098052	1.89814752
C	0.08942594	2.99431440	3.49782108
H	1.10318773	2.60191795	3.62697983
H	0.12357705	4.05214394	3.78907479
C	-0.85351468	2.25124911	4.46449742
H	-0.87749901	1.18015342	4.23497860
H	-0.42814650	2.33282189	5.47341834
C	-2.25456253	2.79633246	4.49348741
H	-2.33789401	3.87299228	4.63979561
C	-3.36961657	2.08001909	4.37687016
H	-3.34084787	1.00251639	4.24146963
H	-4.35099544	2.53773280	4.42869838
N	0.07157568	2.74751233	-1.19458883
C	-0.26144346	3.42541055	-2.45379838
H	1.31346986	2.62366835	-0.86410986
H	-0.35864487	3.27108490	-0.43741564
H	0.35407287	4.32857474	-2.57321908
H	-0.00741301	2.77260116	-3.29196474
C	-1.73333750	3.85233565	-2.55866221
H	-1.95621994	4.54533879	-1.73623097
H	-1.86733015	4.42602986	-3.48291496
C	-2.74690049	2.69604793	-2.53164941
H	-2.56695010	2.09846044	-1.62982052
H	-2.58065564	2.03384892	-3.38769994
C	-4.17264194	3.16926125	-2.53135703
H	-4.45387601	3.82087835	-1.70426206
C	-5.08771795	2.86462990	-3.44743381
H	-4.85449689	2.22286956	-4.29206755
H	-6.10212907	3.24256581	-3.38740557
H	3.19711184	3.81093952	-2.21577199

MP2 Electronic Energy(Ha): 1740.465788917060

B3LYP Electronic Energy(Ha): 1744.953234634828

M06-L Electronic Energy(Ha): 1744.735098055398

Zero point energy correction(kcal/mol): 474.202

Enthalpy correction(kcal/mol): 502.052

Entropy correction(cal/mol): 255.412

Imaginary Frequencies: -1476.90

Deuterated zero point energy correction(kcal/mol): 466.607

Deuterated enthalpy correction(kcal/mol): 494.800

Deuterated entropy correction(cal/mol): 257.484

Deuterated imaginary Frequencies: -1063.33

Product geometry

Zr	-0.01477510	0.72322015	-0.51223050
C	-0.06110365	-1.56239358	-1.49106894
C	-1.36166970	-1.07485903	-1.81767319
H	-2.28264831	-1.38232674	-1.34495576
C	0.83356949	-0.86406348	-2.35945916
H	1.90473834	-0.99740450	-2.38493643
C	0.10774312	0.04415096	-3.15846701
H	0.51326776	0.70292618	-3.91327797
C	-1.25815490	-0.08840897	-2.82129357
H	-2.07494467	0.44845370	-3.27816927
B	0.34642753	-2.51700239	-0.23352949
C	0.34570553	-4.11006241	-0.50122161
C	1.77777370	-1.89957066	0.29296804
C	-0.62302314	-2.00022756	0.98633082
N	-0.94690722	-0.74859655	1.08236783
N	2.01047425	-0.62560089	0.28905286
O	2.75289845	-2.67079500	0.81433033
O	-1.02572272	-2.77483602	2.00836634
C	-1.62039699	-0.52009966	2.37239294
C	-1.83855184	-1.95081891	2.89620213

C	3.35532482	-0.39064897	0.84640381
C	3.79982006	-1.79215216	1.30911353
N	1.49010298	2.44559628	-1.55131203
H	-0.97761467	0.07878958	3.02385220
H	4.01769872	0.01655895	0.07589575
C	2.85134131	2.07838106	-2.03153066
H	3.47763291	1.80464826	-1.18255918
H	2.77781165	1.21053855	-2.69073891
C	3.34751048	3.29828540	-2.81041271
C	2.07008558	3.75459356	-3.52841645
H	2.09320927	4.80625911	-3.82097696
H	1.92772448	3.16555382	-4.43898260
C	0.92876347	3.46332004	-2.51809559
H	0.08021794	3.00634523	-3.02901407
C	0.44183256	4.70808209	-1.78076097
H	-0.03127141	5.40075988	-2.48133715
H	-0.29519092	4.43894842	-1.02205536
C	0.06501301	-4.63118193	-1.77316735
H	-0.15947851	-3.94682587	-2.58519169
C	0.62714310	-5.04149686	0.51362087
H	0.84855597	-4.68757351	1.51450114
C	0.62827801	-6.41315897	0.27337605
H	0.84921625	-7.10322966	1.08186175
C	0.06402262	-6.00344299	-2.02616182
H	-0.15836448	-6.36911202	-3.02385724
C	0.34628238	-6.90218191	-1.00156735
H	0.34607733	-7.97045881	-1.19181699
H	-1.49208670	-2.11574314	3.91576107
H	-2.87250701	-2.28922953	2.80400277
H	-2.55632104	0.02346913	2.23210928
H	3.83850120	-1.89882153	2.39533943
H	4.74679928	-2.12224495	0.88237890
H	3.32181788	0.33442622	1.66291339

H	3.70355200	4.07020107	-2.12050428
H	4.16378975	3.06087095	-3.49588616
N	0.70077982	1.82658376	1.22414007
H	1.21100305	1.18965406	1.82786599
C	0.21540549	2.94284923	2.02362836
H	-0.28689974	3.66230987	1.36552337
H	-0.54309492	2.63306437	2.76506086
C	1.31223353	3.72136559	2.77419942
H	2.04517057	4.09163414	2.04840317
H	0.85617111	4.60306763	3.24363672
C	2.05725974	2.91539741	3.85659487
H	2.56367721	2.05468940	3.40712230
H	2.84986697	3.55373655	4.26825198
C	1.17913314	2.45401256	4.98613467
H	0.61863299	3.23631038	5.49752447
C	1.04848294	1.19722813	5.40355732
H	1.58885448	0.38201395	4.93080130
H	0.40894419	0.93748313	6.23978526
N	-1.63688958	2.04879024	-0.50587764
C	-2.81646961	2.50246972	-1.23235061
H	1.59725581	2.87996802	-0.63394437
H	-1.58685428	2.58410035	0.35861857
H	-2.71827619	3.56896919	-1.49086134
H	-2.88160438	1.96697470	-2.18134363
C	-4.14075058	2.32872947	-0.46684054
H	-4.05667341	2.83152075	0.50570115
H	-4.93702193	2.84853232	-1.01289144
C	-4.54669646	0.86106410	-0.25521401
H	-3.69750255	0.33522220	0.19539022
H	-4.72902397	0.38653475	-1.22576881
C	-5.75890664	0.70625921	0.61747735
H	-5.67802180	1.13126551	1.61824165
C	-6.89731274	0.11500651	0.26550635

H -7.02987837 -0.31968788 -0.72093291

H -7.73602538 0.03969880 0.94856734

H 1.27152933 5.23244139 -1.29524113

MP2 Electronic Energy(Ha): 1740.505263742711

B3LYP Electronic Energy(Ha): 1744.997615687805

M06-L Electronic Energy(Ha): 1744.779485940294

Zero point energy correction(kcal/mol): 476.980

Enthalpy correction(kcal/mol): 505.295

Entropy correction(cal/mol): 261.963

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.499

Deuterated enthalpy correction(kcal/mol): 497.202

Deuterated entropy correction(cal/mol): 264.334

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H5

Reactant geometry

Zr 0.75211013 0.97302841 -0.22861400

C 0.05316279 -1.08813706 -1.38985750

C -0.92919738 -0.13831292 -1.79541939

H -1.95230704 -0.11818081 -1.44959769

C 1.24529515 -0.71895909 -2.09360266

H 2.19763301 -1.22300695 -2.01920358

C 1.01027286 0.44341544 -2.85468663

H 1.72971248 0.96426688 -3.46929876

C -0.34227467 0.81330265 -2.66488519

H -0.83820537 1.65110328 -3.13576061

B -0.05175414 -2.14157362 -0.14396389

C -0.51005869 -3.64886921 -0.49818780

C 1.41721740 -2.00009599 0.59200092

C -0.96575811 -1.38169345 1.00066471

N -0.92239781 -0.09705571 1.17949256

N	1.98686850	-0.84076388	0.70282527
O	2.07451591	-3.02254226	1.16215597
O	-1.67306640	-2.06602062	1.91996527
C	-1.61500845	0.23109754	2.43819783
C	-2.28314831	-1.10142362	2.82281459
C	3.23663848	-0.98364021	1.46841776
C	3.32105350	-2.50442840	1.71301675
N	-0.85734827	2.82551554	-0.13640885
N	2.23865246	2.36918818	-0.61451018
C	3.26293302	2.95010220	-1.45943015
H	2.90505707	3.88436259	-1.92327394
H	-0.88484147	0.57201084	3.17822006
H	4.08286577	-0.60176310	0.89271072
C	-2.30657993	2.76820879	-0.43236194
H	-2.42166852	2.46946985	-1.47626759
H	-2.73626703	1.96710433	0.17021980
C	-3.04407808	4.08633673	-0.18135743
C	4.46049331	3.27209857	-0.50813584
C	3.88864925	3.09686470	0.92230878
H	4.17266242	3.90766324	1.59847344
H	3.53871657	2.27455808	-2.27276329
C	2.36128709	3.01279500	0.71411144
H	1.97736832	4.05101245	0.64929387
H	4.23815911	2.15958875	1.36457462
C	1.49806246	2.17146727	1.66675023
H	0.83856431	2.78511213	2.29279411
H	-0.41111696	3.53564914	-0.71424076
H	2.11701439	1.58311369	2.34993346
C	-0.57875298	-4.66269856	0.47348459
H	-0.31354151	-4.43512356	1.50002917
C	-0.86411143	-4.00715360	-1.80754232
H	-0.82194944	-3.25494142	-2.58892759
C	-0.97854582	-5.95851040	0.15705682

H	-1.01889984	-6.71636727	0.93335275
C	-1.26680290	-5.30200522	-2.13653524
H	-1.53268387	-5.54166229	-3.16141162
C	-1.32597081	-6.28521783	-1.15319771
H	-1.63741531	-7.29420789	-1.40281211
C	-4.55846920	3.99435019	-0.45913627
H	-4.72696725	3.63511132	-1.48020477
H	-4.97489676	5.00763929	-0.41209859
C	-5.29679292	3.11961326	0.51708015
H	-5.24210522	3.42929535	1.56063049
C	-5.99778986	2.03313733	0.20497436
H	-6.08680414	1.68760908	-0.82065059
H	-6.51756660	1.45484250	0.96038797
H	-3.35985753	-1.11063895	2.64015080
H	-2.34457052	1.03196397	2.29446750
H	-2.08667666	-1.42601293	3.84409098
H	3.36067555	-2.78337629	2.76607986
H	4.14224296	-2.98699509	1.18101632
H	3.17854213	-0.40990492	2.39623434
H	5.29770236	2.59367207	-0.68733539
H	4.82828079	4.28715539	-0.67755625
H	-2.88356511	4.40350552	0.85690785
H	-2.61151161	4.86905306	-0.81529772
H	-0.70978888	3.12449967	0.82549339

MP2 Electronic Energy(Ha): 1489.174591321482

B3LYP Electronic Energy(Ha): 1493.002774912113

M06-L Electronic Energy(Ha): 1492.818895201521

Zero point energy correction(kcal/mol): 378.517

Enthalpy correction(kcal/mol): 401.454

Entropy correction(cal/mol): 226.182

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.110

Deuterated enthalpy correction(kcal/mol): 397.221

Deuterated entropy correction(cal/mol): 227.317

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.80649947	0.78238900	0.10711139
C	0.00847810	-1.18600435	1.34600688
C	0.99373467	-0.21338416	1.69166993
H	2.00878041	-0.19565114	1.32185797
C	-1.17651591	-0.78404010	2.04264209
H	-2.12320382	-1.30298900	2.02123595
C	-0.93755227	0.42730626	2.72764222
H	-1.64596940	0.97233166	3.33434079
C	0.41719425	0.77928712	2.51148986
H	0.91224058	1.64991842	2.91560792
B	0.10877352	-2.29948025	0.15192558
C	0.65397552	-3.76238623	0.55685756
C	-1.38902120	-2.26081858	-0.52825802
C	0.95345308	-1.53482987	-1.04383541
N	0.77661984	-0.27106838	-1.28603035
N	-2.03664543	-1.14188458	-0.65002548
O	-1.98339210	-3.33219057	-1.07529452
O	1.78222282	-2.16639515	-1.88702798
C	1.53791878	0.10930241	-2.48705938
C	2.30891868	-1.18236878	-2.82710859
C	-3.25158329	-1.38125448	-1.45255190
C	-3.29886423	-2.91613160	-1.54601151
N	0.59943678	2.63057326	-0.19479978
N	-1.76363806	2.77429047	0.58911906
C	-2.61123353	3.39809226	1.62246290
H	-2.04578759	4.12368236	2.21855869
H	0.85219062	0.41459115	-3.28234021
H	-4.13426241	-0.96277353	-0.96495504
C	1.97604358	2.88379121	0.23172588

H	2.05166960	2.68147793	1.30368956
H	2.67787467	2.19126595	-0.25432142
C	2.43333488	4.32461224	-0.02914071
C	-3.77455185	4.07286881	0.85635341
C	-3.83404179	3.29210243	-0.46453290
H	-4.34085464	3.83344940	-1.26742941
H	-2.99820406	2.64670763	2.32029554
C	-2.35708055	3.02924437	-0.77360357
H	-1.92533034	3.95773597	-1.18158948
H	-4.35432957	2.33696298	-0.32174649
C	-1.99058347	1.81328173	-1.63596351
H	-1.44433526	2.08492493	-2.54556440
H	-0.49909312	3.05529907	0.40683069
H	-2.88972807	1.27731347	-1.95209016
C	0.76239498	-4.80819568	-0.37624075
H	0.47168761	-4.63589523	-1.40696365
C	1.04414546	-4.04919536	1.87339015
H	0.97568246	-3.26958045	2.62550185
C	1.23292496	-6.06829330	-0.01601202
H	1.30274236	-6.85308819	-0.76271648
C	1.51759941	-5.30762695	2.24598600
H	1.81036617	-5.49227426	3.27478958
C	1.61395271	-6.32444052	1.30055437
H	1.98092232	-7.30526160	1.58423931
C	3.89587218	4.59419165	0.37812990
H	4.04761729	4.31356657	1.42638444
H	4.07476665	5.67496396	0.31578656
C	4.90631360	3.89141523	-0.48634139
H	4.86136212	4.13136748	-1.54891366
C	5.82969373	3.03255650	-0.06283263
H	5.91697607	2.76251261	0.98542761
H	6.53608644	2.57296708	-0.74514891
H	3.38330048	-1.10568425	-2.65404408

H	2.20175463	0.94897771	-2.27276756
H	2.13024468	-1.55717225	-3.83457664
H	-3.43203090	-3.30319282	-2.55526377
H	-4.04202380	-3.36483549	-0.88351906
H	-3.15031987	-0.90299907	-2.43012513
H	-4.71082201	4.05126817	1.41912263
H	-3.53582567	5.12174274	0.65481111
H	2.30820514	4.55581963	-1.09543294
H	1.77217861	5.00955782	0.51213374
H	0.50100227	2.91565059	-1.16696635

MP2 Electronic Energy(Ha): 1489.137320634531

B3LYP Electronic Energy(Ha): 1492.965899682640

M06-L Electronic Energy(Ha): 1492.777662397526

Zero point energy correction(kcal/mol): 375.394

Enthalpy correction(kcal/mol): 397.892

Entropy correction(cal/mol): 221.401

Imaginary Frequencies: -1522.74

Deuterated zero point energy correction(kcal/mol): 371.937

Deuterated enthalpy correction(kcal/mol): 394.576

Deuterated entropy correction(cal/mol): 222.176

Deuterated imaginary Frequencies: -1095.85

Product geometry

Zr	0.40993212	-0.81610423	0.02348574
C	-0.69836159	1.06034227	1.18177633
C	-1.72336607	0.06315309	1.18270743
H	-2.61245119	0.08009511	0.56835725
C	0.26958436	0.60501057	2.12840212
H	1.18545918	1.11739977	2.38080274
C	-0.12195788	-0.65120449	2.64366691
H	0.41085541	-1.23780012	3.37943935
C	-1.36979415	-0.97968980	2.06393646
H	-1.94379681	-1.86924113	2.27267961

B	-0.52282810	2.28954765	0.12040169
C	-1.21781722	3.69325465	0.51449622
C	1.09666082	2.36090192	-0.15262646
C	-0.99409791	1.64745848	-1.32295391
N	-0.70162035	0.41986510	-1.62120802
N	1.83655310	1.29828669	-0.19527579
O	1.71603345	3.51945946	-0.45849794
O	-1.60842763	2.33918744	-2.29527111
C	-1.12382590	0.13011943	-3.00013129
C	-1.80338001	1.44622877	-3.43288148
C	3.18392932	1.69125902	-0.65161271
C	3.12672360	3.22935778	-0.64729168
N	-0.53553769	-2.62586275	-0.46327439
N	2.34539602	-1.98228135	0.81176190
C	3.50420611	-1.48609064	1.59823871
H	3.38858479	-1.75224962	2.65034474
H	-0.25471201	-0.12113245	-3.61354417
H	3.95733717	1.30519862	0.01650519
C	-1.69393047	-3.45365272	-0.14552472
H	-2.41345517	-2.86679672	0.43131148
H	-2.21563458	-3.74777347	-1.06583496
C	-1.34200922	-4.72280404	0.64793717
C	4.73284331	-2.10927818	0.92328041
C	4.35542499	-2.04672547	-0.56360957
H	4.91195300	-2.75512609	-1.18030304
H	3.53859614	-0.39640327	1.53387714
C	2.83696408	-2.32998978	-0.61717003
H	2.67335225	-3.40523795	-0.73184297
H	4.55477131	-1.04637959	-0.95749494
C	1.98252708	-1.53878019	-1.60206334
H	1.58913894	-2.17239590	-2.40255263
H	1.99783956	-2.83086969	1.24728392
H	2.55023643	-0.73393836	-2.07447806

C	-1.17998896	4.81397222	-0.33359838
H	-0.67185099	4.74182916	-1.28893015
C	-1.89006433	3.85118554	1.73563546
H	-1.94441250	3.01038677	2.41995043
C	-1.77781926	6.02187528	0.01647873
H	-1.72881279	6.86636880	-0.66401635
C	-2.49228254	5.05671019	2.09781172
H	-3.00361096	5.14050455	3.05177589
C	-2.43859691	6.14955072	1.23765895
H	-2.90553061	7.08945950	1.51321001
C	-2.55793477	-5.61505651	0.96919107
H	-3.31658265	-5.03210941	1.50380021
H	-2.23091565	-6.40521551	1.65726415
C	-3.17645015	-6.25909251	-0.24073654
H	-2.50565593	-6.87684694	-0.83805988
C	-4.44551049	-6.14011336	-0.62061180
H	-5.15232301	-5.53596332	-0.05943909
H	-4.82606018	-6.64406413	-1.50202186
H	-2.87768139	1.35032821	-3.59573090
H	-1.80449657	-0.72389649	-3.01669928
H	-1.34681290	1.91591283	-4.30423180
H	3.44635975	3.69397384	-1.57978188
H	3.67383127	3.67766798	0.18521868
H	3.37336129	1.28303686	-1.64875114
H	5.65714326	-1.57635909	1.15851674
H	4.85496830	-3.14774586	1.24962927
H	-0.60002609	-5.30350092	0.08502792
H	-0.85605037	-4.42415681	1.58347537
H	-0.06049902	-3.03717039	-1.26250314

MP2 Electronic Energy(Ha): 1489.172248308476

B3LYP Electronic Energy(Ha): 1493.004950457762

M06-L Electronic Energy(Ha): 1492.821295728928

Zero point energy correction(kcal/mol): 379.128

Enthalpy correction(kcal/mol): 401.632

Entropy correction(cal/mol): 217.842

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.763

Deuterated enthalpy correction(kcal/mol): 397.463

Deuterated entropy correction(cal/mol): 218.945

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H6

Reactant geometry

Zr	0.83086759	-1.17001169	0.66083915
C	-0.37506299	0.95499736	1.33536139
C	-1.16219786	-0.16757938	1.75309641
H	-2.12296825	-0.43887245	1.33649566
C	0.78050105	0.93347705	2.16204252
H	1.59460186	1.64050811	2.09905182
C	0.72919846	-0.18247131	3.03650788
H	1.46672077	-0.45020603	3.77803458
C	-0.49287591	-0.86242896	2.79154185
H	-0.84863345	-1.73959465	3.31304533
B	-0.72887782	1.92238539	0.06956923
C	-2.19028029	2.63941444	0.21168517
C	0.47374926	3.02198540	-0.14761633
C	-0.63769214	0.94589584	-1.24618916
N	-0.16744693	-0.27079796	-1.23739739
N	1.71992857	2.77272215	-0.35995340
O	0.13380972	4.33908129	-0.09152908
O	-1.01318315	1.38410400	-2.45953923
C	-0.19699612	-0.82176812	-2.60877945
C	-0.82835670	0.31673271	-3.42938139
C	2.43731223	4.05686745	-0.47950972
C	1.33214025	5.12058229	-0.31469240

N	0.26208315	-3.10348505	0.15432080
N	2.68303160	-0.04932436	-0.34906262
C	3.31007050	-0.31428210	-1.66488845
H	2.88411762	0.35037572	-2.41804822
H	0.81346453	-1.06834513	-2.94209416
H	3.20989933	4.13173259	0.29259450
C	-0.97804571	-3.77203362	-0.23197862
H	-1.74091295	-3.00791628	-0.42114010
H	-0.84677327	-4.31182579	-1.17991749
C	-1.50739495	-4.74859369	0.82766876
C	4.80933731	-0.09856213	-1.41921484
C	5.01664087	-0.71911104	-0.02638861
H	5.84857939	-0.26537394	0.51622890
H	3.12235399	-1.34881075	-1.97180278
C	3.66236615	-0.52106428	0.71445849
H	3.74691462	0.28162649	1.45120813
H	5.22917811	-1.78805292	-0.11467998
C	2.98997696	-1.74107679	1.34046423
H	3.24713017	-1.89287237	2.39006881
H	2.48980077	0.96656962	-0.29370146
H	3.27436063	-2.65098297	0.79061973
C	-2.83497903	2.72370430	1.45627103
H	-2.36703531	2.27950913	2.32825175
C	-2.84820412	3.24791124	-0.87217769
H	-2.39006637	3.22476873	-1.85353879
C	-4.06178429	3.36863174	1.61608737
H	-4.52319878	3.41362485	2.59777343
C	-4.07604642	3.88987430	-0.72603301
H	-4.55117029	4.34619768	-1.58911950
C	-4.69264732	3.95305508	0.52199693
H	-5.64852635	4.45287979	0.63924691
C	-2.82733000	-5.43945042	0.43143675
H	-3.59409744	-4.68500140	0.22225090

H	-3.18372978	-6.01306596	1.29639226
C	-2.69938510	-6.37038266	-0.74260764
H	-1.96347335	-7.16697857	-0.63240772
C	-3.40431389	-6.30101917	-1.86845347
H	-4.15085643	-5.52777582	-2.02465016
H	-3.26788667	-7.01718677	-2.67102604
H	-1.80799901	0.06773619	-3.83936429
H	-0.78746403	-1.73940218	-2.63262597
H	-0.18903970	0.69705833	-4.22641122
H	1.17624744	5.73221481	-1.20559822
H	1.47477398	5.77552244	0.54662721
H	2.93889061	4.12036328	-1.45004292
H	5.43381692	-0.55610830	-2.19024178
H	5.02652602	0.97393189	-1.40445562
H	-0.74219625	-5.51038954	1.02558970
H	-1.65037559	-4.20383082	1.76614457
H	0.99432355	-3.79260526	0.31877683

MP2 Electronic Energy(Ha): 1489.161498953282

B3LYP Electronic Energy(Ha): 1493.003771275588

M06-L Electronic Energy(Ha): 1492.810681542651

Zero point energy correction(kcal/mol): 378.139

Enthalpy correction(kcal/mol): 401.147

Entropy correction(cal/mol): 229.761

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.287

Deuterated enthalpy correction(kcal/mol): 396.638

Deuterated entropy correction(cal/mol): 235.220

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.08162165	-1.11425887	0.33917114
C	-0.77074621	1.19585183	1.15444945
C	-1.94921225	0.38105708	1.07102995

H	-2.75711994	0.52940206	0.36760547
C	-0.00941859	0.65131781	2.22223649
H	0.95220429	1.02030874	2.54915521
C	-0.68472901	-0.47689170	2.76548478
H	-0.35221828	-1.08342805	3.59581009
C	-1.90222983	-0.63461833	2.05918286
H	-2.65710123	-1.38410570	2.24854875
B	-0.37097815	2.35557684	0.07946773
C	-1.45974999	3.57199850	0.01177370
C	1.14709592	2.90904536	0.38984629
C	-0.25792026	1.56580064	-1.35942899
N	-0.24350281	0.26763721	-1.49576684
N	2.23685165	2.22059902	0.41807621
O	1.27981881	4.23538766	0.66685004
O	-0.15546171	2.24040474	-2.51534130
C	-0.19941955	-0.07764391	-2.93222686
C	-0.01719324	1.29122259	-3.60897562
C	3.34947719	3.12406236	0.77142203
C	2.68316170	4.50957248	0.89214059
N	-0.53276651	-2.86805479	-0.32705547
N	2.22497434	-0.71234910	-0.01002415
C	2.95881462	-0.90303788	-1.28854787
H	2.99298212	0.04157389	-1.83276390
H	0.61993981	-0.76565875	-3.14417832
H	3.81483648	2.80010949	1.70830295
C	-0.98322978	-4.19526637	-0.66096572
H	-1.13346634	-4.26655272	-1.74816896
H	-0.21296864	-4.94225281	-0.41546563
C	-2.29528338	-4.58115255	0.04003177
C	4.33203994	-1.43565904	-0.86397597
C	3.96104288	-2.38783196	0.27988144
H	4.78721008	-2.59190752	0.96359167
H	2.44532295	-1.64441029	-1.90819754

C	2.77806984	-1.69952949	1.00228918
H	3.15061756	-1.11392853	1.84792285
H	3.63067908	-3.34710700	-0.13132369
C	1.64221744	-2.63194462	1.46153318
H	1.39444856	-2.50532563	2.51632602
H	2.36732454	0.27267316	0.27880208
H	1.92900408	-3.68179378	1.34147941
C	-2.45382239	3.71527153	0.99208695
H	-2.51396503	2.99141544	1.79750728
C	-1.43190591	4.55362100	-0.99532282
H	-0.67824436	4.49822350	-1.77183981
C	-3.37040769	4.76755748	0.97286362
H	-4.12126326	4.84246279	1.75337929
C	-2.34407921	5.60539221	-1.02808919
H	-2.28880782	6.34222455	-1.82363356
C	-3.32275758	5.71809233	-0.04191358
H	-4.03464547	6.53665210	-0.06409056
C	-2.81075679	-5.98293702	-0.33962884
H	-2.93334233	-6.05377628	-1.42642925
H	-3.81073702	-6.10722869	0.09518301
C	-1.93406223	-7.10448075	0.14471937
H	-1.75922713	-7.13225851	1.22030888
C	-1.37823889	-8.04122090	-0.61878524
H	-1.52326532	-8.05661731	-1.69508008
H	-0.76381590	-8.82921644	-0.19773416
H	-0.77908620	1.52535463	-4.35173895
H	-1.13165958	-0.57127860	-3.21841142
H	0.97233340	1.43259623	-4.04766289
H	3.01491859	5.22147896	0.13336481
H	2.78569214	4.96612917	1.87788064
H	4.12177726	3.09581625	-0.00318041
H	4.86499003	-1.92955551	-1.67972653
H	4.95675544	-0.61348562	-0.50060872

H -2.14805293 -4.52080781 1.12462001

H -3.05460289 -3.83422788 -0.21265616

H 0.51801595 -2.95608478 0.52157402

MP2 Electronic Energy(Ha): 1489.125151659596

B3LYP Electronic Energy(Ha): 1492.959685088214

M06-L Electronic Energy(Ha): 1492.765478444510

Zero point energy correction(kcal/mol): 375.814

Enthalpy correction(kcal/mol): 398.385

Entropy correction(cal/mol): 229.434

Imaginary Frequencies: -1490.65

Deuterated zero point energy correction(kcal/mol): 372.291

Deuterated enthalpy correction(kcal/mol): 394.981

Deuterated entropy correction(cal/mol): 230.038

Deuterated imaginary Frequencies: -1092.40

Product geometry

Zr -0.13829018 -1.12239114 0.19762621

C -0.74132376 1.14140663 1.20375768

C -1.92463945 0.32933074 1.21246273

H -2.80285013 0.50366302 0.60524956

C 0.12658139 0.55117132 2.15962811

H 1.11595010 0.91067440 2.40394211

C -0.48313380 -0.61262944 2.71057461

H -0.07529045 -1.24705409 3.48571584

C -1.77130364 -0.73833272 2.13095982

H -2.50284737 -1.49858437 2.36194206

B -0.43203839 2.31258243 0.11141993

C -1.47238597 3.56888964 0.18359096

C 1.13599313 2.79657885 0.24074651

C -0.49146282 1.56657031 -1.36152566

N -0.48761679 0.27018972 -1.55575858

N 2.18664522 2.05725720 0.11760161

O 1.36723741 4.10824120 0.51318499

O	-0.52037443	2.28359015	-2.49092470
C	-0.61901457	-0.01225176	-3.00176792
C	-0.48078636	1.38156137	-3.63375619
C	3.37766816	2.90279752	0.33649206
C	2.79941420	4.31642534	0.54666785
N	-0.60491309	-2.83001527	-0.39792342
N	2.23437755	-0.92383994	0.03089149
C	2.80456862	-1.29878035	-1.29537227
H	2.40159809	-0.63838263	-2.06439991
H	0.15095954	-0.70924753	-3.33537749
H	3.93825598	2.54797009	1.20813001
C	-1.12022256	-4.13741313	-0.68385420
H	-1.37033996	-4.22250057	-1.75457255
H	-0.35229233	-4.90290636	-0.49650769
C	-2.37580040	-4.48976253	0.13107288
C	4.31876715	-1.17011093	-1.10607450
C	4.53146072	-1.71567678	0.31702879
H	5.36695472	-1.23412705	0.82818514
H	2.51502539	-2.32493919	-1.53450430
C	3.18512147	-1.47886423	1.06441501
H	3.29734984	-0.70677461	1.82910731
H	4.74746539	-2.78703807	0.28251919
C	2.65420753	-2.75333814	1.71782946
H	1.73350140	-2.56860350	2.27673224
H	2.29574871	0.11486028	0.08324373
H	3.39413815	-3.14794610	2.42010393
C	-2.39084236	3.69125999	1.23751559
H	-2.41995903	2.92732255	2.00655932
C	-1.47854655	4.60136826	-0.77188950
H	-0.78248069	4.56350008	-1.60151081
C	-3.26824396	4.77227060	1.33635328
H	-3.96077889	4.82953265	2.17039683
C	-2.35190417	5.68243203	-0.68655418

H	-2.32474242	6.45886215	-1.44500998
C	-3.25585214	5.77365977	0.37082882
H	-3.93734169	6.61507748	0.44082569
C	-2.95317818	-5.88399202	-0.18248861
H	-3.17688724	-5.96390704	-1.25250007
H	-3.91134009	-5.98347656	0.34419101
C	-2.06065409	-7.02039427	0.23253196
H	-1.77434344	-7.03109600	1.28436711
C	-1.61365173	-7.98922462	-0.56188074
H	-1.86971782	-8.02177898	-1.61689885
H	-0.97991003	-8.78604158	-0.18851046
H	-1.29737588	1.65482341	-4.30051825
H	-1.59105452	-0.47212383	-3.19522260
H	0.47248869	1.53701802	-4.14259592
H	3.05785209	5.01641669	-0.25072827
H	3.05519304	4.76205377	1.50901193
H	4.04731771	2.84792077	-0.52706453
H	4.88733185	-1.71820140	-1.86015645
H	4.60811073	-0.11722274	-1.16708972
H	-2.13235034	-4.42074463	1.19779891
H	-3.13976402	-3.72971560	-0.06319131
H	2.44885484	-3.52405116	0.97067525

MP2 Electronic Energy(Ha): 1489.169107889255

B3LYP Electronic Energy(Ha): 1493.008396330441

M06-L Electronic Energy(Ha): 1492.813497029376

Zero point energy correction(kcal/mol): 379.286

Enthalpy correction(kcal/mol): 402.109

Entropy correction(cal/mol): 220.649

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.965

Deuterated enthalpy correction(kcal/mol): 397.926

Deuterated entropy correction(cal/mol): 221.541

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H7

Reactant geometry

Zr	0.38167211	0.24646342	-0.81044026
C	-0.48771777	-1.93859835	-1.61116267
C	-1.59118792	-1.07703975	-1.87227336
H	-2.50861938	-1.05285627	-1.30358601
C	0.48898747	-1.60906870	-2.60964840
H	1.45384405	-2.08185901	-2.72326166
C	0.01408990	-0.55628086	-3.40964751
H	0.54379373	-0.08292293	-4.22277735
C	-1.27635086	-0.21141813	-2.94288356
H	-1.91113556	0.55790145	-3.35884959
B	-0.25928008	-2.89641987	-0.31409188
C	-0.72429161	-4.43844504	-0.44763265
C	1.33880664	-2.67865810	0.01880670
C	-0.93307167	-2.07358037	0.93865506
N	-0.98449235	-0.77890762	0.96951640
N	1.88973346	-1.51345140	-0.13153580
O	2.15748776	-3.64658730	0.46109958
O	-1.34632115	-2.69447641	2.06286329
C	-1.43201904	-0.35500307	2.30916372
C	-1.85268817	-1.67902346	2.97204039
C	3.32847105	-1.61393854	0.17266117
C	3.46451278	-3.05140518	0.71079997
N	0.49172948	4.17902323	-1.35465132
H	-0.60734289	0.13684782	2.83393193
H	3.91231422	-1.45078054	-0.73888785
C	0.21503455	5.01728675	-2.53877923
H	-0.32971001	4.41808687	-3.27496824
H	-0.41807595	5.86543244	-2.26758064
C	1.59587661	5.41686177	-3.08229199

C	2.45192085	4.15846838	-2.81852190
H	2.54659592	3.55676400	-3.72513682
H	3.46374937	4.41778044	-2.49627244
C	1.68575596	3.33555439	-1.72042018
H	2.30598986	3.23648890	-0.82851037
C	1.24515618	1.94627898	-2.18524806
H	0.66790271	2.06715733	-3.11046326
H	2.15608276	1.39894051	-2.50017217
C	-1.33568777	-4.90854758	-1.61949217
H	-1.49295237	-4.21994667	-2.44359983
C	-0.54271390	-5.37222988	0.58755513
H	-0.07516730	-5.05633024	1.51370073
C	-0.94809158	-6.69847101	0.46094774
H	-0.79129573	-7.39222898	1.28118500
C	-1.74653613	-6.23490536	-1.75772030
H	-2.21602945	-6.56213412	-2.68024381
C	-1.55390967	-7.13736498	-0.71573124
H	-1.87059596	-8.17021516	-0.81749365
H	-1.40947083	-1.85158345	3.95233804
H	-2.93594971	-1.80218564	3.03809338
H	-2.26187749	0.35336822	2.24317617
H	3.64736101	-3.09645171	1.78642750
H	4.21003166	-3.65373917	0.19296672
H	3.63246895	-0.85476429	0.89516543
H	1.57410377	5.70638651	-4.13598724
H	1.97703445	6.27341911	-2.51596176
H	0.77663326	4.81026115	-0.60900060
N	1.44647810	1.08503044	0.85559185
H	1.79504415	0.33791407	1.44783492
C	1.41389464	2.31575615	1.62940200
H	1.01198122	3.11918192	1.00677917
H	0.73310528	2.24073054	2.49831073
C	2.78361461	2.78031287	2.16008525

H	3.46783099	2.90127604	1.31370597
H	2.66435841	3.76991568	2.62172059
C	3.43363956	1.83157093	3.18659641
H	3.60338630	0.84795518	2.73663446
H	4.42644167	2.22861260	3.43432348
C	2.64665358	1.67866344	4.45816708
H	2.42711697	2.60372818	4.99105236
C	2.21821858	0.52838666	4.97237561
H	2.41524412	-0.42144206	4.48335395
H	1.66868703	0.49055242	5.90642696
N	-1.21660908	1.98553133	-0.27226037
C	-2.65237029	2.01404646	-0.62781946
H	-0.74676719	2.82811194	-0.65506234
H	-1.11834350	2.04606204	0.73794168
H	-2.71880019	1.96105779	-1.71498643
H	-3.12185678	1.10618445	-0.23878424
C	-3.40992359	3.25586448	-0.13858565
H	-2.91175741	4.15385785	-0.52216878
H	-4.41089046	3.24234486	-0.58353455
C	-3.55385724	3.35685078	1.39099401
H	-2.55699946	3.37086032	1.85187984
H	-4.06783459	2.46679788	1.77141678
C	-4.29671091	4.58978006	1.82426813
H	-3.84217899	5.53892435	1.54284769
C	-5.44364699	4.59903022	2.49633168
H	-5.93500818	3.67806756	2.79625894
H	-5.93328373	5.52555646	2.77360868

MP2 Electronic Energy(Ha): 1740.460794435599

B3LYP Electronic Energy(Ha): 1744.955587120810

M06-L Electronic Energy(Ha): 1744.734160523193

Zero point energy correction(kcal/mol): 477.487

Enthalpy correction(kcal/mol): 505.440

Entropy correction(cal/mol): 256.158

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.683

Deuterated enthalpy correction(kcal/mol): 496.997

Deuterated entropy correction(cal/mol): 258.248

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.04732185	0.08854005	-0.67616675
C	-1.05420851	-2.11709875	-1.23267598
C	-2.21154395	-1.31090400	-1.02817333
H	-2.86535149	-1.36427054	-0.16976885
C	-0.50245155	-1.67512147	-2.48177202
H	0.37345031	-2.08644530	-2.96185875
C	-1.25592001	-0.59761606	-2.97753026
H	-1.07259405	-0.05238462	-3.89144898
C	-2.31662090	-0.36097608	-2.06414741
H	-3.08024443	0.39435884	-2.17348872
B	-0.34260857	-3.12053286	-0.15742888
C	-0.80647269	-4.66469305	-0.16346512
C	1.25598029	-2.86117821	-0.44144289
C	-0.50537083	-2.33669485	1.27638223
N	-0.46445381	-1.04113934	1.33009849
N	1.69163650	-1.66328389	-0.67753857
O	2.18335341	-3.83110605	-0.46597400
O	-0.57255402	-2.95319230	2.46611971
C	-0.44204715	-0.60859885	2.73654345
C	-0.67892888	-1.92697221	3.49791813
C	3.13228876	-1.73100181	-0.98806797
C	3.47819878	-3.20494059	-0.69919105
N	-0.47616078	4.61455453	-1.39405717
H	0.52448590	-0.15159680	2.96823711
H	3.30185934	-1.45592991	-2.03396749
C	0.07928587	5.93841891	-1.68595327

H	-0.62878871	6.72781301	-1.42083631
H	1.01829553	6.13151880	-1.13859235
C	0.36711689	5.87331008	-3.20140913
C	0.51096721	4.35657832	-3.50043819
H	-0.28972895	4.01822347	-4.16234856
H	1.46108715	4.10611607	-3.97800485
C	0.37165664	3.65544781	-2.12731231
H	1.37912117	3.60416644	-1.67946805
C	-0.22393623	2.24706426	-2.17137210
H	-1.13441631	2.27529075	-2.77988395
H	0.48733907	1.61787780	-2.73035457
C	-1.78954223	-5.12474339	-1.05189410
H	-2.24324967	-4.42417159	-1.74585222
C	-0.25196993	-5.61403059	0.71246613
H	0.51162893	-5.30609230	1.41901625
C	-0.65551475	-6.94663947	0.70306919
H	-0.20558715	-7.65282569	1.39385800
C	-2.20194429	-6.45756881	-1.07072287
H	-2.96548268	-6.77741053	-1.77279855
C	-1.63536362	-7.37564786	-0.19135589
H	-1.95198719	-8.41333081	-0.20135367
H	0.06631808	-2.14395829	4.26221008
H	-1.67715946	-2.00154676	3.93284285
H	-1.22032282	0.13261635	2.92679808
H	4.07763539	-3.33986193	0.20329815
H	3.95564289	-3.72313261	-1.53000146
H	3.70886113	-1.03789118	-0.37254472
H	-0.46291963	6.29936171	-3.76808533
H	1.26366667	6.44047539	-3.45976924
H	-0.49759473	4.41803065	-0.39939257
N	1.63531757	1.03128960	0.19161204
H	2.29975901	0.34404051	0.53052478
C	1.93804043	2.32134679	0.79963917

H	1.22799319	3.06441804	0.43009160
H	1.80544437	2.28475129	1.89414961
C	3.35547427	2.84607807	0.51177547
H	3.50138373	2.89041125	-0.57215885
H	3.42731193	3.87552095	0.88577751
C	4.49377126	2.01359728	1.13547940
H	4.47021581	0.98820596	0.75130768
H	5.44739519	2.44070597	0.80001923
C	4.47722796	1.99299489	2.63845498
H	4.51260804	2.96859675	3.12283671
C	4.42988168	0.90304427	3.40013443
H	4.39787584	-0.09276509	2.96708292
H	4.43452624	0.96291891	4.48274231
N	-1.27935198	1.71848778	0.32888299
C	-2.71250712	1.85613737	0.58702689
H	-0.80436037	2.09845713	-0.84233315
H	-0.73251755	2.09510217	1.09589722
H	-3.24613249	1.57935160	-0.32397446
H	-3.04263414	1.14313670	1.36000488
C	-3.15746898	3.27049026	0.99033261
H	-2.85607958	3.97318514	0.20600663
H	-4.25263735	3.28867058	1.02991385
C	-2.61350018	3.73791230	2.35273375
H	-1.51490653	3.73921866	2.32611126
H	-2.90854929	3.02604137	3.13263370
C	-3.08182602	5.11615717	2.72697655
H	-2.81217448	5.91140391	2.03301580
C	-3.79549068	5.41970624	3.80697456
H	-4.09202564	4.66024963	4.52468016
H	-4.10942000	6.43631876	4.01499537

MP2 Electronic Energy(Ha): 1740.417103130825

B3LYP Electronic Energy(Ha): 1744.914249874793

M06-L Electronic Energy(Ha): 1744.690292936216

Zero point energy correction(kcal/mol): 473.887

Enthalpy correction(kcal/mol): 501.758

Entropy correction(cal/mol): 256.332

Imaginary Frequencies: -1570.51

Deuterated zero point energy correction(kcal/mol): 466.200

Deuterated enthalpy correction(kcal/mol): 494.429

Deuterated entropy correction(cal/mol): 258.401

Deuterated imaginary Frequencies: -1137.42

Product geometry

Zr	0.03864259	-0.48245887	-0.45304934
C	0.58832148	-2.18611085	1.26342928
C	1.80835202	-1.44902051	1.16295878
H	2.72294750	-1.81465524	0.71701806
C	-0.33739061	-1.29627879	1.89375719
H	-1.36830715	-1.52466858	2.12073524
C	0.26650049	-0.03231290	2.08351512
H	-0.18926699	0.83709583	2.53539699
C	1.61029368	-0.13341149	1.62841449
H	2.34450553	0.65779375	1.65834993
B	0.22350218	-3.57696514	0.47425689
C	0.50357858	-4.95943570	1.25538655
C	-1.32455567	-3.35872621	-0.04333345
C	0.99600704	-3.41873979	-0.97814479
N	0.96883520	-2.29172338	-1.62356921
N	-1.72468941	-2.21751516	-0.50681055
O	-2.22483219	-4.35601827	-0.09649314
O	1.65493892	-4.40979946	-1.59226086
C	1.72310911	-2.42367495	-2.88170562
C	2.13704208	-3.91017955	-2.87627456
C	-3.10179000	-2.36138023	-1.01136612
C	-3.46286130	-3.81391931	-0.63782187
N	0.34786255	5.90707498	1.06289879

H	1.09316833	-2.16686558	-3.73682059
H	-3.76786515	-1.63568630	-0.53640644
C	-0.46746160	7.07930580	0.69341058
H	0.19221927	7.91949784	0.44723063
H	-1.06269514	6.86371387	-0.19654061
C	-1.29985842	7.41414372	1.94005661
C	-0.29508167	7.13698063	3.06863109
H	0.32455600	8.02343600	3.24061411
H	-0.77292415	6.88747455	4.01841174
C	0.59082813	5.97295864	2.53468947
H	0.26203332	5.02815641	2.98158659
C	2.07513837	6.16207788	2.84772617
H	2.45342635	7.07002017	2.36921310
H	2.23979190	6.24955784	3.92677397
C	1.00609255	-4.96356226	2.56492008
H	1.21053006	-4.01647795	3.05419013
C	0.25782066	-6.21343438	0.66964914
H	-0.13258818	-6.26306833	-0.34143411
C	0.49948321	-7.40342311	1.35086375
H	0.29800769	-8.35410310	0.86714245
C	1.25193473	-6.14932444	3.25799996
H	1.64114881	-6.11289960	4.27061247
C	0.99925879	-7.37660644	2.65229715
H	1.18881982	-8.30204898	3.18593197
H	1.65808429	-4.50016827	-3.65879085
H	3.21422835	-4.07160129	-2.91035030
H	2.57772749	-1.74314416	-2.87933214
H	-3.75524938	-4.43123131	-1.48718637
H	-4.22473361	-3.88641294	0.13990434
H	-3.13010168	-2.18473843	-2.09076837
H	-1.68191720	8.43830793	1.94779104
H	-2.15726619	6.73574235	2.01042293
H	-0.17966764	5.06746223	0.85392856

N	-1.59729264	0.66540564	-1.11447748
H	-2.49504344	0.19439768	-1.14908612
C	-1.78613608	2.08183167	-1.41691144
H	-0.80819332	2.52702341	-1.62033393
H	-2.38368151	2.19866477	-2.33195666
C	-2.44711319	2.89782527	-0.29029764
H	-1.81590146	2.83576576	0.60348051
H	-2.47100676	3.95283249	-0.59518284
C	-3.87364811	2.45233454	0.08442026
H	-3.85939301	1.41482646	0.43320206
H	-4.20754748	3.05900565	0.93611693
C	-4.86774010	2.60306035	-1.03326355
H	-4.93825805	3.59840726	-1.47168386
C	-5.65129373	1.63931793	-1.50972282
H	-5.62438851	0.63231436	-1.10292578
H	-6.35676957	1.82104510	-2.31270380
N	1.36128886	0.82861635	-1.39732277
C	2.75453205	1.25678020	-1.31861562
H	2.66192563	5.31885139	2.47692454
H	0.93552947	1.21259433	-2.23965451
H	3.24663034	0.68774024	-0.52602463
H	3.28791075	1.00541430	-2.24941613
C	2.95230702	2.75629004	-1.03730613
H	2.42893814	3.01450960	-0.11004587
H	4.01929055	2.94156822	-0.86425609
C	2.47001185	3.67822198	-2.17062295
H	1.40353966	3.48967399	-2.35102961
H	2.99888176	3.42989905	-3.09881063
C	2.65363328	5.13570475	-1.85103260
H	2.12691690	5.49320636	-0.96629812
C	3.40469730	5.98013666	-2.55302591
H	3.94683865	5.66200073	-3.43947604
H	3.50499718	7.02190876	-2.26885784

MP2 Electronic Energy(Ha): 1740.469345880918

B3LYP Electronic Energy(Ha): 1744.990822496390

M06-L Electronic Energy(Ha): 1744.748425443006

Zero point energy correction(kcal/mol): 476.341

Enthalpy correction(kcal/mol): 504.949

Entropy correction(cal/mol): 266.288

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.974

Deuterated enthalpy correction(kcal/mol): 496.978

Deuterated entropy correction(cal/mol): 268.808

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H8

Reactant geometry

Zr	0.44506405	-0.03854454	-0.55270884
C	0.16067149	2.27063452	-1.46073038
C	1.29865591	1.71684475	-2.13894698
H	2.32753225	2.00467937	-1.97763958
C	-0.96339332	1.59656753	-2.00792709
H	-1.98873130	1.74935997	-1.70040672
C	-0.53071554	0.61046380	-2.93234181
H	-1.15989236	-0.05368632	-3.50942120
C	0.88093741	0.69628428	-3.02359557
H	1.51534245	0.10660306	-3.66882074
B	0.19377032	3.12580721	-0.06006909
C	0.01619298	4.72618830	-0.17772308
C	-0.89075988	2.38733317	0.95611871
C	1.58451103	2.62226977	0.67240772
N	1.88402841	1.36252908	0.69685904
N	-0.99177086	1.09705009	1.07913721
O	-1.64513225	3.10240819	1.81236781
O	2.46175058	3.43357664	1.28543183

C	3.17484324	1.17602214	1.37642421
C	3.51451922	2.60175700	1.86024235
C	-1.85824581	0.79968728	2.23522906
C	-2.46182227	2.17228214	2.57525773
N	1.58055169	-1.54496011	-0.42298700
N	-0.38471066	-3.11391946	1.81261976
C	-0.07270172	-2.62049813	3.16679771
H	-1.01052773	-2.45462319	3.70736557
H	3.08040385	0.46170496	2.19714709
H	-2.61797463	0.05503736	1.98940656
C	2.59630998	-2.54409409	-0.57399250
H	3.36726542	-2.43528853	0.20989975
H	2.18541121	-3.55849055	-0.43443778
C	3.30275681	-2.50388935	-1.94020199
C	0.76641600	-3.72364045	3.87815591
C	0.62115624	-4.96531285	2.96417854
H	0.38480261	-5.87616268	3.51972782
H	0.44641910	-1.66278025	3.10177576
H	0.40713467	-2.88989368	1.20269033
C	-0.49524117	-4.58042024	1.96573501
H	-1.46604136	-4.77292668	2.44269857
H	1.54859560	-5.14966932	2.41321756
C	-0.44800624	-5.31975047	0.63561798
H	-0.53912117	-6.39753634	0.79350002
H	-1.26471132	-5.00787282	-0.02048069
H	0.49915040	-5.13739786	0.11901071
C	0.11447196	5.57787693	0.93636606
H	0.31974455	5.15520612	1.91425078
C	-0.24598931	5.33577233	-1.41363822
H	-0.32451204	4.71435666	-2.30002252
C	-0.04161279	6.95696301	0.82521421
H	0.04239364	7.58381465	1.70761800
C	-0.40562314	6.71640369	-1.53789908

H	-0.60725868	7.15177895	-2.51167108
C	-0.30418762	7.53447372	-0.41650977
H	-0.42598402	8.60887947	-0.50698384
C	4.40711109	-3.56592482	-2.10977647
H	5.14720301	-3.46836157	-1.30703776
H	4.93805277	-3.36076670	-3.04865007
C	3.89431741	-4.97852051	-2.15360831
H	3.14772570	-5.18193904	-2.92160477
C	4.27959934	-5.97287801	-1.35786721
H	5.02125116	-5.82175123	-0.57885831
H	3.87470990	-6.97379093	-1.45897544
H	1.81254339	-3.42612636	3.97469701
H	0.39145764	-3.91278813	4.88681778
H	2.54881163	-2.62356013	-2.72724635
H	3.73476821	-1.50699882	-2.07577014
H	3.46829919	2.71633948	2.94467491
H	4.47046645	2.97987178	1.49865428
H	3.91255259	0.77811571	0.67454879
H	-2.39412002	2.44768828	3.62697151
H	-3.49502683	2.28341323	2.23765381
H	-1.25413738	0.39465597	3.05373823
N	-1.47901355	-1.53508076	-0.56902327
H	-1.39499850	-2.03841038	0.32801134
H	-1.17620482	-2.21494610	-1.26417575
C	-2.88522826	-1.15959850	-0.83165679
C	-3.87124489	-2.32730470	-0.73450654
H	-3.15984530	-0.37362985	-0.12460772
H	-2.93427536	-0.70962970	-1.82583988
H	-3.58481388	-3.10971557	-1.44702708
H	-3.80530615	-2.77605856	0.26375245
C	-5.32279545	-1.89807750	-1.01458797
H	-5.39348214	-1.46347261	-2.01743241
H	-5.59622659	-1.10271854	-0.30800003

C	-6.30210184	-3.03096849	-0.88543003
H	-6.35470291	-3.50240775	0.09528754
C	-7.07780442	-3.48956557	-1.86273230
H	-7.06022186	-3.05101074	-2.85612274
H	-7.76185507	-4.31584315	-1.70626083

MP2 Electronic Energy(Ha): 1740.474704338550

B3LYP Electronic Energy(Ha): 1744.981390186089

M06-L Electronic Energy(Ha): 1744.744216785469

Zero point energy correction(kcal/mol): 477.276

Enthalpy correction(kcal/mol): 505.842

Entropy correction(cal/mol): 264.147

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.553

Deuterated enthalpy correction(kcal/mol): 497.446

Deuterated entropy correction(cal/mol): 266.173

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.72637967	-0.00763959	0.02607777
C	-1.70648310	-2.22501311	-0.45760005
C	-2.53193638	-1.65260915	0.56538751
H	-2.55895651	-1.96946144	1.59829275
C	-2.01380698	-1.48710679	-1.63718160
H	-1.54915242	-1.63122872	-2.60262081
C	-2.92174093	-0.44585112	-1.33277106
H	-3.31974708	0.28016268	-2.02689998
C	-3.25459649	-0.55384408	0.04421098
H	-3.95683651	0.06749757	0.58029864
B	-0.37452055	-3.16495327	-0.22867198
C	-0.55225338	-4.75309896	-0.44061711
C	0.79170178	-2.45491342	-1.16884288
C	0.17668597	-2.71632423	1.26048620
N	0.18546669	-1.46605385	1.61327945

N	0.94519460	-1.16558072	-1.20831262
O	1.65252807	-3.15327635	-1.92457744
O	0.68280731	-3.56587624	2.16201237
C	0.75542257	-1.33661964	2.96460911
C	1.11655862	-2.79392655	3.32319031
C	2.00523703	-0.83201968	-2.17899716
C	2.61071647	-2.20992197	-2.49542939
N	-0.63535947	1.63182338	1.11239902
N	3.19468354	1.74165290	0.07788762
C	4.01326129	0.75794472	0.81108942
H	4.62510027	0.19959218	0.09442846
H	1.62514915	-0.67575700	2.95316999
H	1.55722289	-0.36231316	-3.06048968
C	-0.91970703	2.66736437	2.07450663
H	0.00906311	3.00328423	2.56586746
H	-1.32719504	3.56005038	1.57640168
C	-1.90337507	2.22446473	3.16724996
C	4.93545705	1.54427354	1.79493945
C	4.67980689	3.02919848	1.45201619
H	5.59367068	3.62857412	1.45033360
H	3.36642850	0.03479917	1.31132278
H	2.33519635	1.91370489	0.59730079
C	3.99238200	2.98458686	0.06935522
H	4.76779510	2.85934220	-0.69899759
H	3.99322127	3.48013071	2.17665539
C	3.15614766	4.20981017	-0.27002100
H	3.77641613	5.10981562	-0.27750758
H	2.68787060	4.10996792	-1.25119991
H	2.36256006	4.35588542	0.47013703
C	0.51602488	-5.65368675	-0.28801741
H	1.49921502	-5.27677003	-0.02583790
C	-1.79650036	-5.30292628	-0.78244010
H	-2.64750736	-4.64157738	-0.91081688

C	0.35268200	-7.02491304	-0.46549464
H	1.20015098	-7.69148123	-0.33982241
C	-1.97265874	-6.67513091	-0.96296989
H	-2.95079606	-7.06437503	-1.22730862
C	-0.89650538	-7.54332781	-0.80466442
H	-1.02729256	-8.61130940	-0.94390538
C	-2.25344760	3.32981522	4.18273480
H	-1.33740384	3.73346995	4.62943389
H	-2.82434597	2.87360870	5.00197834
C	-3.06879485	4.45099045	3.59994923
H	-4.00598616	4.15259933	3.13002463
C	-2.74602823	5.74110869	3.62051848
H	-1.82325548	6.08912889	4.07551785
H	-3.39177329	6.49673163	3.18725622
H	4.69924536	1.32612394	2.83876373
H	5.98311269	1.27372236	1.64091936
H	-2.81922070	1.86215255	2.68631792
H	-1.47307074	1.36848239	3.69890834
H	2.18628714	-2.96387798	3.44938914
H	0.58450908	-3.18006719	4.19252445
H	0.01944985	-0.90299726	3.64571521
H	3.57020850	-2.38228264	-2.00279338
H	2.70320473	-2.43142953	-3.55757216
H	2.71513661	-0.12695262	-1.74411258
N	-0.11686960	1.75983284	-1.38324262
H	0.85755358	1.74586742	-1.67220020
H	-0.29060888	2.05542117	-0.07165821
C	-0.94586218	2.43336368	-2.37867200
C	-0.47309279	3.85492810	-2.71426319
H	-1.01047226	1.85344176	-3.31410432
H	-1.96939574	2.48815263	-1.98870943
H	-0.45726695	4.45383244	-1.79789353
H	0.56259932	3.81034969	-3.07567378

C -1.35297524 4.54680850 -3.77053574

H -2.38799994 4.59737114 -3.41443874

H -1.36328924 3.92742622 -4.67799687

C -0.87555094 5.92717017 -4.12268222

H 0.13316891 5.98930213 -4.53042073

C -1.57349145 7.04790934 -3.96380213

H -2.58180410 7.03641990 -3.56004765

H -1.16652538 8.01629677 -4.23268454

MP2 Electronic Energy(Ha): 1740.429347831817

B3LYP Electronic Energy(Ha): 1744.943050221881

M06-L Electronic Energy(Ha): 1744.699697157414

Zero point energy correction(kcal/mol): 472.734

Enthalpy correction(kcal/mol): 501.594

Entropy correction(cal/mol): 274.460

Imaginary Frequencies: -1617.77

Deuterated zero point energy correction(kcal/mol): 464.856

Deuterated enthalpy correction(kcal/mol): 494.118

Deuterated entropy correction(cal/mol): 277.981

Deuterated imaginary Frequencies: -1162.62

Product geometry

Zr -0.30781161 -0.12400171 -0.40238758

C -0.77274869 2.13726053 -1.26524564

C -0.01606935 1.49675428 -2.29741983

H 1.01290818 1.71620307 -2.54218701

C -2.05669673 1.51147485 -1.29779898

H -2.87967039 1.73909716 -0.63452545

C -2.05575883 0.47113703 -2.25227711

H -2.87762591 -0.18832888 -2.48855492

C -0.78079632 0.46166116 -2.87994852

H -0.46990639 -0.19947532 -3.67556172

B -0.18092580 3.08056392 -0.06242759

C -0.31523111 4.67639873 -0.25066273

C	-0.89244437	2.46420304	1.29853402
C	1.34213933	2.52340913	0.21020689
N	1.63024924	1.26009649	0.14026276
N	-0.90801063	1.18411813	1.51435169
O	-1.49807887	3.21106832	2.23387695
O	2.32098007	3.31266824	0.68745888
C	2.96329948	1.04958876	0.73779242
C	3.50167254	2.48208743	0.88052734
C	-1.67816073	0.90855943	2.73983245
C	-1.93908488	2.31973887	3.30172396
N	1.14276707	-1.62706443	-0.75244391
N	0.49887000	-3.00222751	2.30914590
C	0.93192342	-2.34265437	3.55276011
H	0.08948224	-2.32278046	4.25202352
H	2.85630174	0.54482303	1.70445148
H	-2.59643381	0.37267152	2.48587994
C	2.44756105	-1.69822713	-1.40401392
H	2.81072500	-0.68004195	-1.57666458
H	3.19344739	-2.18336153	-0.75591002
C	2.41902820	-2.43531279	-2.75067986
C	2.09916969	-3.18769595	4.14938724
C	2.09169515	-4.49156200	3.31476877
H	2.17824883	-5.39034926	3.93034768
H	1.21184868	-1.30655711	3.35084344
H	1.07925143	-2.67364488	1.53621975
C	0.76016536	-4.43784538	2.52900661
H	-0.04207239	-4.80955713	3.18086736
H	2.92626128	-4.49983914	2.60583255
C	0.74810191	-5.23662682	1.23315660
H	0.92551474	-6.29683741	1.43074509
H	-0.21226712	-5.14275533	0.72102068
H	1.53492552	-4.88871870	0.55545964
C	0.10689580	5.58496070	0.73545247

H	0.53739282	5.20919155	1.65763829
C	-0.86109431	5.22550958	-1.42033261
H	-1.20182985	4.55923221	-2.20656622
C	-0.00798102	6.96196179	0.56451924
H	0.32833655	7.63413109	1.34778394
C	-0.98103377	6.60351184	-1.60352232
H	-1.40891531	6.99152118	-2.52255399
C	-0.55407338	7.47916140	-0.60958304
H	-0.64535660	8.55167449	-0.74587965
C	3.78241352	-2.48249524	-3.46849797
H	4.15215141	-1.46403637	-3.63328396
H	3.62819803	-2.92114384	-4.46272718
C	4.82671549	-3.28874936	-2.74715292
H	4.55330714	-4.32066343	-2.52630779
C	6.02918237	-2.85323547	-2.38130125
H	6.35007308	-1.83517837	-2.58216569
H	6.73958408	-3.49805880	-1.87613180
H	3.05587566	-2.66798192	4.06282768
H	1.93666131	-3.38428763	5.21180130
H	2.05777764	-3.46001739	-2.59155975
H	1.68527962	-1.94830255	-3.40091577
H	3.92054004	2.71511135	1.85851912
H	4.22273817	2.74692646	0.10376275
H	3.59270236	0.42435935	0.10568456
H	-1.34352728	2.54972989	4.18738780
H	-2.98706786	2.53692681	3.50484762
H	-1.10660068	0.28120823	3.42669165
N	-1.69539572	-1.52739850	0.24432620
H	-1.25128131	-2.12851258	0.94810887
H	0.70710594	-2.54624024	-0.78050972
C	-3.10371628	-1.87478822	0.13623492
C	-3.35007060	-3.23765386	-0.53190903
H	-3.58145329	-1.88514530	1.12919262

H	-3.61996476	-1.10046013	-0.43975935
H	-2.89953972	-3.23040889	-1.52971208
H	-2.82759275	-4.01398283	0.04036673
C	-4.84404269	-3.59257196	-0.63812065
H	-5.36652604	-2.82722599	-1.22289957
H	-5.28232940	-3.57076619	0.36918364
C	-5.08494253	-4.94342467	-1.24971879
H	-4.65481837	-5.78859702	-0.71299553
C	-5.75465972	-5.17241164	-2.37556267
H	-6.20023553	-4.36272213	-2.94616158
H	-5.88524810	-6.17488380	-2.76742982

MP2 Electronic Energy(Ha): 1740.475669583765

B3LYP Electronic Energy(Ha): 1744.992981859093

M06-L Electronic Energy(Ha): 1744.753677407367

Zero point energy correction(kcal/mol): 475.931

Enthalpy correction(kcal/mol): 504.908

Entropy correction(cal/mol): 274.623

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.208

Deuterated enthalpy correction(kcal/mol): 496.658

Deuterated entropy correction(cal/mol): 278.565

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction C1

Reactant geometry

Zr	-0.34338449	-0.64558275	0.05202671
C	0.04275658	1.35054323	-1.34455025
C	1.01581816	0.39308307	-1.77566228
H	2.07400276	0.44155520	-1.56407545
C	-1.20633824	0.86361070	-1.83797580
H	-2.16679811	1.33452106	-1.68054974
C	-1.01712517	-0.38520355	-2.46763623

H	-1.78260133	-1.00364436	-2.91382350
C	0.37261108	-0.68106915	-2.43187136
H	0.84797105	-1.55304116	-2.85698646
B	0.24684778	2.50986013	-0.20383877
C	0.51462919	4.01210727	-0.72519787
C	-1.07570426	2.32626033	0.77604452
C	1.37299156	1.90333753	0.82824103
N	1.41348691	0.64105539	1.12701295
N	-1.43047105	1.15241353	1.20480792
O	-1.86214110	3.34016438	1.16633089
O	2.18729699	2.69284306	1.54930762
C	2.29876714	0.46241822	2.29460113
C	2.98542260	1.83274413	2.41274026
C	-2.68627433	1.27553854	1.96544575
C	-2.87429432	2.80134175	2.06761141
N	-2.16007586	-1.68639236	0.15959491
H	1.69742438	0.21551046	3.17605949
C	-2.71328349	-2.41788527	1.29378303
H	-1.94603939	-2.47522490	2.07538897
H	-3.56176272	-1.87541604	1.74612571
C	-3.19009493	-3.85385304	0.99556312
C	-4.47860012	-3.96338222	0.16063973
H	-4.97916268	-4.90999205	0.40597289
H	-5.18495061	-3.18918273	0.49304183
C	-4.38179389	-3.90874358	-1.34424964
C	0.61624878	4.29620856	-2.09508429
H	0.50741652	3.48742423	-2.81077492
C	0.66099998	5.09696600	0.15674488
H	0.59285709	4.92806183	1.22622153
C	0.89597081	6.39065029	-0.30123205
H	1.00384290	7.20457274	0.40893139
C	0.85175862	5.58826075	-2.56618642
H	0.92421096	5.76955502	-3.63395591

C	0.99276871	6.64296264	-1.66914056
H	1.17555874	7.64994749	-2.02937899
H	-2.59962564	0.79760433	2.94362533
H	-3.49586927	0.78195223	1.42071860
H	-2.66946558	3.19603726	3.06472729
H	-3.84603565	3.15912386	1.72959230
H	3.00789414	-0.34967090	2.13890278
H	2.97588555	2.26061660	3.41427355
H	4.00715398	1.83419943	2.02644939
H	-2.38066444	-4.42333154	0.52732020
H	-3.38224167	-4.33294641	1.96267521
H	-2.82561505	-1.66511860	-0.60435553
N	0.72829502	-2.31928859	0.73621236
H	0.13289453	-3.14174371	0.80137789
C	2.12102641	-2.73096232	0.85192910
H	2.76085435	-1.87426438	0.61746728
H	2.36454125	-3.02590789	1.88620086
C	2.49852435	-3.89067888	-0.08212453
H	2.28040433	-3.59656499	-1.11487684
H	1.85960966	-4.75482944	0.13685036
C	3.97382217	-4.31166115	0.04407977
H	4.18738627	-4.61365529	1.07540692
H	4.60603886	-3.43771641	-0.16531047
C	4.34902939	-5.42412936	-0.89361456
H	4.23021863	-5.20814449	-1.95489194
C	4.78952221	-6.62431522	-0.52799444
H	4.92293987	-6.88625609	0.51767149
H	5.03568961	-7.38771256	-1.25747706
H	-5.34805203	-3.91606906	-1.84751857
C	-3.28559233	-3.90243495	-2.09883140
H	-3.35809530	-3.90414751	-3.18089373
H	-2.28796750	-3.89095291	-1.67694431

MP2 Electronic Energy(Ha): 1489.151591155486

B3LYP Electronic Energy(Ha): 1493.008758707171

M06-L Electronic Energy(Ha): 1492.814077130686

Zero point energy correction(kcal/mol): 377.008

Enthalpy correction(kcal/mol): 400.529

Entropy correction(cal/mol): 225.389

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.855

Deuterated enthalpy correction(kcal/mol): 396.609

Deuterated entropy correction(cal/mol): 226.769

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	1.14420205	0.64663358	0.17517740
C	1.39714740	-1.83907801	-0.06736604
C	2.10680566	-1.39390809	-1.22067713
H	1.74937266	-1.46637139	-2.23813923
C	2.24604776	-1.52832907	1.04291784
H	2.03376341	-1.74573137	2.07931856
C	3.40251870	-0.87072516	0.58008798
H	4.22625553	-0.52874496	1.19238928
C	3.31708152	-0.78881917	-0.83201942
H	4.05916890	-0.36406594	-1.49298958
B	-0.15208746	-2.35790013	-0.01592810
C	-0.40338027	-3.94264115	-0.19006276
C	-0.69619918	-1.71161586	1.38729311
C	-0.91692361	-1.40627491	-1.11763916
N	-0.61602414	-0.15086177	-1.24858415
N	-0.32328440	-0.52179484	1.72805692
O	-1.51844759	-2.33229614	2.25154700
O	-1.90028023	-1.84763184	-1.91963045
C	-1.43662342	0.43359334	-2.32321403
C	-2.39771692	-0.71461080	-2.68790284
C	-0.86792836	-0.20615391	3.05920419

C	-1.80264489	-1.40030303	3.33653908
N	2.73182332	2.13309197	0.74403371
H	-1.96018046	1.32439003	-1.97309641
C	2.68866617	3.51034049	1.25320592
H	1.97254524	3.60228659	2.07803450
H	3.67030574	3.78495103	1.65448460
C	2.32994829	4.46690332	0.10568283
C	3.07393660	3.93966180	-1.12151335
H	2.75114259	4.45263927	-2.03152032
H	4.14629844	4.12573432	-1.00131319
C	2.84330402	2.44714849	-1.28751907
C	0.66048206	-4.83093856	-0.40503466
H	1.67155952	-4.43938470	-0.45660681
C	-1.69110115	-4.50289412	-0.12912308
H	-2.54635948	-3.85629436	0.03779956
C	-1.90598910	-5.87081853	-0.27499750
H	-2.91462510	-6.26872828	-0.22152309
C	0.45798463	-6.20364347	-0.55296370
H	1.30627441	-6.86076394	-0.71753371
C	-0.82881994	-6.73019312	-0.48851658
H	-0.99247910	-7.79678307	-0.60217095
H	-1.38995075	0.74987753	3.05354105
H	-0.05208673	-0.13706737	3.78663171
H	-2.86181088	-1.14060848	3.27950277
H	-1.60726914	-1.91358704	4.27753651
H	-0.79855935	0.72936149	-3.16089631
H	-3.42832908	-0.53201262	-2.37738873
H	-2.38301089	-0.99283094	-3.74136774
H	1.25436827	4.45736210	-0.08564087
H	2.61128625	5.49664711	0.34220454
H	3.62674030	1.71436621	0.95781247
N	-0.15323474	2.20480377	0.78721295
H	0.27403535	3.08093128	1.06227134

C	-1.59837013	2.34495420	0.86360393
H	-2.06083772	1.41389340	0.52021483
H	-1.94023936	2.48619466	1.90425902
C	-2.15420608	3.52066291	0.04108156
H	-1.84094401	3.40880689	-1.00309163
H	-1.70328852	4.45494603	0.39730801
C	-3.68681692	3.64432603	0.12066476
H	-3.99542206	3.76186829	1.16524907
H	-4.13313409	2.70407418	-0.23226690
C	-4.22979981	4.78334643	-0.69504947
H	-4.02854033	4.73802508	-1.76508228
C	-4.90692881	5.82191320	-0.21413107
H	-5.13164139	5.91232003	0.84468427
H	-5.26447016	6.61732354	-0.85836380
H	3.75150660	1.87155624	-1.42221783
C	1.68215120	1.89363638	-1.88302908
H	1.83868173	1.10019398	-2.60484929
H	0.86133881	2.56889457	-2.10214101

MP2 Electronic Energy(Ha): 1489.138655066754

B3LYP Electronic Energy(Ha): 1492.972279143780

M06-L Electronic Energy(Ha): 1492.793575531836

Zero point energy correction(kcal/mol): 377.793

Enthalpy correction(kcal/mol): 400.144

Entropy correction(cal/mol): 212.151

Imaginary Frequencies: -353.02

Deuterated zero point energy correction(kcal/mol): 373.573

Deuterated enthalpy correction(kcal/mol): 396.147

Deuterated entropy correction(cal/mol): 213.474

Deuterated imaginary Frequencies: -351.15

Product geometry

Zr	-1.01951092	-0.64116594	0.25962192
C	-1.36075245	1.84803453	0.24989287

C	-2.30504305	1.44739885	-0.73822682
H	-2.19678959	1.60262294	-1.80222837
C	-1.90413691	1.40155135	1.49858766
H	-1.46437378	1.56214950	2.47206344
C	-3.10236405	0.69563071	1.26523608
H	-3.74431725	0.26554883	2.02309083
C	-3.35096696	0.72618144	-0.13405619
H	-4.20283521	0.29618037	-0.64095878
B	0.14725616	2.42472201	-0.01802827
C	0.30073847	4.01807794	-0.22177791
C	0.98755715	1.78975794	1.23781004
C	0.71288694	1.50786141	-1.25624839
N	0.42162281	0.24682380	-1.34939998
N	0.83694199	0.54700453	1.55908367
O	1.77976873	2.51641807	2.05083460
O	1.55547161	1.96831093	-2.19417149
C	1.12589332	-0.33904720	-2.50170189
C	1.90120966	0.86295396	-3.07879314
C	1.51492489	0.31637734	2.84941306
C	2.33549048	1.60379325	3.03938540
N	-2.79473396	-2.36353466	0.50499470
H	1.78552797	-1.14624331	-2.17345128
C	-2.69541450	-3.74761753	1.05716750
H	-1.94671800	-3.79490912	1.85059039
H	-3.65650660	-4.04048968	1.49335996
C	-2.37512477	-4.63859988	-0.14880460
C	-3.15841910	-3.96833238	-1.28440268
H	-2.80030796	-4.24494929	-2.27688148
H	-4.21599389	-4.24896217	-1.21748042
C	-2.98274724	-2.45700294	-1.02647803
C	-0.81385027	4.86925971	-0.20645496
H	-1.80046036	4.44351293	-0.05289199
C	1.55364259	4.62364442	-0.42056419

H	2.44650740	4.00704274	-0.43953739
C	1.68767228	5.99837971	-0.59550732
H	2.67178670	6.43133424	-0.74600393
C	-0.69279408	6.24854635	-0.38064800
H	-1.57871398	6.87571236	-0.36207342
C	0.56106346	6.81992264	-0.57663146
H	0.66157052	7.89177541	-0.71219656
H	2.13655147	-0.57759590	2.82488444
H	0.76651099	0.17767226	3.63833487
H	3.39569309	1.47035659	2.80939853
H	2.23416706	2.06696514	4.02014213
H	0.40913741	-0.75967635	-3.20942101
H	2.98473462	0.74225887	-3.05048671
H	1.59595707	1.13956546	-4.08852058
H	-1.30418060	-4.62267806	-0.36749924
H	-2.66346340	-5.67732211	0.02405605
H	-3.59940415	-1.90851413	0.91763315
N	0.18067164	-2.25926802	0.88860637
H	-0.29409741	-3.15502435	0.92892580
C	1.61235701	-2.50315163	1.01185325
H	2.14442893	-1.57072497	0.80475140
H	1.88362522	-2.79715541	2.04015863
C	2.13248638	-3.59172459	0.05950048
H	1.88947747	-3.30902953	-0.97109638
H	1.60207898	-4.53192365	0.25511721
C	3.64651145	-3.83665709	0.19375170
H	3.88524389	-4.12759850	1.22262652
H	4.17163175	-2.89001346	0.00559935
C	4.15949189	-4.88159065	-0.75621260
H	4.02704890	-4.66401867	-1.81571223
C	4.73373108	-6.02822950	-0.40431910
H	4.88700157	-6.29005499	0.63862581
H	5.07489150	-6.74526436	-1.14257991

H -3.90016751 -1.92053399 -1.27262582

C -1.78284549 -1.76157681 -1.65181392

H -2.06262926 -1.16122401 -2.51964098

H -1.01908675 -2.48382372 -1.95884649

MP2 Electronic Energy(Ha): 1489.161602480934

B3LYP Electronic Energy(Ha): 1492.992620370393

M06-L Electronic Energy(Ha): 1492.811590407919

Zero point energy correction(kcal/mol): 379.374

Enthalpy correction(kcal/mol): 401.748

Entropy correction(cal/mol): 213.709

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 375.020

Deuterated enthalpy correction(kcal/mol): 397.591

Deuterated entropy correction(cal/mol): 214.862

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction C2

Reactant geometry

Zr -0.07686467 1.48753827 -0.24000905

C 0.26009834 -0.69908412 -1.41055598

C -0.75184929 0.00888247 -2.14358179

H -1.80309024 -0.24005011 -2.16429703

C 1.47351577 -0.02076498 -1.70073476

H 2.44188228 -0.27218047 -1.28982474

C 1.21063900 1.10616560 -2.52421611

H 1.94251670 1.80306522 -2.90982778

C -0.17542045 1.11535606 -2.81261420

H -0.69241838 1.82347591 -3.44361943

B 0.00536141 -1.71683088 -0.14657784

C 0.12702091 -3.29823980 -0.44459446

C 0.99464927 -1.16785172 1.06832468

C -1.44211517 -1.22614931 0.47486156

N	-1.69320840	0.03770985	0.61611914
N	1.13763893	0.09169301	1.35599301
O	1.64754417	-2.01813943	1.87801722
O	-2.41205420	-2.05132527	0.89290408
C	-3.03620759	0.21754146	1.18919276
C	-3.50044342	-1.23560060	1.42603512
C	2.01453128	0.22008365	2.53460568
C	2.33143315	-1.24362909	2.90196482
N	-1.09064729	3.05985208	-0.02855412
H	-2.98467581	0.80169707	2.11047827
H	2.91507766	0.78701639	2.28409846
C	-1.60626252	4.38304463	0.09742373
H	-2.49250646	4.54408614	-0.53628741
H	-1.92987637	4.57618799	1.13378954
C	-0.53794012	5.43098356	-0.28103825
C	0.82901109	5.09960211	0.33662986
H	1.50053160	5.95381170	0.16948750
H	0.74610174	4.97123381	1.42057603
C	1.50561112	3.91085824	-0.27982415
C	2.19557234	2.94434053	0.36509630
C	0.50339690	-3.76799846	-1.71156524
H	0.71141188	-3.04995559	-2.49843081
C	-0.13531844	-4.27065461	0.53604942
H	-0.43295196	-3.95806730	1.53147492
C	-0.02716511	-5.63288403	0.26932380
H	-0.23855838	-6.35574162	1.05117174
C	0.61623072	-5.13038463	-1.99098259
H	0.91000160	-5.45602713	-2.98393430
C	0.35114807	-6.07035620	-0.99944973
H	0.43629733	-7.13114730	-1.21090901
H	-0.43578072	5.46343836	-1.37200182
H	-0.85899269	6.42819577	0.03943212
H	-3.61628432	-1.49202761	2.47998810

H	-4.40862980	-1.50534696	0.88730559
H	-3.67340011	0.76063270	0.48715832
H	1.93308199	-1.54871474	3.87059326
H	3.39212432	-1.49124275	2.85509732
H	1.49822908	0.75192622	3.33858763
H	2.83250754	2.25220366	-0.17220319
H	2.24729311	2.93195091	1.44872314
H	1.54667051	3.92557189	-1.36775479

MP2 Electronic Energy(Ha): 1237.838461232390

B3LYP Electronic Energy(Ha): 1241.011076227988

M06-L Electronic Energy(Ha): 1240.866324315554

Zero point energy correction(kcal/mol): 279.525

Enthalpy correction(kcal/mol): 297.259

Entropy correction(cal/mol): 181.305

Imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.15002444	1.47680877	0.35564552
C	-0.38744200	-0.77935388	1.39242444
C	0.52847102	-0.04435569	2.21586833
H	1.59327282	-0.21821133	2.27866456
C	-1.66343684	-0.19969566	1.64354753
H	-2.58697353	-0.49039063	1.16259353
C	-1.52669801	0.90101091	2.52245905
H	-2.32367273	1.53665537	2.88301079
C	-0.15842586	0.99232288	2.89030268
H	0.27196593	1.70611708	3.57780389
B	0.00220479	-1.73692233	0.11400018
C	-0.01439351	-3.33100490	0.35827757
C	-0.98131576	-1.20605159	-1.10624505
C	1.43322233	-1.12309585	-0.42742906
N	1.60186245	0.15815321	-0.52502477
N	-1.15594907	0.05705305	-1.34477420

O	-1.63348572	-2.04326829	-1.93126347
O	2.47263142	-1.86977356	-0.83055001
C	2.94366132	0.44247356	-1.05752499
C	3.52631527	-0.96923788	-1.28608919
C	-2.09035495	0.21060903	-2.47317770
C	-2.32159694	-1.24254883	-2.93420322
N	0.86767812	3.12456373	0.29211703
H	2.87426867	1.02370062	-1.98052579
H	-3.01122710	0.69512389	-2.13635464
C	1.71058359	4.28014550	0.15487024
H	2.31730354	4.44614215	1.05569659
H	2.41479973	4.11709619	-0.67363540
C	0.84950798	5.53714927	-0.13890171
C	-0.47350796	5.04123119	-0.71890114
H	-1.21407762	5.84991234	-0.75098617
H	-0.35160662	4.66895141	-1.74060735
C	-1.01179793	3.94371370	0.16284380
C	-1.93989484	2.95375297	-0.26287812
C	-0.35596309	-3.87075496	1.60694112
H	-0.61379168	-3.19779420	2.41859104
C	0.31137482	-4.24684329	-0.65707362
H	0.58319648	-3.87849608	-1.64101417
C	0.29707043	-5.62206252	-0.44020350
H	0.55452904	-6.30011901	-1.24794796
C	-0.37425158	-5.24689188	1.83682514
H	-0.64390441	-5.62776644	2.81689151
C	-0.04722355	-6.12993289	0.81197071
H	-0.05955971	-7.20103325	0.98469341
H	0.65136605	6.07642450	0.79323320
H	1.36180749	6.23250482	-0.80877122
H	3.72471998	-1.19722878	-2.33403148
H	4.41862710	-1.17966056	-0.69619661
H	3.52102541	1.02825455	-0.33783790

H	-1.87254319	-1.46759937	-3.90338123
H	-3.36782204	-1.54681359	-2.94402170
H	-1.65233323	0.83370162	-3.25701819
H	-2.78260718	2.73557878	0.38441369
H	-2.15305246	2.90203811	-1.32765396
H	-1.09548701	4.24764269	1.20463156

MP2 Electronic Energy(Ha): 1237.832745918439

B3LYP Electronic Energy(Ha): 1241.003430203992

M06-L Electronic Energy(Ha): 1240.856767958702

Zero point energy correction(kcal/mol): 279.262

Enthalpy correction(kcal/mol): 296.435

Entropy correction(cal/mol): 177.712

Imaginary Frequencies: -272.67

Product geometry

Zr	-0.42238309	1.42053567	0.35290130
C	-0.85397423	-0.85524674	1.21968224
C	-0.29584516	-0.12115350	2.31461190
H	0.70176394	-0.25093612	2.71032762
C	-2.17317762	-0.33445719	1.05692405
H	-2.87698686	-0.64382429	0.29724096
C	-2.38185303	0.73995642	1.94839627
H	-3.27972726	1.33400314	2.03791790
C	-1.20716579	0.87340118	2.74148696
H	-1.05911601	1.57802640	3.54729954
B	-0.02624638	-1.73923342	0.10534233
C	-0.02830046	-3.34084126	0.28712365
C	-0.61662152	-1.19454065	-1.34313659
C	1.47115162	-1.04207533	0.05085723
N	1.61181046	0.24925919	0.06609638
N	-0.79307955	0.07333234	-1.56402274
O	-0.92402188	-2.00129613	-2.36762995
O	2.60823223	-1.73715100	-0.08692328

C	3.03340915	0.59203118	-0.11163533
C	3.71814455	-0.79067491	-0.12309361
C	-1.33039748	0.26533889	-2.92185146
C	-1.35564129	-1.17009647	-3.48709250
N	0.46495168	3.25584827	0.54624733
H	3.17462789	1.14147120	-1.04650257
H	-2.32276889	0.71951471	-2.87114947
C	1.49547240	4.22506908	0.85640312
H	1.31315308	4.68482327	1.84003902
H	2.47957658	3.75088336	0.90148621
C	1.40073696	5.31569504	-0.25683512
C	0.05932059	5.02819946	-0.97600816
H	-0.52986025	5.93055582	-1.15872276
H	0.23402277	4.54370851	-1.94112085
C	-0.67812055	4.04077903	-0.04979359
C	-1.67901067	3.05054093	-0.66748515
C	-0.68601186	-3.94733406	1.36721699
H	-1.20307880	-3.32186280	2.08799219
C	0.62406679	-4.19698763	-0.61683872
H	1.14690962	-3.77559243	-1.46921226
C	0.62085797	-5.57956552	-0.45311753
H	1.13489137	-6.21071813	-1.17124809
C	-0.69617500	-5.33153898	1.54214520
H	-1.21611153	-5.76542766	2.39038055
C	-0.04147117	-6.15473001	0.63073257
H	-0.04632935	-7.23176140	0.76129569
H	1.42258936	6.31718196	0.17931392
H	2.24340443	5.24719199	-0.94843919
H	4.29739422	-0.99340008	-1.02347248
H	4.33739384	-0.97729855	0.75531557
H	3.38291313	1.22703628	0.70513289
H	-0.65238310	-1.33051316	-4.30537825
H	-2.34539765	-1.51125336	-3.78956514

H -0.68714311 0.93308895 -3.49969105

H -2.71326902 3.25103678 -0.38668756

H -1.60456892 3.04531916 -1.75918944

H -1.16117027 4.61137126 0.75989779

MP2 Electronic Energy(Ha): 1237.844204486033

B3LYP Electronic Energy(Ha): 1241.018846647552

M06-L Electronic Energy(Ha): 1240.869847590433

Zero point energy correction(kcal/mol): 279.895

Enthalpy correction(kcal/mol): 297.370

Entropy correction(cal/mol): 182.547

Imaginary Frequencies: -0.00

Equatorial Reaction H2

Reactant geometry

Zr -0.79817460 0.95064599 0.68297521

C 0.09258395 -1.21003755 1.49456197

C 1.14252387 -0.31674314 1.85703352

H 2.10357796 -0.26287237 1.36640949

C -0.97985248 -0.91346513 2.40101857

H -1.93690806 -1.41368613 2.42675982

C -0.61937121 0.17186690 3.22563963

H -1.23028652 0.62925556 3.98994445

C 0.70496254 0.54511459 2.88547531

H 1.27292781 1.33868843 3.35095799

B 0.00609134 -2.11487674 0.13690853

C 0.55013774 -3.63242982 0.22609757

C -1.57036496 -1.95224922 -0.31608863

C 0.69867200 -1.19576241 -1.05057442

N 0.60829489 0.10094683 -1.07809524

N -2.16450263 -0.80747529 -0.19249031

O -2.31265830 -2.93212773 -0.85406088

O 1.25468866 -1.75040165 -2.14223535

C	1.07110321	0.58243248	-2.39286823
C	1.70031292	-0.67511630	-3.01616445
C	-3.55610046	-0.92540771	-0.65909253
C	-3.62254708	-2.37707793	-1.17826033
N	0.91005307	2.71524174	0.42442977
N	-1.89150200	2.17407510	-0.65301500
C	-2.53572861	2.40552757	-1.92675168
H	-2.73762679	1.46649914	-2.45384136
H	0.21864319	0.95965118	-2.96624844
H	-4.24676937	-0.74560162	0.16984720
C	2.38194994	2.58460356	0.47540562
H	2.64835049	2.24124647	1.47728593
H	2.67276868	1.78982167	-0.21230791
C	3.13312923	3.87941244	0.15214056
C	-3.83980061	3.21088489	-1.60793104
C	-3.73045912	3.55720274	-0.10245209
H	-4.35636518	2.88616279	0.49329652
H	-1.89970637	3.00675862	-2.60183421
C	-2.24822767	3.28438523	0.24113171
H	-1.67178197	4.20055191	-0.01087704
H	-4.03527053	4.58303046	0.12234491
C	-1.86623121	2.77869677	1.63581795
H	-2.74673537	2.37361202	2.15520524
H	0.59739608	3.39921936	1.10930851
H	-1.41949422	3.53069896	2.29338563
C	0.46761799	-4.52811462	-0.85440093
H	0.02221962	-4.19880443	-1.78676900
C	1.13371495	-4.12018424	1.40493255
H	1.21266243	-3.46206464	2.26440265
C	0.94142092	-5.83445422	-0.76444177
H	0.85987349	-6.49903604	-1.61897205
C	1.61267602	-5.42677065	1.50673325
H	2.05744483	-5.76867530	2.43607804

C	1.51852069	-6.29108255	0.41985820
H	1.88808441	-7.30860864	0.49319787
C	4.66594346	3.70724944	0.16021537
H	4.98613076	3.28329345	1.11817237
H	5.12092262	4.70256733	0.09159107
C	5.18142124	2.85904196	-0.97031759
H	4.97047221	3.23293059	-1.97221388
C	5.86382328	1.72487004	-0.83838739
H	6.10405392	1.31483622	0.13799311
H	6.21750330	1.16976474	-1.69983842
H	2.79212519	-0.66325494	-2.99657898
H	1.79223936	1.39656207	-2.29034645
H	1.35764251	-0.89845617	-4.02569864
H	-3.75163880	-2.44852957	-2.25948573
H	-4.37471434	-2.99164552	-0.68412935
H	-3.76847909	-0.18674909	-1.43284970
H	-3.89845663	4.11068563	-2.22589478
H	-4.73567989	2.62147501	-1.81831565
H	2.81505954	4.25223586	-0.83002348
H	2.85541290	4.65003477	0.88029252
H	0.61729986	3.08330410	-0.47921834

MP2 Electronic Energy(Ha): 1489.164132764631

B3LYP Electronic Energy(Ha): 1492.993336913236

M06-L Electronic Energy(Ha): 1492.811009208805

Zero point energy correction(kcal/mol): 378.371

Enthalpy correction(kcal/mol): 401.207

Entropy correction(cal/mol): 220.940

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 369.593

Deuterated enthalpy correction(kcal/mol): 392.954

Deuterated entropy correction(cal/mol): 225.304

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-0.74622674	0.86779117	0.44810558
C	0.31584363	-1.19181140	1.36590779
C	1.31218774	-0.20652350	1.62216907
H	2.25072411	-0.11845967	1.09361240
C	-0.75346275	-0.89401149	2.27659718
H	-1.66975172	-1.45717798	2.37726521
C	-0.45022714	0.27756289	2.99622725
H	-1.06569756	0.74807540	3.74929517
C	0.83775009	0.71145465	2.58178512
H	1.35850013	1.57718434	2.96285815
B	0.24324183	-2.21806999	0.09017914
C	0.92178818	-3.66957653	0.26573906
C	-1.36495369	-2.22595532	-0.24722933
C	0.79497500	-1.33092816	-1.17930764
N	0.49766034	-0.07269942	-1.29337500
N	-2.03791337	-1.11892369	-0.25840983
O	-2.07787260	-3.34530390	-0.45329599
O	1.48826798	-1.84572253	-2.20469795
C	0.99014839	0.43653641	-2.58331459
C	1.76422413	-0.77034092	-3.15085102
C	-3.47096017	-1.44328417	-0.39620227
C	-3.45227095	-2.94689124	-0.72526604
N	0.61637845	2.64808637	-0.01086844
N	-2.30803586	1.88305029	-0.52175467
C	-3.29503323	1.89210543	-1.58515522
H	-3.48388737	0.89323849	-1.98029094
H	0.14804672	0.73210546	-3.21612794
H	-3.99152532	-1.22512801	0.54243775
C	2.03724978	2.90689257	0.21115955
H	2.27405916	2.67734276	1.25394144
H	2.66725629	2.23690131	-0.39206171
C	2.43177745	4.36137626	-0.07430462

C	-4.55661985	2.56538777	-0.97108341
C	-4.01729669	3.33268424	0.26773661
H	-4.37739515	2.87537884	1.19320109
H	-2.93517598	2.50285509	-2.43082847
C	-2.48208836	3.16528807	0.17829474
H	-2.08785128	3.98629048	-0.45247827
H	-4.31680318	4.38378630	0.28043270
C	-1.64137788	3.06991882	1.44627934
H	-2.16492884	2.49272097	2.21857651
H	-0.31789372	2.94664096	0.88508641
H	-1.40334336	4.04055987	1.89225327
C	0.88950460	-4.63453854	-0.75582654
H	0.39669201	-4.40188212	-1.69427891
C	1.57308022	-4.03133401	1.45395397
H	1.61923076	-3.31617946	2.26926160
C	1.47425244	-5.88862164	-0.60180072
H	1.42976546	-6.60959917	-1.41209336
C	2.16270885	-5.28499173	1.62049111
H	2.65776131	-5.52988812	2.55493371
C	2.11565836	-6.22041839	0.59102908
H	2.57201459	-7.19692888	0.71480075
C	3.91719016	4.66972547	0.19902347
H	4.16010223	4.42969021	1.24017220
H	4.06553397	5.75124852	0.08659027
C	4.87116349	3.95669937	-0.71926350
H	4.72337782	4.13840377	-1.78401415
C	5.86170406	3.15529410	-0.33721387
H	6.05062732	2.94576615	0.71151554
H	6.52366504	2.68436056	-1.05523178
H	2.84483782	-0.62191297	-3.17309785
H	1.62483078	1.31200336	-2.43490981
H	1.42299807	-1.09607618	-4.13302835
H	-3.65509951	-3.15732041	-1.77780893

H	-4.10738694	-3.55449600	-0.10231210
H	-3.94422368	-0.85365386	-1.17988415
H	-5.04521139	3.22609047	-1.69154204
H	-5.29112618	1.81335830	-0.67272274
H	2.19959574	4.59992101	-1.12114948
H	1.80908965	5.02251934	0.53744492
H	0.31016760	3.08238650	-0.87757755

MP2 Electronic Energy(Ha): 1489.129947591430

B3LYP Electronic Energy(Ha): 1492.959354416006

M06-L Electronic Energy(Ha): 1492.774353165244

Zero point energy correction(kcal/mol): 375.512

Enthalpy correction(kcal/mol): 397.875

Entropy correction(cal/mol): 216.682

Imaginary Frequencies: -1552.87

Deuterated zero point energy correction(kcal/mol): 367.738

Deuterated enthalpy correction(kcal/mol): 390.585

Deuterated entropy correction(cal/mol): 220.881

Deuterated imaginary Frequencies: -1114.30

Product geometry

Zr	-0.51647878	0.80997334	0.21081491
C	0.45894687	-1.22034702	1.31987137
C	1.47609909	-0.23393285	1.49715610
H	2.43130259	-0.22694520	0.99085061
C	-0.61849856	-0.80644776	2.16148676
H	-1.56122739	-1.32208436	2.27552169
C	-0.30779749	0.43792356	2.75895109
H	-0.92672860	0.99328816	3.44842669
C	1.00580140	0.79007302	2.34402003
H	1.54313366	1.67834041	2.64101894
B	0.37911507	-2.32883912	0.11319667
C	1.02751357	-3.77760853	0.39605967
C	-1.22062005	-2.33660027	-0.27543806

C	0.98759207	-1.53866042	-1.19529656
N	0.71595432	-0.28437635	-1.40348417
N	-1.87877295	-1.23738594	-0.46543710
O	-1.94037310	-3.47153238	-0.33861772
O	1.72805469	-2.11988831	-2.14554997
C	1.31575163	0.15274211	-2.67615232
C	2.03104893	-1.12265168	-3.16790808
C	-3.30802490	-1.57198254	-0.62332412
C	-3.30405256	-3.11033329	-0.69551943
N	0.53499430	2.56886650	-0.21337215
N	-2.30143495	1.86948991	-0.21654765
C	-3.01820554	1.75291658	-1.48915141
H	-2.86776464	0.77595022	-1.95237896
H	0.53951879	0.49036374	-3.36799539
H	-3.87361406	-1.18914882	0.23180253
C	1.89536307	3.07663191	-0.09416120
H	2.50958001	2.32837634	0.41713885
H	2.35307197	3.21515683	-1.08496252
C	1.98465996	4.40366356	0.67429747
C	-4.49724180	2.06481443	-1.16613030
C	-4.40727691	2.96484507	0.08986710
H	-4.92790985	2.50729594	0.93565540
H	-2.64619726	2.50621470	-2.20693918
C	-2.88836873	3.06380241	0.40216372
H	-2.49667442	3.95961491	-0.11847890
H	-4.84649074	3.95340722	-0.06687758
C	-2.58592163	3.22284042	1.88747704
H	-2.96715171	2.36587578	2.45083618
H	-1.51245724	3.31459787	2.06945365
H	-3.06687973	4.12506372	2.27636031
C	1.00326558	-4.80523293	-0.56257753
H	0.53404835	-4.62661993	-1.52487029
C	1.64697536	-4.07191997	1.61935361

H	1.68530301	-3.30673127	2.38829187
C	1.56564440	-6.05479873	-0.31638867
H	1.52806996	-6.82533418	-1.08011601
C	2.21386998	-5.32034880	1.87843348
H	2.68439334	-5.51197211	2.83767962
C	2.17574231	-6.31861927	0.90942353
H	2.61472097	-7.29133746	1.10512976
C	3.41908957	4.95307357	0.80630473
H	4.06134368	4.20775339	1.28911345
H	3.39107157	5.82078231	1.47773616
C	4.03186531	5.37793109	-0.49952522
H	3.47079084	6.12608166	-1.05972283
C	5.17914769	4.92952062	-1.00162694
H	5.77524217	4.18599345	-0.48062545
H	5.56833721	5.29280118	-1.94623229
H	3.11571431	-1.02562130	-3.22043884
H	1.99875955	0.98685400	-2.50580820
H	1.65506415	-1.50085980	-4.11858019
H	-3.49689749	-3.49453679	-1.69956311
H	-3.97600298	-3.59654871	0.01110011
H	-3.72592115	-1.11916912	-1.52365201
H	-5.00188216	2.55329670	-2.00356203
H	-5.04429591	1.14541260	-0.94522735
H	1.35376078	5.14986451	0.17399214
H	1.55713708	4.26123078	1.67216341
H	-0.03954208	3.24599536	-0.70958637

MP2 Electronic Energy(Ha): 1489.181921971053

B3LYP Electronic Energy(Ha): 1493.021664971341

M06-L Electronic Energy(Ha): 1492.835228881296

Zero point energy correction(kcal/mol): 378.145

Enthalpy correction(kcal/mol): 401.178

Entropy correction(cal/mol): 224.312

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 370.017

Deuterated enthalpy correction(kcal/mol): 393.409

Deuterated entropy correction(cal/mol): 226.725

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H3

Reactant geometry

Zr	-0.56035629	-0.93375041	-0.41620684
C	-0.17944918	1.28892309	-1.43139521
C	0.80228401	0.44069936	-2.03556896
H	1.86124775	0.46299689	-1.82307252
C	-1.42628410	0.88148520	-1.99446797
H	-2.39229277	1.30025390	-1.74974538
C	-1.22264273	-0.22671284	-2.84881189
H	-1.98066093	-0.74635234	-3.41545084
C	0.17009076	-0.50022265	-2.87638774
H	0.65498489	-1.27768828	-3.44838845
B	0.03035175	2.22893961	-0.10386586
C	0.35370870	3.78850983	-0.35329780
C	-1.31878299	1.92207141	0.79749511
C	1.12794166	1.41759007	0.81100348
N	1.10888642	0.12124525	0.88810811
N	-1.71615433	0.70744590	1.02042027
O	-2.09933348	2.89025590	1.30490077
O	2.00324639	2.02441748	1.62543437
C	2.03026330	-0.31294245	1.95418228
C	2.77281633	0.98821262	2.30565875
C	-3.00944615	0.75530447	1.72776020
C	-3.16123908	2.24928811	2.06910269
N	0.70226771	-2.61701826	-0.34873665
N	-2.31901135	-2.09625272	-0.24284376
C	-3.35919045	-2.44441942	-1.21470054

H	-3.01638158	-2.30923883	-2.23930651
H	1.45923661	-0.71202847	2.79873278
H	-3.80354078	0.38863890	1.07075194
C	2.11090554	-2.84944464	-0.63466958
H	2.26263806	-3.14782074	-1.68643949
H	2.65753264	-1.90931804	-0.51433626
C	2.74473418	-3.92831767	0.25683352
C	-3.74129894	-3.91537986	-0.90931887
C	-3.30905126	-4.11300600	0.56325829
H	-2.49477362	-4.83980153	0.63721283
H	-4.24675734	-1.80277153	-1.07775096
C	-2.80213684	-2.71842666	1.00361206
H	-4.12166384	-4.46639742	1.20372160
C	0.47722608	4.30719773	-1.65055665
H	0.34820547	3.64253766	-2.49895981
C	0.52819047	4.69376494	0.70776841
H	0.44363632	4.34022371	1.73018707
C	0.75988667	5.65352623	-1.88377627
H	0.84800792	6.01893641	-2.90208439
C	0.81055322	6.03926520	0.48793373
H	0.93889273	6.71004249	1.33173264
C	0.92813883	6.52671827	-0.81316256
H	1.14794000	7.57468146	-0.98822159
C	4.24187190	-4.16983541	-0.02457643
H	4.39198879	-4.36336482	-1.09259620
H	4.55077095	-5.08003571	0.50450242
C	5.12868528	-3.03750209	0.41427818
H	5.10625496	-2.81127873	1.48065070
C	5.92125500	-2.31749951	-0.37542462
H	5.98261672	-2.50660541	-1.44302951
H	6.54341074	-1.51968901	0.01474213
H	3.78963423	1.02194041	1.90968512
H	2.69908233	-1.09700208	1.60081996

H	2.78805824	1.22725036	3.36814294
H	-2.98716300	2.46963008	3.12449749
H	-4.10868785	2.68898794	1.75984438
H	-2.99551317	0.12403288	2.61835885
H	-4.80878519	-4.09253770	-1.06151691
H	-3.20083714	-4.59764025	-1.56911868
H	2.60100255	-3.65609846	1.30909962
H	2.20046762	-4.86871308	0.10774144
H	0.18989235	-3.49216139	-0.40600197
H	-3.68030601	-2.14878530	1.36045401
C	-1.78518169	-2.76825311	2.14188942
H	-0.89915945	-3.33962813	1.85662361
H	-1.46099476	-1.76724568	2.44580271
H	-2.23180526	-3.24152540	3.02103483

MP2 Electronic Energy(Ha): 1489.188262613862

B3LYP Electronic Energy(Ha): 1493.023835953352

M06-L Electronic Energy(Ha): 1492.839896140525

Zero point energy correction(kcal/mol): 378.279

Enthalpy correction(kcal/mol): 401.233

Entropy correction(cal/mol): 221.340

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.217

Deuterated enthalpy correction(kcal/mol): 397.375

Deuterated entropy correction(cal/mol): 222.658

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.24905709	0.64968188	-0.43326998
C	-0.27734983	-1.52829711	-1.45612337
C	-1.32222207	-0.64449178	-1.88366409
H	-2.34218997	-0.66414690	-1.52648512
C	0.87910979	-1.11181573	-2.17844555
H	1.86465927	-1.54596682	-2.08563566

C	0.57978516	0.03933067	-2.94480552
H	1.26463461	0.58081488	-3.58175338
C	-0.80091736	0.32662153	-2.76723239
H	-1.34832953	1.13245220	-3.23354906
B	-0.28861464	-2.47716466	-0.11455294
C	-0.66763624	-4.03111803	-0.32072768
C	1.18952426	-2.20516859	0.57897378
C	-1.24882682	-1.66507106	0.95202876
N	-1.18377142	-0.37019924	1.05155106
N	1.69565607	-1.01529709	0.70668965
O	1.95288299	-3.21168647	1.03315643
O	-2.08847155	-2.25528011	1.80782971
C	-2.09020466	0.09659896	2.11398138
C	-2.70766841	-1.21936244	2.63191871
C	3.05411617	-1.13854533	1.27467046
C	3.15187178	-2.63476294	1.62372120
N	-0.46584621	2.46104372	-0.22645888
N	2.06584163	2.15688040	-0.29443903
C	2.78597853	2.57741889	-1.49856478
H	2.08324216	2.80966112	-2.30369995
H	-1.53196617	0.63415217	2.88394115
H	3.79969028	-0.83164785	0.53521652
C	-1.34808415	3.58573535	-0.41976833
H	-0.91812701	4.30423412	-1.13826224
H	-2.29564133	3.25214469	-0.86285217
C	-1.65535412	4.34772682	0.88142655
C	3.63766092	3.80204013	-1.07482830
C	3.72941757	3.68402533	0.46667428
H	3.19800108	4.50927618	0.94915708
H	3.44612594	1.77427578	-1.86473999
C	3.01840526	2.34900012	0.80625894
H	4.75932548	3.70029313	0.83354644
C	-0.97782408	-4.53739570	-1.59140038

H	-0.95419317	-3.86883631	-2.44607877
C	-0.71582688	-4.94053233	0.74998718
H	-0.48570494	-4.59800672	1.75357319
C	-1.31830040	-5.87578596	-1.79012856
H	-1.55316287	-6.23122670	-2.78831452
C	-1.05451294	-6.27811267	0.56419074
H	-1.08268820	-6.95230235	1.41435652
C	-1.35798726	-6.75346106	-0.71096135
H	-1.62161884	-7.79538707	-0.85951850
C	-2.60685989	5.54644975	0.69267254
H	-2.19862707	6.23228072	-0.05835681
H	-2.64347828	6.10532023	1.63697054
C	-4.00959916	5.15969349	0.31273836
H	-4.51327554	4.48307514	1.00352504
C	-4.66692469	5.57682882	-0.76585951
H	-4.20977486	6.25116573	-1.48405158
H	-5.68492765	5.26393719	-0.96983429
H	-3.78576913	-1.28738600	2.48770603
H	-2.83220616	0.78251906	1.70033942
H	-2.46550510	-1.44060126	3.67151156
H	3.11995128	-2.83004140	2.69737666
H	4.01178294	-3.14043882	1.18705157
H	3.17905770	-0.49575657	2.14752157
H	4.61926242	3.79253469	-1.55502603
H	3.14445001	4.73252173	-1.36416556
H	-2.08386025	3.64658445	1.60722634
H	-0.71282277	4.70176243	1.31207363
H	0.83152328	2.67876285	-0.17064368
H	3.77847761	1.54916340	0.77962284
C	2.36063980	2.34471438	2.18443547
H	1.61817523	3.14315111	2.26081145
H	1.85533188	1.39705329	2.39214830
H	3.11005334	2.49831377	2.96655528

MP2 Electronic Energy(Ha): 1489.140485764990

B3LYP Electronic Energy(Ha): 1492.976015021364

M06-L Electronic Energy(Ha): 1492.784077062376

Zero point energy correction(kcal/mol): 374.910

Enthalpy correction(kcal/mol): 397.973

Entropy correction(cal/mol): 231.012

Imaginary Frequencies: -1631.29

Deuterated zero point energy correction(kcal/mol): 371.651

Deuterated enthalpy correction(kcal/mol): 394.839

Deuterated entropy correction(cal/mol): 231.815

Deuterated imaginary Frequencies: -1173.56

Product geometry

Zr	-0.02912700	-0.74668978	-0.21978925
C	0.41813275	1.42311068	-1.38890652
C	1.49497999	0.54118929	-1.74334997
H	2.51222110	0.61705442	-1.38702035
C	-0.70962575	0.93999970	-2.10274428
H	-1.70283179	1.36344482	-2.05354103
C	-0.36308422	-0.24301521	-2.80722354
H	-1.00965215	-0.82460228	-3.45034859
C	1.01796078	-0.48058084	-2.59483252
H	1.59961783	-1.28433950	-3.02112437
B	0.39149792	2.44886650	-0.10938651
C	0.64833119	4.01220684	-0.42252991
C	-1.01981776	2.13483150	0.70363960
C	1.43816867	1.76368207	0.96613630
N	1.39851941	0.48711085	1.18172597
N	-1.48285628	0.93826058	0.91087937
O	-1.70067307	3.12688571	1.30926504
O	2.35316376	2.43778910	1.68038277
C	2.44028127	0.11698060	2.15156606
C	3.02540848	1.48537310	2.55990247

C	-2.61846827	1.02822615	1.84867320
C	-2.84726627	2.54485290	1.98433469
N	0.76929931	-2.38095937	0.25090384
N	-2.24950898	-1.86101834	-0.49470248
C	-3.34877163	-1.09672882	-1.17395645
H	-3.21618635	-1.17175762	-2.25280184
H	2.00793979	-0.42796869	2.99329695
H	-3.49865525	0.51193274	1.45889292
C	1.55191805	-3.56278069	0.44250462
H	2.26722071	-3.42043526	1.27184006
H	0.91759128	-4.41025767	0.75201942
C	2.34916284	-3.98535889	-0.80408650
C	-4.69910203	-1.68743399	-0.69106120
C	-4.30554391	-2.90315166	0.16109203
H	-4.26060562	-3.80998432	-0.45247155
H	-3.25600184	-0.04536114	-0.90756380
C	-2.89278314	-2.57188450	0.66522116
H	-5.00195587	-3.09678261	0.97970053
C	0.78271623	4.47220541	-1.74095468
H	0.71601534	3.75854096	-2.55597474
C	0.75049777	4.97730617	0.59458141
H	0.65748192	4.67126055	1.63116530
C	1.00342921	5.81814858	-2.03563011
H	1.10292045	6.13604694	-3.06882735
C	0.97196238	6.32289020	0.31357167
H	1.04718467	7.03979822	1.12537748
C	1.09895774	6.75116355	-1.00734314
H	1.27246132	7.79886971	-1.22996804
C	3.21661641	-5.24310657	-0.59921945
H	3.90051282	-5.09167813	0.24390862
H	3.84523895	-5.37438139	-1.48983094
C	2.42565417	-6.50357912	-0.38561430
H	1.71018773	-6.74639549	-1.17166273

C	2.53627285	-7.32598492	0.65413545
H	3.23337833	-7.12752473	1.46302248
H	1.93884450	-8.22741052	0.73480855
H	4.09800051	1.58043355	2.39265286
H	3.17610524	-0.53668256	1.67624963
H	2.79398702	1.76889253	3.58813062
H	-2.85387896	2.90728036	3.01198788
H	-3.74753946	2.89318288	1.47359923
H	-2.35242103	0.55777114	2.80150584
H	-5.23915764	-0.95286951	-0.08846801
H	-5.34986018	-1.95675024	-1.52465849
H	1.64744662	-4.14956718	-1.63082272
H	2.99003696	-3.15002263	-1.10443938
H	-1.93953103	-2.59555018	-1.13005716
H	-2.96515093	-1.84092506	1.47752847
C	-2.09724358	-3.77625619	1.14296485
H	-2.00544641	-4.52123935	0.34536038
H	-1.09387676	-3.48502307	1.45079634
H	-2.61461635	-4.24872768	1.98218508

MP2 Electronic Energy(Ha): 1489.175710482546

B3LYP Electronic Energy(Ha): 1493.007455141485

M06-L Electronic Energy(Ha): 1492.820323498178

Zero point energy correction(kcal/mol): 379.059

Enthalpy correction(kcal/mol): 402.061

Entropy correction(cal/mol): 224.123

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.729

Deuterated enthalpy correction(kcal/mol): 397.891

Deuterated entropy correction(cal/mol): 225.130

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H4

Reactant geometry

Zr	0.93317268	0.77361477	-0.27162131
C	0.38543699	-1.48077012	-1.24865093
C	-0.25667150	-0.53110296	-2.09302049
H	-1.32508581	-0.38526942	-2.16478680
C	1.78974668	-1.32731807	-1.49545953
H	2.56708341	-1.90732362	-1.01850271
C	1.99681418	-0.30808751	-2.44712652
H	2.94653573	0.02297966	-2.84312989
C	0.72266449	0.19991368	-2.81072924
H	0.53212706	0.95748411	-3.55522063
B	-0.29097091	-2.47171853	-0.14389365
C	-0.02125288	-4.05519135	-0.41227896
C	0.30958201	-1.94768819	1.27740654
C	-1.88580021	-2.12642677	-0.04661762
N	-2.43563034	-1.21410643	0.67110268
N	0.87221183	-0.78192698	1.41938559
O	0.18945174	-2.65041319	2.41161190
O	-2.72158021	-2.84805940	-0.85659317
C	-3.88436004	-1.22783822	0.39022910
C	-4.07102070	-2.38666620	-0.61257246
C	1.16461214	-0.54876135	2.84601942
C	0.77220113	-1.88436490	3.50156800
N	2.85112745	1.42479994	0.30659338
H	-4.44523585	-1.38411623	1.31677252
H	2.21957492	-0.30456078	2.98248359
C	3.02314022	2.58550085	1.19233416
H	2.12359354	3.20897619	1.23056859
H	3.22095672	2.27643247	2.23096886
C	4.25112217	3.32115299	0.63096063
C	5.15440483	2.16629387	0.14641387
H	5.61965650	2.39215808	-0.81540230
H	5.96476694	1.98077800	0.85620593

C	4.21733167	0.91830086	0.05184356
C	0.55817194	-4.52214855	-1.60159822
H	0.85424836	-3.80929134	-2.36404468
C	-0.39603221	-5.03273885	0.52703730
H	-0.85034249	-4.72376082	1.46207007
C	-0.19774807	-6.39206953	0.29762131
H	-0.50029742	-7.11602302	1.04816952
C	0.75949775	-5.88173009	-1.84420679
H	1.20827403	-6.20224130	-2.77949799
C	0.38414673	-6.82537854	-0.89282908
H	0.53940532	-7.88361166	-1.07581087
H	-4.64820210	-3.22217698	-0.20958596
H	-4.50690120	-2.08111991	-1.56580889
H	-4.19558602	-0.26244584	-0.02219999
H	0.01844064	-1.79019196	4.28299307
H	1.62413338	-2.44892528	3.88413187
H	0.56889435	0.29220455	3.20936695
H	3.95409126	3.95870254	-0.20806889
H	4.73709924	3.96203606	1.37095198
N	-0.62970296	1.67055903	0.78589390
H	-1.27282318	0.92443464	1.06994376
C	-1.13548953	2.96130976	1.22721108
H	-0.48167612	3.75604127	0.84741583
H	-2.13250094	3.16458742	0.80885677
C	-1.20456153	3.12237250	2.75775772
H	-0.22698749	2.85945179	3.17553288
H	-1.37556756	4.18107179	2.99330378
C	-2.29833569	2.27845731	3.44310458
H	-2.22029849	1.23055624	3.13648498
H	-2.11735597	2.30147324	4.52544405
C	-3.68953276	2.78598636	3.18063880
H	-3.87803345	3.81610491	3.48379328
C	-4.67806956	2.08906313	2.62712488

H	-4.53678649	1.06126311	2.30928006
H	-5.66255626	2.51897805	2.47829757
N	1.02768953	3.08808425	-1.41148256
C	0.41181697	3.73343979	-2.60645124
H	2.03373515	3.03536377	-1.55689488
H	0.90927543	3.72437977	-0.62545258
H	0.96306637	4.65065938	-2.84640296
H	0.54021620	3.05696076	-3.45357915
C	-1.06587813	4.08872899	-2.43687070
H	-1.19295612	4.68732121	-1.52633643
H	-1.33857898	4.74730504	-3.26844693
C	-2.03389938	2.89279830	-2.41415137
H	-1.77061873	2.23599201	-1.57865115
H	-1.91475991	2.31124331	-3.33473475
C	-3.46774809	3.32118224	-2.27600367
H	-3.71472702	3.86633396	-1.36584299
C	-4.42885672	3.08740959	-3.16517188
H	-4.23251955	2.54567535	-4.08586343
H	-5.44745244	3.42148993	-3.00342793
H	4.25116928	0.49291612	-0.95339239
C	4.63700359	-0.18225889	1.03910454
H	4.63030270	0.18899699	2.06864720
H	3.96041965	-1.03689131	0.97870520
H	5.65127130	-0.53070911	0.81859595

MP2 Electronic Energy(Ha): 1740.488175405661

B3LYP Electronic Energy(Ha): 1744.986827214917

M06-L Electronic Energy(Ha): 1744.764244712055

Zero point energy correction(kcal/mol): 476.440

Enthalpy correction(kcal/mol): 505.171

Entropy correction(cal/mol): 268.041

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.914

Deuterated enthalpy correction(kcal/mol): 497.008

Deuterated entropy correction(cal/mol): 270.388

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.28354681	0.58310509	-0.34951832
C	0.10999704	-1.64745073	-1.46344231
C	-0.81434079	-0.82146077	-2.18572730
H	-1.89088946	-0.88561867	-2.13529470
C	1.40152352	-1.22229951	-1.88457404
H	2.33612705	-1.63439393	-1.53544109
C	1.27733830	-0.12782702	-2.76469164
H	2.08108605	0.41085480	-3.24400933
C	-0.10745067	0.11112600	-2.96064514
H	-0.54070165	0.84874233	-3.61673230
B	-0.25808946	-2.66101552	-0.24063616
C	-0.33470496	-4.23539031	-0.58150101
C	0.77032778	-2.24853290	0.96735267
C	-1.63632967	-1.99048775	0.34820853
N	-1.71945643	-0.70488353	0.46988801
N	1.17548079	-1.02538613	1.13406524
O	1.12437611	-3.10450535	1.93917989
O	-2.74104181	-2.68062999	0.67878036
C	-3.09993975	-0.35482142	0.85716571
C	-3.71572660	-1.72554427	1.19138960
C	1.85390458	-0.92076712	2.43929522
C	1.97850784	-2.38927751	2.87793667
N	2.45722442	1.52825144	-0.14073969
H	-3.12364062	0.33549368	1.70208433
H	2.82200703	-0.43301138	2.33863273
C	2.80732685	2.34907584	1.03770562
H	2.04060972	3.11012554	1.19559358
H	2.84738205	1.75761229	1.95962499
C	4.19596879	2.98241492	0.73816272

C	4.61253622	2.37272824	-0.61785726
H	4.35792892	3.05114579	-1.43664921
H	5.68327718	2.16396725	-0.67934242
C	3.74605564	1.10083929	-0.72393945
C	-0.03508513	-4.71849936	-1.86396565
H	0.25097062	-4.01523280	-2.63974458
C	-0.70374139	-5.18975282	0.38236717
H	-0.94595457	-4.86455838	1.38853569
C	-0.76858140	-6.54836798	0.08472846
H	-1.05831196	-7.25714903	0.85418055
C	-0.09608808	-6.07764741	-2.17402144
H	0.14246164	-6.41443054	-3.17801561
C	-0.46359928	-6.99999813	-1.19869782
H	-0.51353302	-8.05799176	-1.43398633
H	-3.81559774	-1.90053157	2.26521234
H	-4.66869477	-1.92352209	0.70280012
H	-3.60445422	0.13880014	0.01935836
H	1.61485237	-2.59303868	3.88439943
H	2.99031885	-2.78520618	2.77030886
H	1.24227513	-0.32298940	3.12186968
H	4.14211483	4.07194288	0.69189076
H	4.91297003	2.73109062	1.52315089
N	-0.53413792	1.71944167	1.24115550
H	-1.09194790	1.08886042	1.80594266
C	-0.63743114	3.05302173	1.81527178
H	-0.03856603	3.75917747	1.23013548
H	-1.67387793	3.42045140	1.75353793
C	-0.17025926	3.17210859	3.27887489
H	0.87360938	2.85181900	3.34560362
H	-0.19570067	4.23259093	3.56202583
C	-0.99871566	2.37077920	4.30155669
H	-0.95620587	1.29981654	4.07492768
H	-0.52272913	2.49137486	5.28357753

C	-2.43232449	2.81137914	4.40985522
H	-2.58718432	3.88047400	4.55374630
C	-3.49557706	2.01289728	4.36354702
H	-3.39376749	0.93897667	4.23447187
H	-4.50374531	2.39704618	4.47020491
N	0.55657073	2.72066063	-1.28600218
C	0.43991232	3.39625394	-2.58468255
H	1.71988344	2.33113319	-0.89979052
H	0.23770193	3.37278811	-0.57521742
H	1.26387691	4.11363403	-2.70914985
H	0.55552251	2.66187645	-3.38495275
C	-0.87347428	4.17170040	-2.77299261
H	-0.94253663	4.93547841	-1.98669668
H	-0.82449300	4.71860731	-3.72165396
C	-2.15002887	3.31340066	-2.75204824
H	-2.15560771	2.71985813	-1.82988476
H	-2.13710128	2.60505808	-3.58698267
C	-3.40482738	4.13708871	-2.81550786
H	-3.54112756	4.85267883	-2.00495548
C	-4.32962045	4.06366371	-3.76870663
H	-4.23615773	3.36912316	-4.59853569
H	-5.21349435	4.69141096	-3.75506258
H	3.58630679	0.82596937	-1.76768216
C	4.41331077	-0.08821715	-0.01303289
H	4.70589956	0.16758405	1.00997432
H	3.74634145	-0.94982857	0.03181200
H	5.32144684	-0.38550458	-0.54646362

MP2 Electronic Energy(Ha): 1740.470256420370

B3LYP Electronic Energy(Ha): 1744.955933342148

M06-L Electronic Energy(Ha): 1744.738392563552

Zero point energy correction(kcal/mol): 474.448

Enthalpy correction(kcal/mol): 502.302

Entropy correction(cal/mol): 255.889

Imaginary Frequencies: -1373.60

Deuterated zero point energy correction(kcal/mol): 466.834

Deuterated enthalpy correction(kcal/mol): 495.029

Deuterated entropy correction(cal/mol): 257.946

Deuterated imaginary Frequencies: -987.51

Product geometry

Zr	-0.03955587	-0.73704592	0.56681164
C	0.10692095	1.58147507	1.46184904
C	-1.19559401	1.20606628	1.90332108
H	-2.12511059	1.54820156	1.47353538
C	1.01580283	0.87468030	2.31023926
H	2.09281831	0.94047912	2.26471820
C	0.28503947	0.08574783	3.22497731
H	0.69240171	-0.53107540	4.01384883
C	-1.08800572	0.28692252	2.96660497
H	-1.90503946	-0.15601542	3.51553711
B	0.45950324	2.47409298	0.14768955
C	0.55399462	4.07261725	0.36584748
C	1.80296560	1.77339677	-0.48237136
C	-0.64153238	1.97381038	-0.96461578
N	-1.04242363	0.74112582	-0.98444076
N	1.97774059	0.48874226	-0.46340294
O	2.73700631	2.48042919	-1.15027169
O	-1.09562411	2.73926523	-1.97226971
C	-1.85063319	0.51409331	-2.19503337
C	-2.03278873	1.93784821	-2.75115049
C	3.15192007	0.17335004	-1.30342863
C	3.77906713	1.55315789	-1.55770983
N	1.19279834	-2.56304891	1.89458740
H	-1.31240460	-0.14548579	-2.88131027
H	3.83316375	-0.51350966	-0.80065431
C	1.17997249	-3.91314505	1.25296456

H	0.14840824	-4.25801738	1.19352699
H	1.54573247	-3.79905148	0.23476220
C	2.09417581	-4.83439929	2.10263127
C	2.70434926	-3.90287744	3.17567702
H	2.15562083	-3.99629532	4.11770822
H	3.75184611	-4.12671854	3.38797826
C	2.51002882	-2.48311541	2.60637087
C	0.40365883	4.64068353	1.63983115
H	0.21574444	3.98987895	2.48787216
C	0.79226913	4.96226397	-0.69651456
H	0.91356215	4.57172511	-1.70088601
C	0.87594227	6.33826677	-0.49916259
H	1.06013336	6.99509928	-1.34376721
C	0.48646016	6.01768101	1.85009162
H	0.36446967	6.42003440	2.85101744
C	0.72345071	6.87424048	0.77895970
H	0.78781640	7.94601530	0.93584802
H	-1.77249749	2.04749906	-3.80334378
H	-3.03265252	2.34173204	-2.58009207
H	-2.79971791	0.03646079	-1.94516829
H	4.02461880	1.75507513	-2.59970934
H	4.65702467	1.74406970	-0.93547937
H	2.83102586	-0.30908336	-2.23342928
H	1.53660726	-5.65510821	2.55774019
H	2.87012831	-5.28401301	1.47944106
N	0.44124358	-1.89036039	-1.17800721
H	0.96292961	-1.31951136	-1.83395454
C	-0.17084122	-2.99707266	-1.89988367
H	-0.61116181	-3.69453855	-1.17785838
H	-1.00379092	-2.66660573	-2.54601640
C	0.79990270	-3.81410527	-2.77247793
H	1.61592371	-4.18898609	-2.14516501
H	0.26544291	-4.69320500	-3.15586180

C	1.40939805	-3.05155088	-3.96570722
H	1.98889963	-2.19132566	-3.61445422
H	2.12807975	-3.71885983	-4.45913182
C	0.39890880	-2.60153226	-4.98357489
H	-0.24727563	-3.38282913	-5.38328214
C	0.24915170	-1.35728726	-5.43096883
H	0.87185194	-0.54394935	-5.06939490
H	-0.48967498	-1.10744359	-6.18426875
N	-1.72024012	-1.97047259	0.77826716
C	-2.84927629	-2.32529019	1.63033031
H	0.48253096	-2.58274157	2.62447220
H	-1.76551352	-2.56355098	-0.04810014
H	-2.78030121	-3.38219248	1.93450486
H	-2.79933032	-1.74077707	2.55096122
C	-4.22867702	-2.11861494	0.97851486
H	-4.25796338	-2.66991249	0.02943320
H	-4.99553054	-2.56992176	1.61938094
C	-4.58134913	-0.64327933	0.72875550
H	-3.75010570	-0.18320013	0.18304986
H	-4.65704901	-0.11592785	1.68607634
C	-5.85506543	-0.46657587	-0.04680866
H	-5.87977698	-0.94017332	-1.02852661
C	-6.93009958	0.19775974	0.36839911
H	-6.95746642	0.68326918	1.33954356
H	-7.81935155	0.28487502	-0.24587089
H	2.42047003	-1.74296904	3.40192348
C	3.63274270	-2.05390119	1.66590419
H	3.74396906	-2.74050832	0.82267999
H	3.43523043	-1.05755520	1.27132159
H	4.58153724	-2.02932894	2.20806756

MP2 Electronic Energy(Ha): 1740.497827043470

B3LYP Electronic Energy(Ha): 1744.989885264503

M06-L Electronic Energy(Ha): 1744.772658880196

Zero point energy correction(kcal/mol): 477.145

Enthalpy correction(kcal/mol): 505.496

Entropy correction(cal/mol): 261.112

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.658

Deuterated enthalpy correction(kcal/mol): 497.394

Deuterated entropy correction(cal/mol): 263.510

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H5

Reactant geometry

Zr	-0.81077216	0.92950598	0.19824294
C	-0.13832528	-1.12298664	1.38983787
C	0.84586733	-0.17264916	1.79100154
H	1.87227485	-0.16329895	1.45547861
C	-1.33362370	-0.73813459	2.07739494
H	-2.29011762	-1.23317258	1.99637777
C	-1.09787412	0.43061647	2.83042454
H	-1.82258081	0.95974631	3.43171546
C	0.25734075	0.78985007	2.64932440
H	0.75544943	1.62773928	3.11785566
B	-0.03527009	-2.18850435	0.15228678
C	0.39925093	-3.69843216	0.52416388
C	-1.49471916	-2.03412564	-0.60430023
C	0.90009481	-1.45108714	-0.98967046
N	0.87401923	-0.16806580	-1.18053194
N	-2.04431855	-0.86729700	-0.73163004
O	-2.16279697	-3.04940617	-1.17445252
O	1.60651680	-2.15282237	-1.89684400
C	1.58017720	0.13967025	-2.43675712
C	2.23801168	-1.20356482	-2.80118271
C	-3.30202658	-0.99523567	-1.48500577

C	-3.36905672	-2.50690578	-1.78965723
N	0.83895718	2.75628949	0.11916866
N	-2.36626008	2.26270122	0.52337554
C	-3.22237575	3.05567678	1.38184329
H	-2.83885305	3.09794928	2.40430245
H	0.85924630	0.47966176	-3.18636110
H	-4.14268660	-0.65078311	-0.87747022
C	2.28181628	2.66550953	0.43860917
H	2.37412598	2.39830668	1.49321088
H	2.69504679	1.83222211	-0.13099757
C	3.06205853	3.95221830	0.15546255
C	-3.30626416	4.46305403	0.70562511
C	-2.71745596	4.25286072	-0.71403577
H	-1.71195846	4.68285723	-0.78305602
H	-4.23119043	2.61593043	1.43359180
C	-2.62624073	2.71887411	-0.86368010
C	-1.52023872	2.09728442	-1.73126070
H	-3.32149290	4.71357268	-1.50010605
H	0.40503464	3.49278850	0.67214900
C	0.46084315	-4.72209127	-0.43761715
H	0.20536142	-4.50057748	-1.46794169
C	0.73996298	-4.04897810	1.83915428
H	0.70257177	-3.28901334	2.61323843
C	0.84143598	-6.02000853	-0.10648166
H	0.87681340	-6.78558348	-0.87540076
C	1.12351490	-5.34582254	2.18277429
H	1.37960980	-5.57931709	3.21155258
C	1.17610311	-6.33889025	1.20900414
H	1.47265705	-7.34947376	1.47003001
C	4.57015905	3.82254942	0.45188026
H	4.71785282	3.48793480	1.48446522
H	5.01786317	4.82096721	0.38024134
C	5.29073777	2.89810926	-0.49126099

H 5.25481504 3.17886530 -1.54378187

C 5.95615991 1.80090116 -0.14115065

H 6.02549254 1.48270867 0.89477353

H 6.46520691 1.18579353 -0.87446409

H 3.31225545 -1.22245025 -2.60501815

H 2.31664579 0.93466611 -2.29574105

H 2.05054993 -1.53564313 -3.82172306

H -3.33223182 -2.74355429 -2.85371331

H -4.22500189 -3.00920161 -1.33817974

H -3.26897741 -0.38210139 -2.38814051

H -4.33938911 4.81703107 0.66913552

H -2.73466704 5.20527141 1.26856975

H 2.92179653 4.24187637 -0.89371902

H 2.64771357 4.76728361 0.76016183

H 0.71310644 3.03810194 -0.85077660

H -3.62240505 2.35403352 -1.17463027

H -0.87512782 2.87358516 -2.16473114

H -1.91611679 1.52041967 -2.57099070

MP2 Electronic Energy(Ha): 1489.174259923573

B3LYP Electronic Energy(Ha): 1493.002315509711

M06-L Electronic Energy(Ha): 1492.818695784316

Zero point energy correction(kcal/mol): 378.519

Enthalpy correction(kcal/mol): 401.441

Entropy correction(cal/mol): 225.900

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.114

Deuterated enthalpy correction(kcal/mol): 397.211

Deuterated entropy correction(cal/mol): 227.039

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr -0.60474811 -0.64058966 -0.16927302

C 0.47845099 1.24565263 -1.27216081

C	1.50763873	0.25684012	-1.31974307
H	2.40268380	0.25573619	-0.71472434
C	-0.50003202	0.81376301	-2.22481253
H	-1.42139579	1.32785886	-2.45372037
C	-0.11106874	-0.42450736	-2.78053813
H	-0.65792049	-0.99711371	-3.51585163
C	1.14374066	-0.76695263	-2.22021879
H	1.72583636	-1.64417812	-2.45719451
B	0.28935080	2.40611423	-0.13243423
C	0.91778526	3.85668661	-0.45699784
C	-1.33186461	2.38787012	0.16538995
C	0.82623691	1.70256398	1.26220876
N	0.64600625	0.43598994	1.49204884
N	-2.00300795	1.27600514	0.16165772
O	-2.03163061	3.48114806	0.49974848
O	1.35888193	2.39379403	2.27937589
C	1.05154903	0.12511857	2.87250394
C	1.66064998	1.45626987	3.35630500
C	-3.39441959	1.54992502	0.56675181
C	-3.42208484	3.08680925	0.68735112
N	0.36432160	-2.68122091	0.35637095
N	-1.93418092	-2.38796937	-0.69857259
C	-2.64906987	-3.20180067	-1.67198624
H	-1.94973783	-3.74658128	-2.31261607
H	0.17815037	-0.18090510	3.45428544
H	-4.09374690	1.17805755	-0.18547137
C	1.57386364	-3.36416457	-0.10946622
H	1.52365195	-3.45112686	-1.19963875
H	2.47752596	-2.77867276	0.10832414
C	1.72313624	-4.76716327	0.48739135
C	-3.55080598	-4.15360134	-0.81522654
C	-3.46340223	-3.60259652	0.63411148
H	-2.77770324	-4.20368000	1.23896594

H	-3.27661128	-2.58204596	-2.32883181
C	-2.86253901	-2.19408271	0.44807673
C	-2.03909831	-1.47256656	1.52135439
H	-4.43138616	-3.58789992	1.14150271
H	-0.81307025	-2.90171681	-0.20154076
C	0.81582764	4.93624844	0.43774208
H	0.29870616	4.80025076	1.38126620
C	1.59881035	4.09702706	-1.65968445
H	1.70066735	3.29077640	-2.37921348
C	1.36227026	6.18405375	0.14875888
H	1.26441412	6.99548819	0.86311455
C	2.15029790	5.34307763	-1.95998415
H	2.67028307	5.49172184	-2.90112231
C	2.03395277	6.39390523	-1.05489399
H	2.46041744	7.36520445	-1.28287745
C	2.97225452	-5.52257263	-0.00382053
H	2.96260043	-5.58362162	-1.09788167
H	2.91314398	-6.55358462	0.36645388
C	4.26989200	-4.91938573	0.45823384
H	4.38421653	-4.82255363	1.53800420
C	5.26355383	-4.51787518	-0.32949387
H	5.19831790	-4.59498505	-1.41082946
H	6.17986400	-4.10336098	0.07547624
H	2.74556817	1.42261779	3.46699129
H	1.77225875	-0.69505340	2.88590466
H	1.21512178	1.84680442	4.27054739
H	-3.74259562	3.45232817	1.66245058
H	-4.00948721	3.57354794	-0.09259968
H	-3.61945923	1.04790745	1.51018587
H	-4.57852104	-4.14335652	-1.18582559
H	-3.19893530	-5.18580504	-0.87141308
H	1.75330479	-4.69016326	1.58271876
H	0.82792766	-5.34951829	0.24486000

H 0.26282821 -2.81701665 1.35789383

H -3.68361097 -1.52915891 0.12500967

H -1.56412117 -2.18927549 2.20292332

H -2.63915221 -0.79433371 2.13112338

MP2 Electronic Energy(Ha): 1489.135230708399

B3LYP Electronic Energy(Ha): 1492.963924517422

M06-L Electronic Energy(Ha): 1492.774986525056

Zero point energy correction(kcal/mol): 375.444

Enthalpy correction(kcal/mol): 398.022

Entropy correction(cal/mol): 223.896

Imaginary Frequencies: -1552.92

Deuterated zero point energy correction(kcal/mol): 371.989

Deuterated enthalpy correction(kcal/mol): 394.708

Deuterated entropy correction(cal/mol): 224.678

Deuterated imaginary Frequencies: -1116.90

Product geometry

Zr -0.42915264 -0.78041159 -0.04391185

C 0.56932389 1.14056471 -1.22263676

C 1.62236061 0.17416522 -1.27884715

H 2.53790955 0.21392146 -0.70592759

C -0.42874985 0.66160375 -2.12578461

H -1.37183893 1.14582788 -2.32927440

C -0.02815534 -0.58197459 -2.66317682

H -0.58307377 -1.18486388 -3.36812003

C 1.25532678 -0.87701031 -2.14435158

H 1.84097231 -1.75188521 -2.38122845

B 0.40240413 2.35236289 -0.13898836

C 1.02928111 3.78343898 -0.54628523

C -1.20451201 2.36329170 0.21053654

C 0.96013235 1.70770275 1.27089131

N 0.71237964 0.46908301 1.56292140

N -1.90289044 1.27470001 0.27444859

O	-1.85009201	3.49663287	0.54952050
O	1.60468393	2.39965990	2.22268036
C	1.21195375	0.16700765	2.91267319
C	1.87266392	1.49565762	3.33694391
C	-3.26146106	1.61521533	0.73880366
C	-3.22295825	3.15082125	0.87596581
N	0.64421916	-2.52115962	0.43861314
N	-2.32134595	-2.16300838	-0.71474897
C	-3.39023180	-2.48248604	-1.68247369
H	-3.00045783	-3.09982551	-2.49293447
H	0.38296534	-0.12219678	3.56369408
H	-4.01077757	1.28806453	0.01259116
C	1.87552924	-3.23818227	0.12519983
H	2.50890496	-2.61335278	-0.50987941
H	2.45459742	-3.42052801	1.04031247
C	1.63830581	-4.58206074	-0.58310828
C	-4.50483743	-3.19148008	-0.84392017
C	-4.08860974	-2.98929280	0.64027588
H	-3.62115458	-3.89280137	1.04567975
H	-3.75693048	-1.55087564	-2.11850498
C	-3.04486836	-1.85853797	0.57199554
C	-1.97349034	-1.57869139	1.61258707
H	-4.93329565	-2.73890344	1.28532648
H	-1.79767861	-3.02398888	-0.54611979
C	1.00072794	4.88969178	0.32086674
H	0.54700605	4.78687446	1.30051142
C	1.63019721	3.98089484	-1.79844192
H	1.67504479	3.15232505	-2.49820883
C	1.54037188	6.12142559	-0.04050380
H	1.50085343	6.95383569	0.65528205
C	2.17356669	5.21057387	-2.17214913
H	2.63055093	5.32498954	-3.15018117
C	2.13086488	6.28833113	-1.29256878

H	2.55237526	7.24687904	-1.57692327
C	2.93329493	-5.35770481	-0.89795105
H	3.60824385	-4.73065726	-1.49160680
H	2.67276489	-6.21762223	-1.52830262
C	3.65356808	-5.85933283	0.32305976
H	3.07114500	-6.50744259	0.97813477
C	4.91351004	-5.58516687	0.64930449
H	5.53455732	-4.94499591	0.02964325
H	5.37217669	-5.99294015	1.54318817
H	2.95507395	1.42855061	3.45311204
H	1.91761876	-0.66584740	2.87727772
H	1.44021480	1.93936118	4.23387655
H	-3.42894674	3.51024031	1.88489421
H	-3.87525086	3.66815576	0.17062512
H	-3.47403505	1.11411159	1.68698020
H	-5.47939865	-2.74395748	-1.05034752
H	-4.57872384	-4.25019902	-1.10070293
H	0.98176024	-5.20435132	0.03858372
H	1.09384960	-4.39306264	-1.51482373
H	0.22567290	-2.94698562	1.26150259
H	-3.59045790	-0.93209917	0.36608405
H	-1.66709524	-2.50359028	2.11941900
H	-2.32295925	-0.88395565	2.38010846

MP2 Electronic Energy(Ha): 1489.165132773166

B3LYP Electronic Energy(Ha): 1492.998533872070

M06-L Electronic Energy(Ha): 1492.813480850473

Zero point energy correction(kcal/mol): 379.178

Enthalpy correction(kcal/mol): 401.811

Entropy correction(cal/mol): 219.575

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.792

Deuterated enthalpy correction(kcal/mol): 397.613

Deuterated entropy correction(cal/mol): 220.634

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H6

Reactant geometry

Zr	-0.77740389	1.15867730	-0.73858312
C	0.39463428	-1.00027767	-1.35586756
C	-0.75189707	-0.96905541	-2.19467183
H	-1.58246102	-1.65639256	-2.12734643
C	1.20983730	0.09744995	-1.78555769
H	2.17053450	0.35793402	-1.36213167
C	0.56715467	0.78711951	-2.84360555
H	0.94683165	1.64929907	-3.37330831
C	-0.66689151	0.12942111	-3.08929369
H	-1.39071298	0.39886337	-3.84356973
B	0.71221545	-1.94860992	-0.06656812
C	2.16075115	-2.69743741	-0.17244615
C	0.62425702	-0.94474536	1.22870854
C	-0.51549178	-3.01874137	0.15480904
N	-1.75578068	-2.73873520	0.36331271
N	0.19014940	0.28487841	1.19072179
O	0.96383498	-1.37332031	2.45612234
O	-0.20708325	-4.34373934	0.10437357
C	-2.50386141	-4.00477455	0.48760914
C	-1.42487139	-5.09542167	0.32493037
C	0.22639092	0.86275302	2.55065305
C	0.75690945	-0.29763426	3.41136847
N	-0.16489769	3.10436897	-0.34170054
N	-2.65896844	0.10298628	0.29648848
C	-3.29282263	0.40887275	1.60011732
H	-3.08991283	1.44671076	1.88565912
H	-3.00557579	-4.05299701	1.45898303
H	0.88270756	1.73532865	2.56811003

C	1.09992318	3.78114310	-0.06367765
H	1.85051241	3.02513079	0.19388701
H	1.47852629	4.29220612	-0.95928375
C	1.00315132	4.79636474	1.08360748
C	-4.79366457	0.21421588	1.34593943
C	-4.97720302	0.80647649	-0.06224777
H	-5.16644540	1.88167718	-0.00014225
H	-2.88572171	-0.24587372	2.37227301
C	-3.62233827	0.56117145	-0.78735674
H	-3.71796602	-0.26183525	-1.50010355
H	-5.81502662	0.35886436	-0.60086651
C	-2.92284484	1.74815021	-1.44537093
H	-3.18943508	2.67847704	-0.92098158
H	-2.48269109	-0.91708101	0.26659502
H	-3.17492599	1.87670378	-2.49928360
C	2.78738181	-3.30123323	0.93240019
H	2.31312590	-3.25279098	1.90519143
C	2.82482817	-2.81503331	-1.40400736
H	2.38104691	-2.37616300	-2.29113098
C	4.00427586	-3.96995036	0.81814278
H	4.45504965	-4.42156724	1.69662430
C	4.04096918	-3.48674081	-1.53184934
H	4.51825657	-3.55685832	-2.50441915
C	4.64096345	-4.06565232	-0.41766807
H	5.58846543	-4.58619933	-0.51010959
C	2.33607651	5.50199158	1.40308456
H	3.10459144	4.75712871	1.63916112
H	2.19452579	6.10198479	2.31108324
C	2.82727862	6.40257459	0.30333318
H	2.13829786	7.19017847	-0.00171181
C	4.00921411	6.31531830	-0.30009479
H	4.72939789	5.54801761	-0.03169789
H	4.30255602	7.00812820	-1.08071894

H	-1.58198217	-5.74635538	-0.53695688
H	-3.27903652	-4.06354662	-0.28326742
H	-1.28589936	-5.71103176	1.21584458
H	0.04859252	-0.65032028	4.16209014
H	1.71440072	-0.08758184	3.88888500
H	-0.76955634	1.19068323	2.85525984
H	-5.02993765	-0.85432979	1.35323852
H	-5.41655528	0.70019345	2.10071291
H	0.24510542	5.54924122	0.83088036
H	0.63865806	4.28389783	1.98009771
H	-0.88245737	3.79027120	-0.57303624

MP2 Electronic Energy(Ha): 1489.160675463183

B3LYP Electronic Energy(Ha): 1493.003310492426

M06-L Electronic Energy(Ha): 1492.810049360966

Zero point energy correction(kcal/mol): 378.097

Enthalpy correction(kcal/mol): 401.125

Entropy correction(cal/mol): 230.103

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.787

Deuterated enthalpy correction(kcal/mol): 396.993

Deuterated entropy correction(cal/mol): 231.155

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.11095606	1.03141171	-0.73838575
C	0.52757402	-1.40905823	-1.32388499
C	-0.39067377	-0.95306899	-2.30610198
H	-1.41399318	-1.28709921	-2.40164135
C	1.73979763	-0.67958527	-1.56634216
H	2.65519933	-0.79300977	-1.00189793
C	1.56135998	0.19794708	-2.66520474
H	2.30375573	0.85934697	-3.08841822
C	0.22802024	0.04096052	-3.11516417

H	-0.22173520	0.55758418	-3.95098004
B	0.27726402	-2.38159260	-0.03893357
C	1.29246368	-3.66130493	0.00978204
C	0.48906703	-1.40327464	1.26708827
C	-1.29953350	-2.84866858	0.01262793
N	-2.33683080	-2.08646020	0.08619282
N	0.57784111	-0.10150374	1.21739001
O	0.57889052	-1.91294144	2.50573354
O	-1.55331066	-4.18494832	-0.05114110
C	-3.54277041	-2.93746067	0.05709669
C	-2.98554313	-4.37485710	0.03701815
C	0.85617211	0.42301413	2.57138805
C	0.69844051	-0.82137352	3.45934101
N	0.75096825	2.83203163	-0.47135968
N	-2.09304448	0.86434380	0.11842036
C	-2.51552677	1.24733988	1.49327893
H	-1.80225244	1.95856724	1.91973597
H	-4.16857572	-2.74180658	0.93280519
H	1.86719387	0.83798833	2.60006018
C	1.30164905	4.16337626	-0.44793206
H	1.97331119	4.31984470	-1.30598139
H	0.50407319	4.91574769	-0.54434366
C	2.08820585	4.43949851	0.84142414
C	-3.87718227	1.92611505	1.30623277
C	-3.66062344	2.70869727	0.00630285
H	-3.10556769	3.62893000	0.21740084
H	-2.54030739	0.35950968	2.12645338
C	-2.79834620	1.77548315	-0.87075652
H	-3.44987009	1.14530466	-1.48456957
H	-4.58712840	2.99182747	-0.49677535
C	-1.74472825	2.47649557	-1.74361518
H	-1.93984468	3.55244511	-1.80014061
H	-2.34256090	-0.13268190	-0.01206999

H	-1.74539294	2.11701147	-2.77359440
C	1.38301239	-4.50670553	1.13047783
H	0.77670184	-4.29892626	2.00419857
C	2.09582656	-3.99913789	-1.09010202
H	2.05689735	-3.38713322	-1.98461010
C	2.22877905	-5.61259893	1.15618685
H	2.26941694	-6.23973767	2.04157982
C	2.94406129	-5.10754102	-1.07819965
H	3.54611486	-5.33468806	-1.95255662
C	3.01818279	-5.91954268	0.04896764
H	3.67801919	-6.78075427	0.06539791
C	2.68494538	5.85884977	0.90839122
H	3.31646092	6.04009759	0.03142959
H	3.34543221	5.90996423	1.78343035
C	1.65219136	6.94595984	1.02246702
H	0.97928223	6.86579953	1.87641061
C	1.50672127	7.97095739	0.18733362
H	2.15161737	8.09514440	-0.67762920
H	0.74282680	8.72545338	0.33886472
H	-3.30389148	-4.96337608	-0.82464983
H	-4.14223258	-2.70831280	-0.83050032
H	-3.19669595	-4.93620620	0.94997876
H	-0.20935194	-0.81009284	4.06604471
H	1.55753612	-1.02721024	4.09667346
H	0.16147387	1.22086036	2.83525730
H	-4.66120311	1.17251972	1.18049035
H	-4.15114740	2.56034916	2.15248588
H	1.42613109	4.27370551	1.69925320
H	2.89385336	3.70253658	0.92095983
H	-0.43454072	2.86313108	-1.11830774

MP2 Electronic Energy(Ha): 1489.124866998297

B3LYP Electronic Energy(Ha): 1492.959369266944

M06-L Electronic Energy(Ha): 1492.765370487885

Zero point energy correction(kcal/mol): 375.890

Enthalpy correction(kcal/mol): 398.396

Entropy correction(cal/mol): 227.526

Imaginary Frequencies: -1488.21

Deuterated zero point energy correction(kcal/mol): 372.368

Deuterated enthalpy correction(kcal/mol): 394.991

Deuterated entropy correction(cal/mol): 228.127

Deuterated imaginary Frequencies: -1091.19

Product geometry

Zr	0.12362812	1.06911650	-0.58855554
C	0.49495905	-1.33002861	-1.35990077
C	-0.52799199	-0.83791729	-2.21249858
H	-1.55101051	-1.18590240	-2.21830298
C	1.66743926	-0.57503073	-1.69877117
H	2.64104525	-0.70115414	-1.24426803
C	1.36066465	0.36556827	-2.71302372
H	2.04682595	1.05878332	-3.17728402
C	-0.01491525	0.21597858	-3.02269424
H	-0.55160219	0.75830559	-3.78914116
B	0.37740865	-2.32840872	-0.07551926
C	1.36594089	-3.62519499	-0.15946486
C	0.72266864	-1.39378045	1.24267546
C	-1.19470961	-2.75913441	0.15415315
N	-2.19121070	-1.96643864	0.36452701
N	0.77608845	-0.08387568	1.25305608
O	0.94902734	-1.95501220	2.43603347
O	-1.49450893	-4.08450956	0.11324558
C	-3.41607144	-2.78286746	0.48598258
C	-2.91024828	-4.23496856	0.37515737
C	1.17682049	0.38215435	2.59876234
C	1.13871053	-0.90892115	3.43115753
N	0.71943759	2.82690980	-0.38248151

N	-2.17990687	0.99985496	0.03393329
C	-2.48728238	1.58185965	1.37207208
H	-2.14899624	2.62057671	1.39892362
H	-3.91342908	-2.58383451	1.43997646
H	2.17368427	0.82623386	2.54768118
C	1.30544381	4.13443141	-0.43568173
H	1.81924699	4.29028012	-1.39855799
H	0.52423197	4.90761421	-0.38456585
C	2.31861319	4.38543968	0.69463401
C	-4.01132667	1.48280982	1.48629340
C	-4.48370063	1.82211393	0.06103722
H	-4.69130763	2.89220352	-0.02423535
H	-1.95309581	1.02509963	2.14319648
C	-3.29857946	1.44385048	-0.87747155
H	-3.55478202	0.58149587	-1.49717915
H	-5.39875195	1.29319329	-0.21122322
C	-2.88488521	2.60239365	-1.78298279
H	-3.73718914	2.92454409	-2.38812715
H	-2.26591815	-0.03230373	0.14558913
H	-2.08262428	2.31534743	-2.46703652
C	1.53391831	-4.51882134	0.91393503
H	1.00521168	-4.34076366	1.84290427
C	2.07013037	-3.92622788	-1.33536762
H	1.96703039	-3.27513875	-2.19637496
C	2.35961473	-5.63628410	0.82335334
H	2.46218428	-6.30151380	1.67527984
C	2.89738489	-5.04557720	-1.43981471
H	3.42172294	-5.24307199	-2.36963722
C	3.04972585	-5.90612992	-0.35750186
H	3.69357762	-6.77633082	-0.43175706
C	2.96207398	5.78564133	0.65730768
H	3.44118458	5.94997712	-0.31452385
H	3.76279958	5.81485791	1.40796681

C	2.00039370	6.90574800	0.94183904
H	1.46819442	6.83679637	1.89088447
C	1.76224697	7.94747921	0.14970816
H	2.26519903	8.06054183	-0.80621419
H	1.05988549	8.72584117	0.42683562
H	-3.35026731	-4.79678602	-0.44994386
H	-4.12223452	-2.52563198	-0.31098367
H	-3.02411852	-4.80788956	1.29791594
H	0.29607890	-0.95682855	4.12358927
H	2.06203058	-1.12425006	3.96709131
H	0.49125229	1.14619005	2.96774403
H	-4.29301918	0.46148340	1.75731710
H	-4.42333588	2.15544417	2.24135326
H	1.81497633	4.23441930	1.65711190
H	3.10375103	3.62475320	0.63048270
H	-2.53983596	3.45831668	-1.19751434

MP2 Electronic Energy(Ha): 1489.168783837613

B3LYP Electronic Energy(Ha): 1493.008435865478

M06-L Electronic Energy(Ha): 1492.813181517582

Zero point energy correction(kcal/mol): 378.666

Enthalpy correction(kcal/mol): 401.341

Entropy correction(cal/mol): 226.167

Imaginary Frequencies: -2.32

Deuterated zero point energy correction(kcal/mol): 374.347

Deuterated enthalpy correction(kcal/mol): 397.158

Deuterated entropy correction(cal/mol): 227.058

Deuterated imaginary Frequencies: -2.32

Equatorial Reaction H7

Reactant geometry

Zr	-0.10971686	0.24332554	-0.82989163
C	-1.31027178	-1.93167357	-0.94191791

C	-2.33752602	-1.06013932	-0.48299142
H	-2.72749143	-1.03867975	0.52356293
C	-1.11930753	-1.59235603	-2.32322565
H	-0.42209148	-2.06991982	-2.99625209
C	-1.95795556	-0.51764719	-2.66792364
H	-2.01967513	-0.04198101	-3.63547314
C	-2.70951004	-0.17427692	-1.51765274
H	-3.45383192	0.60745293	-1.45941282
B	-0.36041542	-2.89877883	-0.03730319
C	-0.83995961	-4.42943593	0.15432864
C	1.11961675	-2.70650697	-0.73304126
C	-0.10444248	-2.06485798	1.35853448
N	-0.08333311	-0.76851059	1.40143102
N	1.48753152	-1.54195343	-1.16802047
O	2.02521298	-3.68722755	-0.87646215
O	0.26263982	-2.68371827	2.49869659
C	0.44411080	-0.34755833	2.71260783
C	0.47431008	-1.66144053	3.51190120
C	2.82756874	-1.64904612	-1.77058350
C	3.22810961	-3.10544411	-1.46058382
N	-1.72554447	3.78302580	-1.72229864
H	1.43583589	0.09622646	2.58188113
H	2.77039060	-1.44961682	-2.84523651
C	-0.90185271	5.01273060	-1.86115398
H	-1.50465639	5.88533963	-1.59959919
H	-0.06890837	4.97610558	-1.15405341
C	-0.37597541	5.06121402	-3.32498201
C	-1.01786314	3.83280400	-4.00177353
H	-1.95952061	4.11880478	-4.48578998
H	-0.37644670	3.38709700	-4.76461672
C	-1.30940440	2.86230384	-2.82920515
H	-2.16692936	2.22751739	-3.06641306
C	-0.12157845	1.99611298	-2.39916709

H	0.72547955	2.64831412	-2.15577442
H	0.21484188	1.41912587	-3.27993022
C	-2.04569897	-4.88210605	-0.40204706
H	-2.65741450	-4.18736519	-0.96879594
C	-0.08548051	-5.37104082	0.87600741
H	0.85404709	-5.06881741	1.32542593
C	-0.51015166	-6.68785411	1.03412330
H	0.09862577	-7.38803843	1.59783111
C	-2.48152648	-6.19889686	-0.25012280
H	-3.42034384	-6.51250527	-0.69597372
C	-1.71381782	-7.10923346	0.47038475
H	-2.04707294	-8.13473215	0.59157888
H	1.42299121	-1.86781829	4.00627923
H	-0.33721671	-1.74133649	4.23873151
H	-0.19717440	0.40462162	3.17723453
H	4.02695165	-3.18910505	-0.72117952
H	3.48888141	-3.69296291	-2.34034323
H	3.50943810	-0.91500580	-1.33855474
H	-0.64471897	5.99341995	-3.82641484
H	0.71334484	4.98914607	-3.34023348
H	-2.69481375	4.03932064	-1.88451794
N	1.73740175	1.11347868	-0.19313247
H	2.37706443	0.43289332	0.20521889
C	2.18406685	2.45404823	0.14691432
H	1.46298024	3.17693913	-0.24856895
H	2.20838550	2.61531741	1.24037092
C	3.56743255	2.83542476	-0.41334022
H	3.54423291	2.72837120	-1.50264379
H	3.75319068	3.89630073	-0.19810799
C	4.74133217	2.00435650	0.14094510
H	4.60209112	0.94580576	-0.10225087
H	5.65518899	2.31918707	-0.37930117
C	4.95382309	2.15965815	1.62093104

H	5.09744581	3.18131241	1.97235419
C	4.98753898	1.16844950	2.50823934
H	4.85599144	0.13269332	2.20777609
H	5.16157512	1.35159387	3.56274919
N	-1.16004293	1.95687511	0.52616550
C	-2.33789204	1.79079320	1.40615843
H	-1.37147967	2.69361003	-0.17591845
H	-0.36864610	2.29150782	1.07099071
H	-3.17584421	1.49937106	0.77134134
H	-2.15338038	0.95230218	2.08210687
C	-2.72584681	3.04472078	2.20163699
H	-2.88360901	3.87611295	1.50487779
H	-3.69084391	2.85797103	2.68545232
C	-1.70848679	3.46023038	3.28021464
H	-0.73194257	3.64282850	2.81196570
H	-1.56999962	2.63857383	3.99198564
C	-2.12280976	4.70127106	4.02024276
H	-2.23463412	5.59846245	3.41266942
C	-2.36763572	4.77198925	5.32495593
H	-2.27117834	3.90354552	5.97001662
H	-2.67076576	5.69916536	5.79776007

MP2 Electronic Energy(Ha): 1740.465559930566

B3LYP Electronic Energy(Ha): 1744.959340600270

M06-L Electronic Energy(Ha): 1744.738437911015

Zero point energy correction(kcal/mol): 477.507

Enthalpy correction(kcal/mol): 505.421

Entropy correction(cal/mol): 255.998

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.727

Deuterated enthalpy correction(kcal/mol): 497.004

Deuterated entropy correction(cal/mol): 258.103

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.01607437	0.16686341	-0.49686580
C	-1.16804311	-1.95759591	-1.03703263
C	-2.25398915	-1.10527904	-0.68643945
H	-2.82533948	-1.16759990	0.22841192
C	-0.70968947	-1.48150961	-2.31094575
H	0.09538315	-1.91075180	-2.88902829
C	-1.44541792	-0.34258602	-2.68296317
H	-1.32221599	0.23106403	-3.58986352
C	-2.40303789	-0.09987158	-1.66246257
H	-3.13345203	0.69542092	-1.65983518
B	-0.42180197	-3.04850766	-0.07694266
C	-0.98148729	-4.56033245	-0.10117730
C	1.15593601	-2.87000594	-0.49910642
C	-0.39583876	-2.32358369	1.39698742
N	-0.25269763	-1.03870046	1.49890924
N	1.64459553	-1.68998033	-0.71627122
O	2.01306192	-3.89237917	-0.64798883
O	-0.40087492	-2.99047655	2.56173362
C	-0.06836853	-0.67692236	2.91361264
C	-0.33473241	-2.00953915	3.63982894
C	3.05624451	-1.82304074	-1.12196141
C	3.31304427	-3.33969472	-1.00292841
N	-1.73737701	4.26820538	-1.79825668
H	0.94782451	-0.30324378	3.07054214
H	3.19289081	-1.45073248	-2.14145539
C	-0.87803699	5.45363407	-2.01471342
H	-1.48975399	6.35818936	-1.99171267
H	-0.15772259	5.53628067	-1.19615055
C	-0.13789778	5.26004699	-3.37370468
C	-0.63749120	3.89166960	-3.88859337
H	-1.47464012	4.02488567	-4.58344740
H	0.13699058	3.33083588	-4.41715978

C	-1.15034505	3.17301666	-2.61185086
H	-1.95219626	2.47492756	-2.86528751
C	-0.05540768	2.43387953	-1.82802685
H	0.72361998	3.14319884	-1.52743330
H	0.45301693	1.75192310	-2.52668957
C	-2.06990050	-4.92019724	-0.90942992
H	-2.54136985	-4.16272106	-1.52767679
C	-0.40894557	-5.58029261	0.67843920
H	0.43478097	-5.35073329	1.32069787
C	-0.89460497	-6.88497450	0.65347859
H	-0.42773745	-7.64759964	1.26891656
C	-2.56533380	-6.22414450	-0.94298122
H	-3.40952266	-6.46560809	-1.58118754
C	-1.97833855	-7.21376452	-0.15990504
H	-2.35913535	-8.22946584	-0.18172908
H	0.45787232	-2.31603128	4.32153639
H	-1.29219002	-2.03253082	4.16345855
H	-0.76532150	0.10963191	3.20758925
H	4.01302024	-3.60242207	-0.20819285
H	3.63228023	-3.80893849	-1.93338674
H	3.71301921	-1.24048389	-0.47179054
H	-0.35588306	6.06571893	-4.07816755
H	0.94427122	5.25123443	-3.22351695
H	-2.65800243	4.47430284	-2.17320615
N	1.83383145	1.01353977	0.16477569
H	2.52075694	0.31086345	0.41404967
C	2.28759054	2.31511954	0.64342342
H	1.47520539	3.03944725	0.54061618
H	2.52773124	2.27217778	1.71720632
C	3.50987459	2.88127972	-0.10273657
H	3.27026671	2.94822468	-1.16867102
H	3.68702025	3.90574472	0.25035304
C	4.80755683	2.06668564	0.06380505

H	4.66635730	1.05164324	-0.32112570
H	5.57954169	2.52750471	-0.56586326
C	5.31160141	2.01146422	1.47894948
H	5.47632000	2.97644439	1.95802733
C	5.57066412	0.90437433	2.16993918
H	5.42908639	-0.08240406	1.73806010
H	5.94506119	0.94023568	3.18685155
N	-1.03904654	1.77421335	0.67896064
C	-2.41028185	1.93073338	1.16006463
H	-0.67493200	2.20561072	-0.52784998
H	-0.37914142	2.14726430	1.35379309
H	-3.08903432	1.66228390	0.34867168
H	-2.62254937	1.22139552	1.97780006
C	-2.75009346	3.35410739	1.62280121
H	-2.55258113	4.03510362	0.78916006
H	-3.82355577	3.40057581	1.84110875
C	-1.97670435	3.80870403	2.87366978
H	-0.89874526	3.78443386	2.66301014
H	-2.15517248	3.10848378	3.69862216
C	-2.34179936	5.20011168	3.30668313
H	-2.16655253	5.98295850	2.56977299
C	-2.86340222	5.52942041	4.48459286
H	-3.05945272	4.78224885	5.24824716
H	-3.11266553	6.55543546	4.73058873

MP2 Electronic Energy(Ha): 1740.418618868332

B3LYP Electronic Energy(Ha): 1744.914886879928

M06-L Electronic Energy(Ha): 1744.690401581373

Zero point energy correction(kcal/mol): 473.748

Enthalpy correction(kcal/mol): 501.792

Entropy correction(cal/mol): 261.535

Imaginary Frequencies: -1602.59

Deuterated zero point energy correction(kcal/mol): 466.045

Deuterated enthalpy correction(kcal/mol): 494.443

Deuterated entropy correction(cal/mol): 263.593

Deuterated imaginary Frequencies: -1162.83

Product geometry

Zr	-0.35103092	-0.56056849	-0.47051458
C	1.11143368	-2.02168530	0.90281436
C	2.05149130	-1.13193488	0.29772158
H	2.75621052	-1.40222946	-0.47645910
C	0.38486099	-1.22050847	1.83902201
H	-0.41673887	-1.57097854	2.47234587
C	0.79959782	0.12727404	1.73982423
H	0.42687180	0.95971127	2.31933639
C	1.84539032	0.17727391	0.77690696
H	2.38929364	1.06348818	0.48594357
B	0.69361591	-3.51124372	0.35831590
C	1.48737166	-4.76964585	0.98016608
C	-0.94454547	-3.55910215	0.51801353
C	0.77998199	-3.36688427	-1.28587548
N	0.31466728	-2.31196844	-1.88405563
N	-1.67797824	-2.52982946	0.23626232
O	-1.61355092	-4.67371953	0.86254694
O	1.28418280	-4.30502676	-2.09822506
C	0.50190271	-2.44433004	-3.33876214
C	1.12813517	-3.84811351	-3.47565567
C	-3.09790816	-2.90796743	0.34874479
C	-3.03504150	-4.35912402	0.86834464
N	1.47966966	6.71200407	0.63803716
H	-0.45564918	-2.35941632	-3.85846747
H	-3.62321910	-2.24422421	1.04102982
C	1.21449694	8.14114358	0.91388073
H	1.57009933	8.74864396	0.07937009
H	0.13566250	8.30180930	0.98693441
C	1.91038514	8.49873194	2.26324316

C	2.52039753	7.16344401	2.75164465
H	3.58424111	7.11813065	2.50000704
H	2.43615921	7.03074273	3.83312315
C	1.75818305	6.08262305	1.94750670
H	2.37950985	5.19803442	1.78068083
C	0.45733039	5.64365209	2.62565685
H	-0.19958263	6.49570970	2.82385255
H	0.66518979	5.15436718	3.58146018
C	2.46957587	-4.59254562	1.96574539
H	2.69605007	-3.58827433	2.30976422
C	1.23487555	-6.09054935	0.57096574
H	0.48283581	-6.27968553	-0.18788343
C	1.92265951	-7.17281647	1.11332893
H	1.70156465	-8.17968758	0.77312926
C	3.16512618	-5.66906591	2.51728196
H	3.91854063	-5.49295405	3.27861046
C	2.89402253	-6.96626989	2.09212499
H	3.43184254	-7.80738746	2.51693105
H	0.48695760	-4.56554094	-3.98926542
H	2.11508575	-3.85023371	-3.93801513
H	1.15390720	-1.64897667	-3.70700266
H	-3.54036272	-5.08222835	0.22816246
H	-3.39529071	-4.47039033	1.89227127
H	-3.58878387	-2.83072565	-0.62604173
H	2.67740705	9.26546514	2.13612229
H	1.18531180	8.89007260	2.98056856
H	2.31643774	6.64242830	0.06781874
N	-2.27900530	0.27683663	-0.43790965
H	-3.02475263	-0.32213200	-0.10000030
C	-2.80911804	1.62030473	-0.66248362
H	-2.07993481	2.18879969	-1.24623443
H	-3.72594363	1.56814690	-1.26637497
C	-3.10554034	2.41860951	0.61997739

H	-2.17556613	2.52906479	1.18776346
H	-3.42279793	3.42957649	0.33293212
C	-4.17435716	1.79671877	1.53891541
H	-3.84932674	0.80553202	1.87168500
H	-4.24720042	2.41616624	2.44214129
C	-5.53585211	1.70329448	0.90845521
H	-5.94035990	2.63719824	0.51841671
C	-6.26638935	0.59679324	0.79866775
H	-5.91145653	-0.35777561	1.17713398
H	-7.24894677	0.60345462	0.34024888
N	0.25506892	0.84531385	-1.89230251
C	1.47938349	1.45921755	-2.39561479
H	-0.08624621	4.94532055	1.98603872
H	-0.52914361	1.11320037	-2.48457501
H	2.33322105	0.98109959	-1.90857996
H	1.59418606	1.26084043	-3.47318116
C	1.58236960	2.97817860	-2.17118314
H	1.50030059	3.18412808	-1.09799171
H	2.58014466	3.30794298	-2.48614823
C	0.52697695	3.80000097	-2.93059578
H	-0.47015863	3.48650035	-2.59621956
H	0.58845964	3.57982421	-4.00336572
C	0.66834006	5.27947879	-2.70597454
H	0.60189483	5.61438081	-1.67097199
C	0.88196358	6.17838766	-3.66360725
H	0.96244972	5.89282789	-4.70892137
H	0.97777239	7.23516255	-3.43911977

MP2 Electronic Energy(Ha): 1740.467709269012

B3LYP Electronic Energy(Ha): 1744.989843094904

M06-L Electronic Energy(Ha): 1744.747517461468

Zero point energy correction(kcal/mol): 475.039

Enthalpy correction(kcal/mol): 499.478

Entropy correction(cal/mol): 235.503

Imaginary Frequencies: -36.69 -35.20 -34.33 -31.13 -28.18 -19.50 -12.97

Deuterated zero point energy correction(kcal/mol): 466.667

Deuterated enthalpy correction(kcal/mol): 491.499

Deuterated entropy correction(cal/mol): 237.920

Deuterated imaginary Frequencies: -36.61 -34.98 -33.54 -31.11 -28.05 -19.46 -12.96

Equatorial Reaction C1-S

Reactant geometry

Zr	-0.34635192	-0.05478315	0.26000669
C	-0.23023373	2.16911107	1.32605848
C	-1.60840523	1.82663480	1.47168374
H	-2.42552120	2.28417579	0.93157825
C	0.47195927	1.28760041	2.20862857
H	1.54358965	1.26082472	2.34082104
C	-0.43677398	0.38540951	2.80709094
H	-0.19450651	-0.39781461	3.51079203
C	-1.73679310	0.72280239	2.34262018
H	-2.65650614	0.23092493	2.62552696
B	0.41842430	3.07598314	0.12643535
C	0.61719014	4.64538411	0.42476202
C	1.75569180	2.24952287	-0.35977472
C	-0.53504329	2.73666787	-1.18536357
N	-0.85175374	1.51487445	-1.49278406
N	1.77445236	0.95307856	-0.41026489
O	2.83079864	2.86249876	-0.88779751
O	-1.03714704	3.68050487	-1.99773523
C	-1.76238708	1.53167183	-2.65083880
C	-1.73605205	3.00881337	-3.08610760
C	2.97287571	0.52926229	-1.16013073
C	3.78199399	1.83101875	-1.27690976
N	-2.12179782	-1.07739616	-0.19672688
H	-1.41175227	0.85693898	-3.43498920

C	-2.33962343	-2.08595641	-1.22906686
H	-1.49572729	-2.05952214	-1.92854579
H	-2.31924432	-3.10104959	-0.79683499
C	-3.63889800	-1.94382982	-2.04208605
C	-4.94084794	-2.26957333	-1.28079328
H	-5.74849470	-2.33893266	-2.02172339
H	-4.86041301	-3.26166234	-0.82126862
C	-5.36044584	-1.26501400	-0.24247270
H	-5.44807853	-0.23604561	-0.58952906
C	-5.66061533	-1.53992631	1.02539470
H	-5.59614703	-2.55039759	1.41856479
C	0.32549764	5.17329293	1.63769414
H	0.01954399	4.51811823	2.44857499
C	1.22259408	5.52929010	-0.57988866
H	1.55294875	5.08410856	-1.51178268
C	1.50935894	6.82449241	-0.34776379
H	2.10322766	7.38922994	-1.06097955
C	0.41702740	6.60984757	1.95598869
H	0.61238580	6.85854108	2.99486681
C	1.06693489	7.51945116	0.87179040
H	1.68413648	8.34548173	1.21174701
H	2.67351556	0.13021537	-2.13508244
H	3.51770527	-0.25367450	-0.63406426
H	4.13240435	2.05873588	-2.28283485
H	4.62242666	1.87639649	-0.58059585
H	-2.75636851	1.19889278	-2.34074154
H	-1.16313094	3.17971629	-3.99985127
H	-2.71958087	3.46660191	-3.18546294
H	-3.70012086	-0.93079730	-2.45489652
H	-3.57508699	-2.62634032	-2.89798612
H	-2.95295463	-0.97069458	0.37237478
H	-5.99040105	-0.76890176	1.71255660
N	0.72865428	-1.85147885	0.31974312

H	0.11054110	-2.66405918	0.32063092
C	2.05292566	-2.29553050	0.72900171
H	2.68647801	-1.42324608	0.92077639
H	2.00053259	-2.83933672	1.68678909
C	2.73844140	-3.21038849	-0.29868271
H	2.82284551	-2.67510600	-1.25131874
H	2.09175824	-4.07390373	-0.48828783
C	4.12477983	-3.70119315	0.15571440
H	4.03667320	-4.23440456	1.10880695
H	4.76334052	-2.82709156	0.34672399
C	4.79477548	-4.58779198	-0.85547269
H	4.97539547	-4.13904067	-1.83196371
C	5.15823560	-5.85126446	-0.65379836
H	4.99991649	-6.34315672	0.30152678
H	5.63092845	-6.43984323	-1.43202844
N	-0.86472084	-4.59242006	1.40411160
H	-1.86593252	-4.48289695	1.27152426
H	-0.62980526	-4.08853402	2.25349746
C	-0.51281187	-6.01221079	1.52864540
H	0.54569846	-6.07159960	1.80135160
H	-1.07365426	-6.53527537	2.31971314
C	-0.72389508	-6.73910108	0.19700085
H	-0.10758799	-6.26240978	-0.57017797
H	-1.77164229	-6.62889294	-0.10954187
C	-0.36616358	-8.22375269	0.31384570
H	-1.07643256	-8.79419626	0.92322412
H	-0.41282374	-8.75740274	-0.70787363
C	0.95414998	-8.78523651	0.22848724
H	1.58058572	-8.01893973	-0.28013324
C	-0.40295626	7.62213032	1.19395265
H	-0.72857749	8.50075584	1.73803206
H	-1.10210033	7.24648047	0.45650276

MP2 Electronic Energy(Ha): 1740.253059073936

B3LYP Electronic Energy(Ha): 1744.782014621743

M06-L Electronic Energy(Ha): 1744.548852853181

Zero point energy correction(kcal/mol): 471.023

Enthalpy correction(kcal/mol): 500.775

Entropy correction(cal/mol): 274.213

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 462.544

Deuterated enthalpy correction(kcal/mol): 492.690

Deuterated entropy correction(cal/mol): 276.826

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-1.27565765	0.54841947	-0.35936977
C	-1.11136249	3.04105313	-0.28426584
C	-1.58545749	2.80533186	-1.61763286
H	-1.00022580	2.90464570	-2.52043065
C	-2.23520402	2.81282923	0.55939088
H	-2.23110563	2.88478781	1.63714747
C	-3.33802449	2.40034113	-0.21814484
H	-4.32141923	2.14654937	0.15319756
C	-2.93528467	2.41384843	-1.57537036
H	-3.55356991	2.17427046	-2.42996794
B	0.44077326	3.27333896	0.17511139
C	0.92769938	4.79892424	0.37842789
C	0.61396980	2.30875863	1.49099918
C	1.26777921	2.42481116	-0.96198712
N	0.82990441	1.27349001	-1.36427583
N	-0.00814143	1.17690572	1.57359034
O	1.44586478	2.58507285	2.51285558
O	2.37842592	2.86723929	-1.57702775
C	1.65147627	0.82360189	-2.50273010
C	2.82137862	1.82335583	-2.49141584
C	0.39814428	0.48411044	2.80512633

C	1.35629634	1.49319236	3.47255258
N	-2.77700117	-0.63283310	-1.53089781
H	1.97636295	-0.20841814	-2.37895288
C	-2.77352763	-1.97738138	-2.11158232
H	-2.93305583	-1.91998114	-3.19373690
H	-1.79128274	-2.42351435	-1.94690927
C	-3.86435769	-2.80475686	-1.41847170
C	-3.71385599	-2.48084871	0.06844714
H	-4.58612474	-2.81314842	0.64302458
H	-2.84069417	-2.98991642	0.48584337
C	-3.57488603	-0.98643892	0.27624519
H	-4.47853997	-0.42606940	0.05220057
C	-2.75117096	-0.44640872	1.31155990
H	-2.15943224	-1.16089806	1.87418358
C	0.04495088	5.87521572	0.20751661
H	-0.98499047	5.67256613	-0.06885215
C	2.24957527	5.11706678	0.73533369
H	2.96951585	4.31826337	0.88020332
C	2.66749550	6.43347448	0.91169055
H	3.69674429	6.64199752	1.18700593
C	0.45161558	7.19865463	0.38186875
H	-0.26018084	8.00610016	0.24081649
C	1.76735255	7.48373595	0.73525053
H	2.08957204	8.51082326	0.87172661
H	0.88498844	-0.46271725	2.55942257
H	-0.47606514	0.26385844	3.42302998
H	2.36342706	1.10753613	3.63415960
H	0.97432976	1.90483244	4.40807730
H	1.06307911	0.87933347	-3.42539435
H	3.74318520	1.39869972	-2.08694478
H	3.02892719	2.28681474	-3.45498602
H	-4.85378522	-2.49703602	-1.77755075
H	-3.76170439	-3.87498562	-1.61938538

H	-3.52586915	-0.09246737	-1.94674689
H	-3.16290920	0.37018944	1.89301200
N	-0.19415986	-1.27702207	-0.28553203
H	-0.75882336	-2.07883986	-0.01151405
C	1.20047274	-1.64197078	-0.10406865
H	1.81877697	-0.74461369	-0.19883672
H	1.38817853	-2.02681863	0.91411705
C	1.69896349	-2.70592473	-1.09972873
H	1.45813245	-2.37387299	-2.11604632
H	1.14087329	-3.63630145	-0.94415395
C	3.20756061	-2.98751224	-0.98521858
H	3.44851084	-3.35483001	0.01829672
H	3.74781301	-2.03730121	-1.10506908
C	3.70927757	-3.96118865	-2.01370439
H	3.50900451	-3.69497405	-3.05141205
C	4.35969894	-5.09313951	-1.75794752
H	4.58505562	-5.39915120	-0.74072376
H	4.69659106	-5.74950253	-2.55254194
N	-0.98936038	-3.90301312	2.13000600
H	-1.89520477	-4.11452526	2.54085058
H	-0.56018975	-3.19805561	2.72197046
C	-0.15553028	-5.11540131	2.07869389
H	0.86080404	-4.81144304	1.81502244
H	-0.08745412	-5.63670786	3.04728462
C	-0.68585403	-6.08514201	1.02234512
H	-0.69545278	-5.57397442	0.05363839
H	-1.72892322	-6.33371629	1.25389614
C	0.12492994	-7.39149736	0.92227108
H	0.11206802	-7.91348538	1.88575889
H	-0.37821721	-8.04945663	0.20259389
C	1.54769498	-7.18418921	0.47874459
H	1.67974631	-6.68176687	-0.47901931
C	2.62696597	-7.56295564	1.15783629

H 2.54916879 -8.06533921 2.11774690

H 3.62709479 -7.39340151 0.77513656

MP2 Electronic Energy(Ha): 1740.435469712616

B3LYP Electronic Energy(Ha): 1744.937857899865

M06-L Electronic Energy(Ha): 1744.714352325830

Zero point energy correction(kcal/mol): 475.251

Enthalpy correction(kcal/mol): 503.638

Entropy correction(cal/mol): 263.036

Imaginary Frequencies: -356.93

Deuterated zero point energy correction(kcal/mol): 466.717

Deuterated enthalpy correction(kcal/mol): 495.490

Deuterated entropy correction(cal/mol): 265.569

Deuterated imaginary Frequencies: -355.74

Product geometry

Zr -1.14354220 0.65021814 -0.43408103

C -1.04737307 3.15391889 -0.43964530

C -1.33063277 2.80871933 -1.80197605

H -0.64027905 2.88728555 -2.62923519

C -2.26310800 2.92794673 0.26702114

H -2.39927093 3.06079364 1.33067586

C -3.23356424 2.40252761 -0.60740769

H -4.24277422 2.11989505 -0.34166662

C -2.65388190 2.33519773 -1.90247195

H -3.14793613 2.02181796 -2.81301485

B 0.42261893 3.45991292 0.21092730

C 0.80120075 5.00524365 0.48197846

C 0.48704022 2.48611708 1.53030902

C 1.42646835 2.66057996 -0.81155619

N 1.14087744 1.46278492 -1.20755733

N -0.05844712 1.30956275 1.52344611

O 1.16149008 2.79448514 2.65008564

O 2.52327027 3.21531827 -1.36409171

C	2.07857659	1.09501287	-2.28572012
C	3.14297457	2.20269973	-2.20569817
C	0.24035875	0.61830528	2.78705837
C	1.04574655	1.67296823	3.57365216
N	-2.97378248	-0.72062118	-1.29976855
H	2.49611034	0.09977088	-2.13683727
C	-2.96455723	-2.01407801	-2.04138259
H	-3.23334718	-1.84542854	-3.08628026
H	-1.95685374	-2.43262950	-2.02734795
C	-3.94704100	-2.91827421	-1.28496524
C	-3.71978790	-2.49740273	0.17220690
H	-4.54039585	-2.77541358	0.83723219
H	-2.80788950	-2.96871200	0.55072009
C	-3.54346296	-0.96811725	0.12252511
H	-4.52861576	-0.49191460	0.14061905
C	-2.60377940	-0.31916081	1.13075535
H	-2.07998271	-1.06785890	1.73057979
C	-0.10209535	6.03999526	0.19840501
H	-1.07566503	5.79183935	-0.21246203
C	2.04792951	5.38357538	1.00977442
H	2.78101779	4.61890524	1.24535673
C	2.37490517	6.71678174	1.24266686
H	3.34790020	6.97190724	1.65106154
C	0.21368794	7.37990836	0.42720833
H	-0.51144734	8.15366247	0.19472312
C	1.45600572	7.72448982	0.95163739
H	1.70735259	8.76461074	1.13147497
H	0.81485100	-0.29116276	2.59208721
H	-0.68504018	0.33121367	3.28998180
H	2.05466652	1.35354567	3.83613798
H	0.53738459	2.03359693	4.46890623
H	1.55131677	1.09158740	-3.24687629
H	4.06121390	1.87578670	-1.71108692

H	3.39129978	2.66373044	-3.16084812
H	-4.97634564	-2.70789646	-1.59545899
H	-3.75356415	-3.97859662	-1.46139783
H	-3.60255996	-0.09063672	-1.78136146
H	-3.12126297	0.36728762	1.80237467
N	-0.10050855	-1.18195376	-0.58185687
H	-0.71123751	-1.99308378	-0.51577023
C	1.25445168	-1.63569439	-0.30710409
H	1.91545544	-0.76677776	-0.25796283
H	1.31941448	-2.11251104	0.68739303
C	1.79021939	-2.64023037	-1.34009968
H	1.76003092	-2.17725583	-2.33314868
H	1.11544213	-3.50280349	-1.38286278
C	3.21553537	-3.13085281	-1.02789728
H	3.23414639	-3.61677969	-0.04610726
H	3.88111918	-2.25907953	-0.95657656
C	3.75365204	-4.07503894	-2.06552190
H	3.84618863	-3.66839446	-3.07226084
C	4.09998577	-5.34106215	-1.85078279
H	4.02112924	-5.79208543	-0.86596531
H	4.47438899	-5.97194580	-2.64935811
N	-0.76859967	-4.24360594	1.65575452
H	-1.54996258	-4.25043476	2.30546646
H	-0.21571318	-3.42247600	1.88050968
C	0.03136209	-5.46736379	1.81184792
H	0.92665183	-5.36424643	1.19276202
H	0.37977364	-5.63056259	2.84492639
C	-0.76442186	-6.69042221	1.35687734
H	-1.06303393	-6.54573604	0.31310942
H	-1.69219606	-6.75057422	1.93900274
C	-0.00047913	-8.01924657	1.50964014
H	0.28216762	-8.17076159	2.55745113
H	-0.68567455	-8.83636103	1.25090209

C 1.22108278 -8.12037376 0.63826312

H 1.05296582 -7.97910609 -0.42905277

C 2.45589637 -8.36922157 1.06569598

H 2.67411516 -8.51615167 2.11950368

H 3.29130989 -8.44443331 0.37874568

MP2 Electronic Energy(Ha): 1740.449641490854

B3LYP Electronic Energy(Ha): 1744.953929370596

M06-L Electronic Energy(Ha): 1744.724486964694

Zero point energy correction(kcal/mol): 475.191

Enthalpy correction(kcal/mol): 498.897

Entropy correction(cal/mol): 223.125

Imaginary Frequencies: -50.70 -48.34 -45.07 -44.16 -42.60 -31.89 -27.53 -18.91

Deuterated zero point energy correction(kcal/mol): 466.559

Deuterated enthalpy correction(kcal/mol): 490.629

Deuterated entropy correction(cal/mol): 225.429

Deuterated imaginary Frequencies: -50.62 -48.17 -44.81 -44.10 -42.51 -31.56 -26.82 -18.64

Equatorial Reaction C2-S

Reactant geometry

Zr -1.06761246 -1.14034076 0.12776513

C -1.86998529 1.23345336 0.13522607

C -2.62542158 0.66604229 -0.92184713

H -2.48226886 0.86747808 -1.97386684

C -2.40323725 0.64731595 1.33435873

H -2.06426796 0.85477279 2.33947242

C -3.44144290 -0.25228639 1.00841598

H -4.00358268 -0.85691919 1.70482191

C -3.56406210 -0.26468706 -0.39474370

H -4.27882605 -0.84251409 -0.96536785

B -0.45960195 2.05370156 0.00043604

C -0.54839124 3.66644928 0.08449299

C 0.49162723 1.37915026 1.16372555

C	0.20685910	1.48448836	-1.39510986
N	0.18995314	0.23291633	-1.72122400
N	0.47037160	0.10273041	1.40734082
O	1.30596511	2.09278159	1.95816151
O	0.75913994	2.31858639	-2.30677102
C	0.71157236	0.10373775	-3.09345427
C	1.27203682	1.50572338	-3.39405035
C	1.29195059	-0.17607713	2.59838373
C	2.00787440	1.16534348	2.83479805
N	1.11413101	-2.39701665	-0.19862279
N	-1.42629785	-2.67183713	1.20055255
C	-2.11782796	-3.81092550	1.69228780
H	-3.21092526	-3.64016555	1.72095401
H	1.47510593	-0.67528557	-3.16443058
H	0.64346536	-0.46658835	3.43060846
C	2.47032077	-1.87167040	-0.45296426
H	2.49358689	-1.48377587	-1.47316675
H	2.62214295	-1.01306385	0.20097547
C	3.58938159	-2.90107358	-0.26337167
C	-1.83103300	-5.06177865	0.82091153
C	-1.67816788	-4.72189206	-0.68812999
H	-2.20802691	-5.48075335	-1.27896019
H	-1.83055345	-4.04136365	2.72928727
C	-2.22210712	-3.38772073	-1.11930782
H	-3.22460081	-3.15906972	-0.76950478
H	-0.63126534	-4.79605681	-0.99796699
C	-1.68595587	-2.58457511	-2.07680765
H	-2.26160631	-1.78587024	-2.52541653
H	0.91961138	-3.17026224	-0.83022743
H	-0.74655004	-2.83847502	-2.55823492
C	0.59007745	4.48617127	-0.00331794
H	1.56606904	4.03045674	-0.13576075
C	-1.77953862	4.31679609	0.25258884

H	-2.68331975	3.72009012	0.32376992
C	0.50672817	5.87388876	0.07255652
H	1.40789178	6.47519669	0.00048729
C	-1.87669475	5.70684961	0.32966723
H	-2.84780077	6.17442289	0.45981980
C	-0.73161605	6.49285555	0.24019572
H	-0.80081777	7.57414478	0.29974688
C	5.00031191	-2.31304847	-0.47105775
H	5.05705627	-1.81995286	-1.44784303
H	5.71592128	-3.14355479	-0.49906253
C	5.41762661	-1.35277531	0.60900624
H	5.45747442	-1.76780570	1.61601483
C	5.74311377	-0.07567784	0.42766509
H	5.72497963	0.38282004	-0.55652465
H	6.05153199	0.55609144	1.25294232
H	0.92625506	1.93747670	-4.33286154
H	-0.10180161	-0.17379731	-3.77372720
H	2.36384092	1.54755629	-3.35884884
H	3.05620167	1.15029854	2.52885469
H	1.93037091	1.54397410	3.85307013
H	1.99238469	-0.99582851	2.42280478
H	-0.90403288	-5.53446898	1.15886971
H	-2.62667415	-5.80018441	0.96771004
H	3.52104688	-3.33364096	0.74291903
H	3.44159096	-3.73014909	-0.96554838
H	1.04096025	-2.80306799	0.73324960

MP2 Electronic Energy(Ha): 1489.145479861277

B3LYP Electronic Energy(Ha): 1492.972085239445

M06-L Electronic Energy(Ha): 1492.794842210303

Zero point energy correction(kcal/mol): 377.583

Enthalpy correction(kcal/mol): 400.899

Entropy correction(cal/mol): 223.461

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.734

Deuterated enthalpy correction(kcal/mol): 396.351

Deuterated entropy correction(cal/mol): 226.742

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-1.21493760	-1.24392669	0.15535697
C	-2.12870422	1.08179292	0.28393149
C	-2.95162632	0.49421473	-0.71286932
H	-2.91813108	0.72836663	-1.76758289
C	-2.49466099	0.42371429	1.50777419
H	-2.07355423	0.62741662	2.48211777
C	-3.47610455	-0.56203586	1.24997620
H	-3.93275662	-1.21707723	1.97719010
C	-3.74778804	-0.53151033	-0.13694669
H	-4.46791870	-1.15081406	-0.65462582
B	-0.74933939	1.93822146	0.02065835
C	-0.85912956	3.54845852	0.04109599
C	0.29996713	1.30893478	1.12693312
C	-0.12911601	1.32059112	-1.38072839
N	-0.15316027	0.05678977	-1.65918399
N	0.39507977	0.02412945	1.29631776
O	1.05940388	2.04786528	1.94780024
O	0.46934518	2.10318719	-2.30271979
C	0.44698595	-0.15403806	-2.98594509
C	1.00445943	1.23690124	-3.34164441
C	1.26289901	-0.24963969	2.45433742
C	1.85417128	1.13735603	2.76590087
N	1.91181400	-2.41195595	-0.65942229
N	-1.08119707	-2.83755271	1.17465884
C	-1.36781700	-4.10941586	1.74597797
H	-2.41925757	-4.16244807	2.07691818
H	1.21612087	-0.92628284	-2.93737870

H	0.66364742	-0.65441175	3.27528600
C	3.07712391	-1.52242279	-0.70493772
H	3.15260170	-1.11405685	-1.71989065
H	2.86741169	-0.66993483	-0.05548354
C	4.42724384	-2.15438626	-0.33675959
C	-1.10314311	-5.27081875	0.74028853
C	-1.13599107	-4.80440456	-0.73308484
H	-1.46501157	-5.64428786	-1.36011351
H	-0.76634369	-4.28318727	2.65054006
C	-2.04908803	-3.64770924	-1.02979398
H	-3.03591480	-3.68950739	-0.57404584
H	-0.13304905	-4.54314626	-1.07771407
C	-1.82111097	-2.70885599	-1.98754728
H	-2.61391935	-2.06543988	-2.34645430
H	2.09241492	-3.26979340	-1.17322646
H	-0.89355436	-2.71563377	-2.54988867
C	0.27151499	4.37297277	-0.09264897
H	1.25083825	3.92011075	-0.20884426
C	-2.09512907	4.19418956	0.18774775
H	-2.99271460	3.59347883	0.29614455
C	0.17607783	5.76169140	-0.08134910
H	1.07143601	6.36672608	-0.18632083
C	-2.20438376	5.58547809	0.19897009
H	-3.17855029	6.05040879	0.31388684
C	-1.06708193	6.37640226	0.06434147
H	-1.14573021	7.45856992	0.07325167
C	5.60366854	-1.15631030	-0.39047400
H	5.59478015	-0.62561353	-1.34943514
H	6.54120395	-1.72453389	-0.35866462
C	5.60906153	-0.16318919	0.73914939
H	5.69248881	-0.59181570	1.73784560
C	5.53809964	1.15968117	0.61377084
H	5.45905434	1.63768417	-0.35801698

H	5.56875752	1.81598090	1.47636755
H	0.67050437	1.62117167	-4.30510012
H	-0.31982882	-0.48580180	-3.69416113
H	2.09438074	1.29136024	-3.29021417
H	2.89468708	1.23889267	2.45273448
H	1.75086440	1.44853401	3.80460555
H	2.03111830	-0.98623608	2.21074557
H	-0.12445597	-5.72114595	0.93045834
H	-1.84129458	-6.06311449	0.90364031
H	4.36577394	-2.59824372	0.66468399
H	4.63099859	-2.98095803	-1.02812857
H	1.67696503	-2.68340177	0.29127148

MP2 Electronic Energy(Ha): 1489.132587663202

B3LYP Electronic Energy(Ha): 1492.965225311903

M06-L Electronic Energy(Ha): 1492.783198014111

Zero point energy correction(kcal/mol): 377.106

Enthalpy correction(kcal/mol): 400.151

Entropy correction(cal/mol): 221.270

Imaginary Frequencies: -40.74

Deuterated zero point energy correction(kcal/mol): 372.422

Deuterated enthalpy correction(kcal/mol): 395.759

Deuterated entropy correction(cal/mol): 223.945

Deuterated imaginary Frequencies: -39.44

Product geometry

Zr	-1.42050406	-0.44471740	0.31335525
C	-1.40356674	2.03135159	0.63725135
C	-2.57012493	1.84318402	-0.15060614
H	-2.67428085	2.13284054	-1.18728757
C	-1.71786899	1.45900574	1.91655087
H	-1.05970505	1.43413895	2.77316857
C	-3.01486459	0.89215472	1.88514982
H	-3.52006652	0.40007657	2.70347658

C	-3.54176463	1.11982091	0.59102405
H	-4.52929537	0.83962707	0.25068336
B	0.10347089	2.35049786	0.06323204
C	0.57057020	3.89503615	0.05379657
C	1.07189595	1.32731468	0.92401813
C	0.19929048	1.58857009	-1.40857986
N	-0.31249851	0.41615334	-1.63483591
N	0.71193172	0.09426721	1.10680029
O	2.25011719	1.66404315	1.46539260
O	0.91855224	2.10035855	-2.42136195
C	0.03346991	-0.01066066	-3.00524186
C	0.99299621	1.09659412	-3.47654136
C	1.71091997	-0.59297212	1.94084005
C	2.82328951	0.46652838	2.07512533
N	0.67729673	-3.23411350	-1.54775798
N	-1.49167514	-2.19143757	1.02822432
C	-1.86022732	-3.50669443	1.44181607
H	-1.88594212	-3.60296157	2.53874286
H	0.48414575	-1.00477392	-2.98099169
H	1.26677358	-0.86995552	2.90091339
C	2.08414060	-3.49864130	-1.22789319
H	2.63255364	-3.61581028	-2.17011108
H	2.49132581	-2.60240981	-0.75106761
C	2.34695771	-4.72473041	-0.34093660
C	-3.24344561	-3.90377564	0.88475335
C	-3.38454767	-3.56725352	-0.60918669
H	-4.29545395	-4.05262539	-0.98694228
H	-1.12467830	-4.25159644	1.09038402
C	-3.54131918	-2.10391066	-0.90217574
H	-4.32735782	-1.61053555	-0.33299554
H	-2.54872427	-3.98271034	-1.18102513
C	-2.92510549	-1.40011777	-1.87255503
H	-3.24305697	-0.39671066	-2.12855079

H	0.25252462	-4.05755355	-1.96495499
H	-2.16943187	-1.86057977	-2.50007485
C	1.86105913	4.28803195	-0.34162576
H	2.57578476	3.53434264	-0.65440399
C	-0.30547445	4.91718664	0.44802577
H	-1.31043332	4.65612024	0.76414508
C	2.25487732	5.62348171	-0.34459785
H	3.26025399	5.89008254	-0.65544818
C	0.07709872	6.25900303	0.44828356
H	-0.62878524	7.02231959	0.76038061
C	1.36162773	6.61838789	0.05104589
H	1.66537556	7.66002294	0.05010199
C	3.83756520	-4.94562347	-0.01007508
H	4.42454561	-4.96644007	-0.93528329
H	3.94537655	-5.93560042	0.44998198
C	4.40706454	-3.91855855	0.92925906
H	3.92779102	-3.86141805	1.90656312
C	5.42924794	-3.10771738	0.66816605
H	5.94300084	-3.12976304	-0.28835550
H	5.79910352	-2.40195690	1.40368504
H	0.70360988	1.57397704	-4.41217909
H	-0.87056505	-0.05851184	-3.62064000
H	2.03249324	0.76917649	-3.54371142
H	3.72738046	0.21531470	1.51798002
H	3.08690572	0.71310066	3.10304226
H	2.05927390	-1.50721580	1.45791701
H	-3.41366278	-4.97528383	1.03894551
H	-4.02225622	-3.37309323	1.44453287
H	1.77440576	-4.62665134	0.58957171
H	1.95992438	-5.61668704	-0.84822135
H	0.14664658	-3.02336322	-0.70214672

MP2 Electronic Energy(Ha): 1489.134227611127

B3LYP Electronic Energy(Ha): 1492.974552235453

M06-L Electronic Energy(Ha): 1492.785767907502

Zero point energy correction(kcal/mol): 376.937

Enthalpy correction(kcal/mol): 400.819

Entropy correction(cal/mol): 237.169

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 372.282

Deuterated enthalpy correction(kcal/mol): 396.461

Deuterated entropy correction(cal/mol): 243.207

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction C3-S

Reactant geometry

Zr	0.35059326	0.04444944	-0.20450074
C	1.06921908	-2.28854359	-0.62765563
C	1.15478654	-1.66982362	-1.91558419
H	0.48395147	-1.85560289	-2.74286360
C	2.14346752	-1.73140716	0.12882351
H	2.36816622	-1.96083953	1.16077994
C	2.82443298	-0.76799903	-0.65088379
H	3.66819726	-0.16680213	-0.34929368
C	2.21176206	-0.73713332	-1.92515401
H	2.50274927	-0.10120490	-2.74816473
B	-0.17168310	-3.19815931	-0.06699339
C	-0.01915263	-4.79912801	-0.20493505
C	-0.37652214	-2.65247372	1.46698657
C	-1.47615268	-2.56260567	-0.83652667
N	-1.63866675	-1.28036456	-0.93464632
N	-0.38293299	-1.38587831	1.73531995
O	-0.48784376	-3.47465747	2.52815238
O	-2.40622350	-3.31353944	-1.45422720
C	-2.80409429	-1.01309011	-1.79787675
C	-3.40344809	-2.41548879	-2.01754584

C	-0.44742014	-1.21195243	3.19808126
C	-0.64262387	-2.65082918	3.71670801
N	-0.06925231	1.35671297	-1.82794992
N	1.29701112	1.30136071	1.20164185
C	2.51992047	1.41003115	1.98680249
H	3.28259548	0.76004063	1.55282143
H	-3.51239394	-0.33310377	-1.31566051
H	0.47791933	-0.75201875	3.55664745
C	-0.32330697	2.78606979	-1.93530194
H	-0.49696260	3.19665191	-0.93479601
H	0.55980652	3.32147955	-2.31581562
C	-1.52434812	3.14249558	-2.82817259
C	3.07066781	2.84430127	2.08615900
C	3.56443697	3.44641470	0.75759212
H	3.71520354	4.52416761	0.90527290
H	2.36464377	1.04755578	3.01756927
H	0.63768385	1.98858807	1.55970307
C	4.85764838	2.85248278	0.27196389
H	5.67999907	2.86443849	0.98788256
H	2.79050939	3.33348506	-0.00640755
C	5.07218274	2.34435532	-0.93882259
H	6.04021450	1.95053658	-1.22841893
H	0.16034069	0.99655273	-2.74848109
H	4.28530110	2.31153699	-1.68613051
C	-1.01904777	-5.68091090	0.23993709
H	-1.92179863	-5.27992954	0.69056977
C	1.12210075	-5.37952938	-0.77704952
H	1.91910121	-4.73459368	-1.13343023
C	-0.88963287	-7.06206957	0.12194460
H	-1.68265215	-7.71285830	0.47725221
C	1.26419995	-6.76221368	-0.90133903
H	2.16246989	-7.17521104	-1.34965905
C	0.25696791	-7.61081279	-0.45146812

H	0.36208227	-8.68668750	-0.54525432
C	-1.78476137	4.65635461	-2.96419855
H	-1.92125274	5.10419744	-1.97299620
H	-2.73286901	4.79362765	-3.50040447
C	-0.70623251	5.39695612	-3.70568342
H	-0.48335902	5.02404616	-4.70534026
C	-0.03267336	6.44925722	-3.24966643
H	-0.21791805	6.85699430	-2.26021867
H	0.72559083	6.94283158	-3.84702481
H	2.28577822	3.49042242	2.50034981
H	3.88914404	2.85705912	2.81758555
H	-1.36529870	2.71077236	-3.82487882
H	-2.42377476	2.65620525	-2.43109326
H	-4.33836442	-2.57594298	-1.47618394
H	-3.54361559	-2.68437389	-3.06415301
H	-2.47321051	-0.53615662	-2.72467640
H	-1.64047153	-2.83367533	4.12102710
H	0.10334865	-2.96906525	4.44477151
H	-1.27439690	-0.55714398	3.48426682
N	-1.72801122	1.13805780	0.71578676
C	-1.97734219	1.97244324	1.91724346
H	-2.16739812	0.22789023	0.83396284
H	-2.16225482	1.55895083	-0.10215165
H	-1.27956554	1.65531116	2.69638478
H	-2.99019388	1.79576144	2.30071182
C	-1.80568206	3.46528953	1.64393720
H	-2.48999180	3.77351391	0.84487385
H	-0.79334634	3.66287325	1.27740683
C	-2.07779835	4.32179595	2.89345343
H	-1.40704827	3.99273585	3.69834452
H	-3.10059387	4.15055543	3.24606371
C	-1.86858336	5.78979354	2.64586951
H	-0.86129026	6.08183824	2.35222237

C	-2.80731197	6.72519414	2.74987552
H	-3.82471823	6.48082101	3.04107649
H	-2.59381892	7.76959908	2.55339820

MP2 Electronic Energy(Ha): 1740.469641904500

B3LYP Electronic Energy(Ha): 1744.980375895094

M06-L Electronic Energy(Ha): 1744.753703836733

Zero point energy correction(kcal/mol): 475.061

Enthalpy correction(kcal/mol): 504.314

Entropy correction(cal/mol): 268.251

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 466.536

Deuterated enthalpy correction(kcal/mol): 496.197

Deuterated entropy correction(cal/mol): 270.832

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	0.08621471	-0.19184500	0.48058495
C	-0.19702179	2.17373806	1.26640589
C	-1.38460765	1.48648192	1.69266670
H	-2.36880122	1.61125188	1.26422138
C	0.83612157	1.69988012	2.11546095
H	1.87617855	1.98723523	2.05818961
C	0.31459875	0.71432034	2.99223573
H	0.86518956	0.17731699	3.75139707
C	-1.07210488	0.60247617	2.74378903
H	-1.75653247	-0.06795089	3.24107033
B	-0.02332357	3.05131851	-0.09863918
C	-0.23442193	4.64818681	0.03575598
C	1.44554268	2.60398045	-0.68645594
C	-1.04001381	2.31383413	-1.16152510
N	-1.13558020	1.01942241	-1.22900374
N	1.85279486	1.37495002	-0.66437865
O	2.30341144	3.49502510	-1.22595526

O	-1.84277176	2.99269851	-1.99707513
C	-2.19040096	0.66713766	-2.19895698
C	-2.58646262	2.03146383	-2.79653922
C	3.22213940	1.32523286	-1.21393520
C	3.46557038	2.76701920	-1.70291576
N	-1.16585790	-1.73637354	0.45966785
N	1.69622192	-1.60420700	1.28123102
C	3.02054583	-1.24373226	1.82045374
H	2.86993958	-0.50106224	2.60518926
H	-1.81847254	-0.02345339	-2.96179308
H	3.92995403	1.02653420	-0.43413832
C	-2.40302912	-2.36872377	0.04947012
H	-2.61533076	-2.14763717	-1.00961082
H	-2.29517184	-3.46099692	0.10434245
C	-3.63797375	-1.96124382	0.87023083
C	3.68138076	-2.52348934	2.39514756
C	2.54851748	-3.55617875	2.57012921
H	2.62381734	-4.08295650	3.52476446
H	3.64394506	-0.77503669	1.05476175
H	1.85775206	-2.22495303	0.48763817
C	1.19105473	-2.86281049	2.49451619
H	1.04209712	-2.17922027	3.33045404
H	2.59017575	-4.32338343	1.79000673
C	0.01951910	-3.59253958	2.11625744
H	-0.81220042	-3.56500237	2.81496500
H	-0.63637970	-2.54145588	1.13529239
H	0.17840494	-4.57174606	1.66690299
C	-0.13870708	5.51409033	-1.06729086
H	0.08140940	5.10586153	-2.04839026
C	-0.51940527	5.23868680	1.27569174
H	-0.60138835	4.60547858	2.15328832
C	-0.31647934	6.88935968	-0.94193379
H	-0.23478608	7.52767499	-1.81630452

C	-0.69934185	6.61551087	1.41461174
H	-0.91835949	7.03614645	2.39110971
C	-0.59841246	7.44830179	0.30408716
H	-0.73729854	8.51961705	0.40591011
C	-4.94237391	-2.61898939	0.37587140
H	-5.10694480	-2.37317060	-0.68034260
H	-5.78199774	-2.18154781	0.93127635
C	-4.97538653	-4.11202097	0.55224193
H	-4.82264667	-4.46707948	1.57119389
C	-5.17373681	-5.00511063	-0.41345005
H	-5.32745075	-4.70234009	-1.44531810
H	-5.19169824	-6.07000878	-0.20990571
H	4.45254535	-2.90215389	1.71874431
H	4.17792410	-2.30129721	3.34262152
H	-3.46661929	-2.21861279	1.92139307
H	-3.74612009	-0.87202295	0.83337043
H	-2.28061736	2.15673263	-3.83692538
H	-3.64620250	2.26685127	-2.70222832
H	-3.02024454	0.17472146	-1.68570983
H	3.49376719	2.85697643	-2.79115669
H	4.35469222	3.23590098	-1.28179007
H	3.30254510	0.59321581	-2.02348100
N	0.78000573	-1.12275562	-1.78404236
C	1.76568474	-2.17879096	-2.12517653
H	1.00535678	-0.25069215	-2.25521558
H	-0.13863295	-1.41227280	-2.11034693
H	2.66226726	-2.02031314	-1.51618796
H	2.08076165	-2.09467737	-3.17313806
C	1.19706862	-3.57763022	-1.88138985
H	0.36590723	-3.75197595	-2.57486946
H	0.76873771	-3.63387588	-0.87565493
C	2.25269609	-4.68121495	-2.07208854
H	3.07601505	-4.50459881	-1.36591493

H	2.68347292	-4.62168578	-3.07796352
C	1.69608469	-6.05923123	-1.84167179
H	1.25688162	-6.23292246	-0.86057318
C	1.69845105	-7.04397867	-2.73466699
H	2.12461598	-6.91384715	-3.72529906
H	1.27878747	-8.01749677	-2.50828342

MP2 Electronic Energy(Ha): 1740.413395837820

B3LYP Electronic Energy(Ha): 1744.908350121204

M06-L Electronic Energy(Ha): 1744.689971403839

Zero point energy correction(kcal/mol): 472.852

Enthalpy correction(kcal/mol): 501.305

Entropy correction(cal/mol): 265.272

Imaginary Frequencies: -802.29

Deuterated zero point energy correction(kcal/mol): 464.862

Deuterated enthalpy correction(kcal/mol): 493.671

Deuterated entropy correction(cal/mol): 267.328

Deuterated imaginary Frequencies: -720.67

Product geometry

Zr	0.31254812	0.54870191	0.34690880
C	0.55601909	-1.92189983	1.05391458
C	1.85893077	-1.31747553	1.04450831
H	2.64815385	-1.54958830	0.34365060
C	-0.12659225	-1.33902195	2.14926359
H	-1.14091907	-1.57281427	2.44300983
C	0.71890733	-0.38606724	2.78351064
H	0.48650630	0.18915753	3.66782956
C	1.96226241	-0.39023075	2.10782451
H	2.83112054	0.19883573	2.36270103
B	-0.00258089	-2.94154825	-0.08696610
C	0.76282014	-4.38284160	-0.11555441
C	-1.62752910	-3.12036497	0.09008733
C	0.21094389	-2.11988456	-1.49051953

N	0.38881452	-0.83294927	-1.55295368
N	-2.54182635	-2.23334336	-0.11370723
O	-2.07051317	-4.32661728	0.54280993
O	0.23465774	-2.74506553	-2.68224652
C	0.66044652	-0.44539709	-2.95134280
C	0.40132479	-1.74832434	-3.72681017
C	-3.85038172	-2.82411609	0.22869156
C	-3.51381796	-4.27610173	0.62396558
N	1.43104301	1.85094934	-0.39621903
N	-0.94972653	2.18296331	1.77497807
C	-2.04373753	1.67731116	2.68339401
H	-2.08798700	0.58997412	2.65173162
H	0.01328621	0.37511238	-3.27414766
H	-4.31491302	-2.26495432	1.04844403
C	2.50940955	2.63200799	-0.92522876
H	2.59491722	2.47892274	-2.01507674
H	2.31385722	3.71010836	-0.80262581
C	3.87363218	2.31107736	-0.29044622
C	-1.72479010	2.21688158	4.08609472
C	-0.95743742	3.50951729	3.79818067
H	-0.34749180	3.84649831	4.63889672
H	-3.00723067	2.06385664	2.34109616
H	-1.38911321	2.73247980	1.04145800
C	-0.10361389	3.15392689	2.57283316
H	0.78296066	2.60521639	2.90031010
H	-1.65216629	4.31920784	3.54520740
C	0.33089842	4.34217356	1.72865164
H	0.98042375	5.00021109	2.31114438
H	0.87587479	4.00292129	0.84808310
H	-0.53694204	4.93066469	1.40873311
C	0.49744669	-5.34563856	-1.10604976
H	-0.22204258	-5.12164319	-1.88605661
C	1.70192931	-4.73932336	0.86349949

H	1.93613929	-4.03437272	1.65388953
C	1.13333771	-6.58409651	-1.12336093
H	0.90098788	-7.29987106	-1.90616836
C	2.34414916	-5.97885071	0.85928983
H	3.06315589	-6.21623851	1.63748801
C	2.06451025	-6.90840756	-0.13740582
H	2.56211341	-7.87273247	-0.14682501
C	5.04494500	3.12158121	-0.87998855
H	5.09321389	2.97268152	-1.96485467
H	5.98011804	2.71938861	-0.46895126
C	4.98488715	4.59251553	-0.57550052
H	4.93968155	4.85008200	0.48292821
C	4.99203273	5.57501562	-1.47239494
H	5.03599118	5.37049744	-2.53818001
H	4.95838923	6.61775599	-1.17645418
H	-2.62975279	2.37088730	4.67672609
H	-1.09282575	1.51253289	4.63225195
H	3.80935283	2.48500184	0.79028223
H	4.07243012	1.24240241	-0.41932130
H	-0.51741358	-1.72742940	-4.31741391
H	1.22988312	-2.06260572	-4.36076079
H	1.69111168	-0.09226659	-3.03562129
H	-3.91828477	-5.02016131	-0.06575131
H	-3.80731835	-4.53841145	1.64183528
H	-4.52859413	-2.76947974	-0.62831275
N	-1.91634600	0.58589536	-0.77973219
C	-3.03106741	1.55824100	-0.82581076
H	-2.26146956	-0.35814659	-0.50584946
H	-1.59779059	0.44381830	-1.73492541
H	-3.32401960	1.80750487	0.19759023
H	-3.91380129	1.10392841	-1.29385139
C	-2.65018128	2.82433266	-1.59321770
H	-2.40691034	2.55724548	-2.62841589

H	-1.73186649	3.25085015	-1.17327466
C	-3.76948510	3.87981231	-1.59992200
H	-4.01043188	4.14636280	-0.56139901
H	-4.68109658	3.45317240	-2.03184421
C	-3.39006547	5.12486931	-2.35235054
H	-2.51414476	5.65508589	-1.98081386
C	-4.02780419	5.60030013	-3.41730513
H	-4.90468017	5.10481393	-3.82369301
H	-3.70032791	6.50292860	-3.92029573

MP2 Electronic Energy(Ha): 1740.485041164148

B3LYP Electronic Energy(Ha): 1744.983099602689

M06-L Electronic Energy(Ha): 1744.752857593456

Zero point energy correction(kcal/mol): 477.391

Enthalpy correction(kcal/mol): 505.906

Entropy correction(cal/mol): 266.891

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.605

Deuterated enthalpy correction(kcal/mol): 497.443

Deuterated entropy correction(cal/mol): 268.864

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H3-S

Reactant geometry

Zr	-0.17160954	0.74565653	-0.61028933
C	-1.58004365	-1.24581060	-1.08377384
C	-2.52478238	-0.26150587	-0.66297917
H	-3.05270637	-0.26335675	0.27986830
C	-1.14920694	-0.82446494	-2.37757888
H	-0.41260161	-1.32738916	-2.98682266
C	-1.77837991	0.39393881	-2.71875029
H	-1.62577540	0.96080910	-3.62504014
C	-2.63254317	0.74458942	-1.65094661

H	-3.25468063	1.62560905	-1.60332873
B	-0.90133706	-2.40944758	-0.15935123
C	-1.58720298	-3.87103837	-0.21589126
C	0.68676910	-2.38030986	-0.57636903
C	-0.85246521	-1.72531499	1.33277675
N	-0.48616483	-0.49142490	1.48073215
N	1.32774869	-1.27985713	-0.82122245
O	1.41192780	-3.51196943	-0.66911395
O	-1.21429798	-2.36041507	2.46204740
C	-0.65766239	-0.10683273	2.89259004
C	-1.02029072	-1.44136446	3.57374795
C	2.70894198	-1.62621430	-1.21837004
C	2.78615443	-3.14064195	-0.95706811
N	-0.95891330	2.48722493	0.32134087
N	1.02484496	1.89321209	-1.97483285
C	0.47900474	3.01227696	-2.75083567
H	-0.38694270	3.44245700	-2.24413449
H	0.25747132	0.32914388	3.30254288
H	2.86714518	-1.37919568	-2.27059576
C	-2.22916222	2.94638512	0.86900939
H	-2.96739758	2.14528839	0.76566517
H	-2.15278315	3.14156785	1.95000556
C	-2.77235973	4.21206541	0.18825205
C	1.64401881	4.03244018	-2.89571280
C	2.91406445	3.22822011	-2.52043733
H	3.30541574	3.55873995	-1.55321992
H	0.13738214	2.69805007	-3.75061567
C	2.41487862	1.76352946	-2.41645264
H	2.99367735	1.20804998	-1.66933888
H	3.72077733	3.34558846	-3.24920432
C	2.56372551	1.03158302	-3.76637075
H	3.61924239	0.89117333	-4.02336416
H	2.07960043	0.05375228	-3.73087429

H	2.09893882	1.59844519	-4.57779898
C	-2.67540563	-4.13069446	-1.06183345
H	-3.06014375	-3.33025042	-1.68579003
C	-1.13182496	-4.94242105	0.57179733
H	-0.29215786	-4.79202821	1.24249893
C	-3.27951301	-5.38706862	-1.12443721
H	-4.12001254	-5.55006110	-1.79186033
C	-1.72650969	-6.20024069	0.51922836
H	-1.34806725	-7.00431170	1.14287011
C	-2.80666426	-6.42920878	-0.33240052
H	-3.27278677	-7.40808375	-0.37613206
C	-4.11589765	4.70423900	0.76255194
H	-4.86333572	3.90529837	0.69912958
H	-4.48001938	5.52140329	0.12664209
C	-4.02935285	5.20346121	2.17828095
H	-3.31130578	6.00576728	2.34956594
C	-4.75080121	4.76087630	3.20453959
H	-5.48013495	3.96509074	3.08475090
H	-4.64486623	5.18054732	4.19877475
H	-1.94459381	-1.41213057	4.14989747
H	-1.44877722	0.64318093	2.97983035
H	-0.21851838	-1.84056012	4.19861892
H	3.39145847	-3.39847470	-0.08495146
H	3.12172555	-3.72544225	-1.81312600
H	3.44439580	-1.07058597	-0.63528322
H	1.69785169	4.43429982	-3.91046299
H	1.50631766	4.88235459	-2.22314993
H	-2.02598633	5.01325278	0.27440902
H	-2.88613301	4.01510545	-0.88260794
H	-0.28421536	3.24723255	0.38730196
N	1.70556146	1.45508156	0.90414705
H	2.14714551	2.18503105	0.34988965
C	2.71944420	0.65317214	1.61667636

H	1.09879680	1.93082671	1.56948313
H	2.22657461	-0.24436524	1.99824804
H	3.45580561	0.31832625	0.88614048
C	3.42276485	1.40147138	2.75325827
H	2.67560137	1.73635533	3.48270826
H	3.89431876	2.30870232	2.35543598
C	4.48256492	0.54873747	3.47913493
H	4.83369344	1.11280948	4.35175726
H	4.02187937	-0.36747993	3.86465287
C	5.66664355	0.19880253	2.61990403
H	6.21124960	1.04498198	2.20150659
C	6.09038672	-1.03335254	2.35199637
H	5.58589313	-1.90808372	2.75189238
H	6.96431340	-1.21287063	1.73610342

MP2 Electronic Energy(Ha): 1740.500060211502

B3LYP Electronic Energy(Ha): 1744.992322272806

M06-L Electronic Energy(Ha): 1744.773357392376

Zero point energy correction(kcal/mol): 476.429

Enthalpy correction(kcal/mol): 505.089

Entropy correction(cal/mol): 265.980

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 467.970

Deuterated enthalpy correction(kcal/mol): 497.016

Deuterated entropy correction(cal/mol): 268.452

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-1.21477253	0.18481327	-0.01262933
C	-1.88087883	-2.17288789	0.28887245
C	-2.50367178	-1.44635313	1.35743516
H	-2.21273135	-1.48770875	2.39714446
C	-2.60850018	-1.81217319	-0.88065670
H	-2.38588559	-2.15206882	-1.88240288

C	-3.57953322	-0.83606674	-0.56144114
H	-4.26142724	-0.36136351	-1.25138196
C	-3.52189790	-0.61123263	0.84040264
H	-4.16615558	0.04420390	1.40841145
B	-0.40212927	-2.88140918	0.32411453
C	-0.36170887	-4.48653217	0.46824852
C	0.40582421	-2.27583001	-0.99154929
C	0.40981706	-2.03888735	1.48907122
N	0.30429058	-0.74760578	1.54056682
N	0.30337461	-1.03429116	-1.38026361
O	1.33301587	-2.99563135	-1.63338353
O	1.23376550	-2.58424028	2.39296965
C	1.13724389	-0.22702626	2.63762845
C	1.80817352	-1.50305769	3.19036583
C	1.35465813	-0.76370004	-2.38324945
C	1.90792448	-2.16555733	-2.68483157
N	-0.92800366	1.98353558	0.73314149
N	-1.64923354	1.77348807	-1.70657805
C	-2.97800604	2.37956579	-1.88948673
H	-3.41710893	2.61569663	-0.91580064
H	1.85755283	0.50094722	2.25960442
H	0.94252192	-0.28079436	-3.26791639
C	-0.83277474	3.07504880	1.67401786
H	-0.47377261	2.70306623	2.64646241
H	-0.08632115	3.80922529	1.34123721
C	-2.16927269	3.79987904	1.90605308
C	-2.74457339	3.64518900	-2.76052045
C	-1.31456824	3.46783796	-3.33379956
H	-0.62176080	4.15826987	-2.84716334
H	-3.67595967	1.69937320	-2.39674638
C	-0.93617392	2.01106422	-2.97011703
H	0.14162416	1.92444057	-2.79150626
H	-1.26496368	3.65614120	-4.40947082

C	-1.33330460	1.02816677	-4.08565282
H	-0.72842777	1.18928931	-4.98418212
H	-1.20601566	-0.00730664	-3.76114435
H	-2.38149623	1.15493947	-4.37027336
C	-1.54530636	-5.23898817	0.49300603
H	-2.49838865	-4.72562182	0.41479101
C	0.84382118	-5.20116150	0.57822539
H	1.78602251	-4.66397565	0.56688127
C	-1.53437437	-6.62846087	0.61801530
H	-2.47063829	-7.17724136	0.63379959
C	0.86711500	-6.58767125	0.70429958
H	1.81669358	-7.10680220	0.78823136
C	-0.32525731	-7.30970708	0.72417859
H	-0.31045086	-8.39005219	0.82269343
C	-2.10573991	4.88306319	3.00040434
H	-1.80233629	4.43202777	3.95218490
H	-3.12041606	5.27432672	3.15099247
C	-1.19065846	6.03054531	2.67421037
H	-1.39485015	6.54417445	1.73485179
C	-0.18249969	6.45537986	3.43043757
H	0.06146930	5.97449794	4.37333119
H	0.43474532	7.29725043	3.13770585
H	1.57889066	-1.70750351	4.23596535
H	0.51341506	0.27735122	3.37973138
H	2.88874703	-1.52794861	3.04499808
H	2.99177976	-2.24674878	-2.61949964
H	1.56829971	-2.56606640	-3.64190012
H	2.11003552	-0.09916378	-1.95227958
H	-3.49586185	3.72515696	-3.54964919
H	-2.81243228	4.55450145	-2.15983493
H	-2.50118675	4.24965391	0.96249517
H	-2.92540456	3.05684635	2.18076090
H	-1.17925939	2.24971174	-0.52564600

N	2.13462861	3.03545086	-0.48104869
H	2.03069026	3.05945206	-1.49106560
C	3.36951440	2.34219350	-0.10643172
H	1.31435506	2.56332357	-0.10682314
H	3.40045738	2.28577711	0.98805920
H	3.43129248	1.30412362	-0.47263162
C	4.59458388	3.11727982	-0.59179489
H	4.52950406	4.13845130	-0.20523859
H	4.55895571	3.19875833	-1.68662810
C	5.93791518	2.48893186	-0.17535103
H	6.73903970	3.18585719	-0.45209333
H	5.97899002	2.38711171	0.91497784
C	6.21952552	1.15910118	-0.81897067
H	6.20612381	1.15404801	-1.90911897
C	6.49182247	0.02614783	-0.17708919
H	6.52319843	-0.01845897	0.90767554
H	6.70531692	-0.89432944	-0.70898390

MP2 Electronic Energy(Ha): 1740.429030516741

B3LYP Electronic Energy(Ha): 1744.933013324890

M06-L Electronic Energy(Ha): 1744.695317723417

Zero point energy correction(kcal/mol): 472.757

Enthalpy correction(kcal/mol): 501.675

Entropy correction(cal/mol): 274.499

Imaginary Frequencies: -1617.25

Deuterated zero point energy correction(kcal/mol): 465.197

Deuterated enthalpy correction(kcal/mol): 494.419

Deuterated entropy correction(cal/mol): 276.589

Deuterated imaginary Frequencies: -1163.12

Product geometry

Zr	0.36683678	0.20810360	-0.53292514
C	0.64983991	2.63786463	-1.06351460
C	1.93976010	2.02860730	-1.22269297

H	2.78149910	2.15398327	-0.55685272
C	-0.11184186	2.19832732	-2.17801795
H	-1.14285219	2.45985867	-2.36542499
C	0.65028868	1.28984667	-2.95371802
H	0.33186280	0.79865000	-3.86256978
C	1.93610006	1.19367769	-2.36472306
H	2.76658706	0.61144368	-2.73549055
B	0.04969620	3.31207847	0.30391581
C	0.03652761	4.92509305	0.37740744
C	-1.42686250	2.60062497	0.55335311
C	0.87944296	2.55473468	1.50815299
N	1.03746666	1.27010531	1.46589737
N	-1.66254098	1.33547640	0.37006245
O	-2.44034119	3.30111363	1.09806214
O	1.42590108	3.16673817	2.57118067
C	1.85243765	0.83755465	2.61104822
C	2.00723988	2.13736643	3.42763468
C	-3.00085690	1.02402274	0.90842961
C	-3.57496820	2.40893167	1.25728919
N	1.38387584	-1.31688704	-0.07978705
N	-1.25394578	-1.38716568	-1.56835535
C	-0.57525395	-2.19628036	-2.63769376
H	0.15101179	-2.84874719	-2.15635502
H	1.34936794	0.04513902	3.16922499
H	-3.61270208	0.49949004	0.17331108
C	2.38764197	-2.31580623	0.13683841
H	2.68639813	-2.34626787	1.20060785
H	1.99723610	-3.32552028	-0.07995744
C	3.65984516	-2.10629400	-0.70297151
C	-1.68283285	-2.96132107	-3.40786842
C	-2.98589568	-2.61256705	-2.66286790
H	-3.18877714	-3.35549485	-1.88659794
H	-0.02125508	-1.53192346	-3.30048894

C	-2.68369566	-1.25488423	-1.99857176
H	-3.28361417	-1.12796295	-1.09545011
H	-3.85681951	-2.57402255	-3.32080256
C	-2.92215686	-0.06806640	-2.92777686
H	-3.97158581	-0.03995121	-3.23364083
H	-2.68485513	0.87020095	-2.42740518
H	-2.31348639	-0.13015757	-3.83358629
C	0.41843314	5.70193474	-0.72650276
H	0.73106663	5.20241546	-1.63793227
C	-0.35183609	5.62294563	1.53430433
H	-0.65244862	5.06729622	2.41624964
C	0.41206334	7.09673615	-0.68678938
H	0.71489897	7.66377764	-1.56155015
C	-0.36103263	7.01428926	1.58697130
H	-0.66557758	7.51916213	2.49857293
C	0.02115483	7.76018236	0.47255813
H	0.01568803	8.84458487	0.51012900
C	4.75469068	-3.16446956	-0.46257484
H	5.00905609	-3.20435629	0.60291538
H	5.66344107	-2.84157184	-0.98727395
C	4.39135633	-4.54081646	-0.94617639
H	4.12174064	-4.61024437	-2.00027554
C	4.38538724	-5.64946481	-0.21074812
H	4.64700034	-5.63323266	0.84326160
H	4.12490998	-6.61324734	-0.63419116
H	3.04015101	2.41870354	3.63059129
H	2.80718214	0.43900786	2.25817543
H	1.44408639	2.13225310	4.36284556
H	-3.93570800	2.50094216	2.28152465
H	-4.35661419	2.73704597	0.56888424
H	-2.90714095	0.37632020	1.78706336
H	-1.72676806	-2.62743850	-4.44697583
H	-1.49837400	-4.03689852	-3.42509731

H	3.38171752	-2.09438394	-1.76326076
H	4.06089622	-1.11264645	-0.47824583
H	-1.29033845	-2.00315246	-0.74282857
N	-1.12455451	-3.01355066	1.05936080
H	-1.56727616	-2.57026862	1.86043637
C	-1.04990599	-4.46841045	1.27686743
H	-0.19290270	-2.59858064	0.97870519
H	-0.48137938	-4.90058965	0.44692216
H	-0.50953362	-4.73181343	2.19607385
C	-2.44519242	-5.09145308	1.31072394
H	-2.96056614	-4.85195126	0.37500405
H	-3.03057040	-4.62348282	2.11360797
C	-2.43850390	-6.61888122	1.51472802
H	-3.46435912	-6.98393662	1.37958592
H	-1.83385198	-7.09509382	0.73484730
C	-1.94873770	-7.05132097	2.86954897
H	-2.49692187	-6.64429320	3.71924107
C	-0.93152908	-7.87659287	3.09859373
H	-0.35488573	-8.30740298	2.28542422
H	-0.63981703	-8.15550768	4.10483797

MP2 Electronic Energy(Ha): 1740.471099904139

B3LYP Electronic Energy(Ha): 1744.972199400037

M06-L Electronic Energy(Ha): 1744.739789849729

Zero point energy correction(kcal/mol): 477.236

Enthalpy correction(kcal/mol): 505.914

Entropy correction(cal/mol): 265.236

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.528

Deuterated enthalpy correction(kcal/mol): 497.528

Deuterated entropy correction(cal/mol): 267.344

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H6-S

Reactant geometry

Zr	-0.13471100	1.97391962	0.45859395
C	2.23978329	1.08624987	0.72677173
C	2.31968996	2.34481022	0.04270619
H	2.61407614	2.47319449	-0.99023120
C	1.82559680	1.40236922	2.04781361
H	1.66280576	0.68417735	2.83956694
C	1.61818297	2.80745815	2.16484769
H	1.33644461	3.34517942	3.05977179
C	1.94522841	3.39489031	0.91695927
H	1.92459145	4.44962374	0.68455791
B	2.33753561	-0.37529501	0.00615035
C	3.78713595	-0.68283859	-0.68006664
C	1.94194719	-1.52021524	1.11477414
C	1.13452012	-0.39414338	-1.12679077
N	0.16691713	0.48555983	-1.21752517
N	0.76952601	-1.78775082	1.59224888
O	2.97051107	-2.22513183	1.65266805
O	1.08767732	-1.35014513	-2.05876322
C	-0.65453394	0.19599996	-2.41386262
C	-0.08914818	-1.14558618	-2.90240676
C	0.92942435	-2.80410743	2.65618397
C	2.42208119	-3.17733898	2.59514582
N	-1.32394196	3.27453021	-0.15719667
N	-1.38463636	0.37853858	1.73835709
C	-2.56542855	-0.18843181	1.01587129
H	-2.22326521	-0.77363976	0.16167893
H	-1.71154987	0.13435440	-2.15246157
H	0.64633539	-2.37854963	3.62555289
C	-2.03420262	4.44158551	-0.59320811
H	-3.00627799	4.51411658	-0.07673410
H	-1.48361179	5.35462482	-0.32372190

C	-2.29700103	4.45278482	-2.10905340
C	-3.29488622	-1.01956336	2.07420234
C	-3.16665001	-0.14850068	3.33249364
H	-3.17485586	-0.73150209	4.25535112
H	-3.19043202	0.63176800	0.65414487
C	-1.83608441	0.63744846	3.16033222
H	-1.06119878	0.22590287	3.81192202
H	-4.00156660	0.55627342	3.38655408
C	-1.99849918	2.12544040	3.46176376
H	-1.04635928	2.65813322	3.40089430
H	-0.68641595	-0.38630011	1.76912349
H	-2.38668428	2.26002895	4.47554219
C	4.02374564	-1.84196161	-1.44086842
H	3.21511924	-2.54523646	-1.60576290
C	4.87948193	0.17943808	-0.50298985
H	4.75356712	1.08060526	0.08679240
C	5.26928205	-2.12003179	-1.99777994
H	5.41083580	-3.02598712	-2.57919826
C	6.13347788	-0.08938814	-1.05373549
H	6.95326921	0.60321054	-0.89026986
C	6.33453258	-1.24098463	-1.80795558
H	7.30674650	-1.45378327	-2.24010261
C	-3.08517353	5.68385257	-2.59777494
H	-4.03869710	5.75415317	-2.06165930
H	-3.33364689	5.53283065	-3.65657475
C	-2.33463607	6.97978087	-2.46373045
H	-1.36428954	7.01294568	-2.95925515
C	-2.75693598	8.05889646	-1.81064728
H	-3.71487035	8.07425981	-1.29890803
H	-2.16402904	8.96560777	-1.76434810
H	0.24865156	-1.13936442	-3.93792705
H	-0.53446448	1.00390910	-3.13944616
H	-0.76147357	-1.98218794	-2.71656507

H	2.60198382	-4.18110403	2.20308798
H	2.95156516	-3.06349218	3.54152284
H	0.27471925	-3.66105326	2.47423035
H	-4.33207010	-1.22914525	1.80492635
H	-2.78315559	-1.97706217	2.20834252
H	-1.33462587	4.39663795	-2.63113540
H	-2.84801334	3.54339877	-2.37221141
H	-2.69651022	2.59401563	2.76347391
N	-1.05707634	-3.44428797	-0.64427717
H	-0.59002616	-2.91803303	0.09320974
H	-0.31256819	-3.84917470	-1.20579114
C	-1.89863086	-4.51160504	-0.08958172
H	-1.33319798	-5.24719465	0.50677627
H	-2.62295151	-4.05000396	0.59070372
C	-2.65314050	-5.24767406	-1.19707973
H	-1.93286710	-5.68248521	-1.90069737
H	-3.23974282	-4.51732994	-1.76476685
C	-3.56909776	-6.36348070	-0.66566041
H	-4.27490991	-5.92421901	0.05278911
H	-2.97726149	-7.10086683	-0.11244622
C	-4.34271959	-7.05370838	-1.75366442
C	-4.26542535	-8.34726085	-2.05080887
H	-3.61677774	-9.01989946	-1.49715380
H	-4.84780169	-8.78300082	-2.85477801
H	-5.00630617	-6.41766341	-2.33856800

MP2 Electronic Energy(Ha): 1740.462053021716

B3LYP Electronic Energy(Ha): 1744.972652506377

M06-L Electronic Energy(Ha): 1744.731273779371

Zero point energy correction(kcal/mol): 475.502

Enthalpy correction(kcal/mol): 499.552

Entropy correction(cal/mol): 230.272

Imaginary Frequencies: -44.23 -42.74 -41.35 -39.41 -34.68 -23.58 -21.97 -16.84

Deuterated zero point energy correction(kcal/mol): 466.470

Deuterated enthalpy correction(kcal/mol): 490.358

Deuterated entropy correction(cal/mol): 226.373

Deuterated imaginary Frequencies: -44.42 -42.84 -41.30 -39.09 -34.93 -28.25 -24.37 -21.38 -15.83

Transition State geometry

Zr	0.21218580	1.51373348	0.71308267
C	2.52409473	0.58684679	0.59301778
C	2.55434245	1.75700010	-0.23940222
H	2.62817384	1.75640060	-1.31833628
C	2.42608110	1.07311492	1.92311139
H	2.35314325	0.46127698	2.80997531
C	2.33224289	2.48963628	1.90388635
H	2.23694432	3.13614507	2.76462224
C	2.44081574	2.91189110	0.55748167
H	2.40450138	3.93241637	0.20595837
B	2.30969313	-0.94617161	0.07288017
C	3.66116572	-1.78583134	-0.21546296
C	1.29845068	-1.64160384	1.16145069
C	1.31568404	-0.73724930	-1.22852326
N	0.26514228	0.03334579	-1.16461232
N	0.32755801	-1.00899884	1.73265273
O	1.39761981	-2.96031889	1.46060550
O	1.56650446	-1.25689688	-2.43743083
C	-0.29737720	0.19023538	-2.52120158
C	0.52151370	-0.81498016	-3.35309018
C	-0.45187772	-1.98581702	2.52577642
C	0.43347182	-3.24290017	2.50776630
N	-0.61138528	3.06246092	-0.09846308
N	-2.06973256	0.81836540	1.49745794
C	-3.33305499	0.94755674	0.71693326
H	-3.58727893	-0.01890772	0.28089572
H	-1.36735460	-0.02749801	-2.53273540
H	-0.63393990	-1.61708518	3.53815272

C	-0.74389798	4.38950953	-0.63607317
H	-0.89806101	5.11999343	0.17712391
H	0.18707702	4.69548290	-1.13521987
C	-1.90656153	4.53459321	-1.63198201
C	-4.36934853	1.47365268	1.71878943
C	-3.53394249	2.44779358	2.55614903
H	-3.96980222	2.67813179	3.53067090
H	-3.17229231	1.67250724	-0.08405240
C	-2.16276131	1.75835804	2.70035449
H	-2.16462667	1.13343956	3.59975845
H	-3.41376985	3.39277890	2.01655938
C	-0.95533376	2.69005318	2.67142791
H	-0.18592013	2.40506059	3.39246446
H	-2.01244736	-0.13606110	1.83169744
H	-1.21849480	3.72413251	2.91326697
C	3.64552285	-3.09654902	-0.72269289
H	2.69572158	-3.56977391	-0.94972618
C	4.92141752	-1.23624822	0.06447697
H	4.97989554	-0.22632085	0.45729932
C	4.81745198	-3.81876510	-0.93371695
H	4.76694895	-4.83099780	-1.32289026
C	6.10266781	-1.94948308	-0.14180065
H	7.05854373	-1.49023215	0.09037222
C	6.05549701	-3.24734197	-0.64173003
H	6.97046143	-3.80839240	-0.80125268
C	-2.06233330	5.96361646	-2.18954985
H	-2.21192776	6.66842220	-1.36360956
H	-2.97512705	5.99809554	-2.79809854
C	-0.90277501	6.41721956	-3.03265795
H	-0.69003077	5.80527251	-3.90926262
C	-0.14017502	7.48048121	-2.79344014
H	-0.31049005	8.11820898	-1.93091849
H	0.68060683	7.75289155	-3.44735992

H	1.00860166	-0.38251528	-4.22660392
H	-0.16587556	1.22329843	-2.85409305
H	-0.04646351	-1.69636174	-3.65612351
H	-0.09191505	-4.16215088	2.24986311
H	0.98445042	-3.39103405	3.43985743
H	-1.41930164	-2.16640432	2.04146730
H	-5.22580934	1.94691825	1.23316053
H	-4.74777928	0.65631698	2.34268533
H	-1.75757657	3.82730463	-2.45654289
H	-2.83675722	4.23912383	-1.13507503
H	-0.82023123	3.08120278	1.24295801
N	-2.31964709	-2.28021014	-0.59701738
H	-1.42940705	-1.78981462	-0.62405368
H	-2.90989009	-1.85198019	-1.30472701
C	-2.14704249	-3.71042491	-0.89461606
H	-1.72600071	-3.89914250	-1.89516898
H	-1.42720733	-4.11654456	-0.17662583
C	-3.47729470	-4.45059601	-0.76139519
H	-4.19703181	-4.03704696	-1.47878550
H	-3.88640344	-4.25313968	0.23520419
C	-3.35803628	-5.96663944	-0.99207512
H	-2.62278445	-6.37173915	-0.28357997
H	-2.96728755	-6.16500172	-1.99592688
C	-4.66587331	-6.68409806	-0.80814650
C	-5.29495687	-7.39133175	-1.74164533
H	-4.88179113	-7.51189400	-2.73881687
H	-6.24262920	-7.87936409	-1.54381404
H	-5.12046912	-6.59111181	0.17763798

MP2 Electronic Energy(Ha): 1740.409510979094

B3LYP Electronic Energy(Ha): 1744.906338896701

M06-L Electronic Energy(Ha): 1744.674831010355

Zero point energy correction(kcal/mol): 471.768

Enthalpy correction(kcal/mol): 493.858

Entropy correction(cal/mol): 210.045

Imaginary Frequencies: -1524.50 -61.86 -61.26 -58.56 -55.74 -52.70 -48.86 -40.99 -38.61 -12.18

Deuterated zero point energy correction(kcal/mol): 463.535

Deuterated enthalpy correction(kcal/mol): 486.050

Deuterated entropy correction(cal/mol): 218.280

Deuterated imaginary Frequencies: -1120.34 -61.58 -60.70 -60.46 -55.11 -52.85 -49.42 -44.74 -38.54 -12.

Product geometry

Zr	-0.78881527	0.96780066	0.93865858
C	1.43114235	2.04132184	0.88382532
C	0.55123953	3.03359116	0.34852277
H	0.50277027	3.33442791	-0.68890039
C	1.12224595	1.97895877	2.27698947
H	1.58455725	1.31513478	2.99266039
C	0.05600550	2.85442419	2.57297373
H	-0.40457899	3.00000617	3.53909964
C	-0.29280400	3.51893556	1.37298794
H	-1.06378924	4.26656017	1.27138431
B	2.34522046	0.96386741	0.05111911
C	3.87071466	1.39019777	-0.25972903
C	2.17836785	-0.41350962	0.93644934
C	1.44347228	0.61449377	-1.27891616
N	0.16353101	0.42984853	-1.19134227
N	1.02000282	-0.81608676	1.35279106
O	3.23364909	-1.14948153	1.34219226
O	1.95549713	0.49835769	-2.51834431
C	-0.38998745	0.20067634	-2.53582654
C	0.87044434	0.14564407	-3.42332328
C	1.22094022	-1.95794619	2.26572187
C	2.72018555	-2.27426965	2.10818231
N	-2.55575756	1.77868221	0.15136102
N	-1.98441063	-1.16641401	0.69302371
C	-3.19926826	-1.54845546	-0.07886390

H	-2.93449201	-2.28613377	-0.83916097
H	-0.97170156	-0.72422347	-2.56706261
H	0.96031634	-1.66388269	3.28688807
C	-3.14645385	3.03853094	-0.28386550
H	-3.84739937	3.43037206	0.47225453
H	-2.35885130	3.78653271	-0.38433695
C	-3.89822382	2.93081492	-1.61895158
C	-4.20253234	-2.08644311	0.95513063
C	-3.84121107	-1.29639822	2.21752546
H	-4.20463065	-1.75462049	3.13938071
H	-3.60939181	-0.67945838	-0.60203473
C	-2.30800882	-1.22064478	2.19457234
H	-1.90573324	-2.16654325	2.57735831
H	-4.25588623	-0.28373514	2.16531666
C	-1.66480562	-0.00993048	2.86492019
H	-0.93670100	-0.28723237	3.63044337
H	-1.26193191	-1.85093301	0.46741404
H	-2.41080557	0.63832116	3.33512906
C	4.74952775	0.55112998	-0.96611980
H	4.39851035	-0.41376647	-1.31886892
C	4.38528786	2.62301939	0.16701270
H	3.74034447	3.30085280	0.71705006
C	6.06550699	0.91904633	-1.23283821
H	6.71601490	0.24492846	-1.78152739
C	5.70228978	3.00366363	-0.09347145
H	6.06537697	3.96611479	0.25324554
C	6.54942656	2.15169801	-0.79598311
H	7.57437356	2.44241978	-1.00150289
C	-4.53584980	4.25624365	-2.08113729
H	-5.20709543	4.63671506	-1.30308199
H	-5.16121501	4.04931775	-2.95910018
C	-3.53178487	5.31528625	-2.44426711
H	-2.82040138	5.04135825	-3.22345987

C	-3.45317347	6.52796950	-1.90353518
H	-4.13819851	6.84758030	-1.12371511
H	-2.70574711	7.24616035	-2.22135738
H	0.87048377	0.86535733	-4.24160579
H	-1.06337896	1.01908595	-2.80349239
H	1.08115252	-0.84916477	-3.82138837
H	2.91292229	-3.18394243	1.53373180
H	3.27091121	-2.32165877	3.04711010
H	0.58235370	-2.80036652	1.99071710
H	-5.23919008	-1.95281020	0.63720940
H	-4.03934548	-3.15656170	1.11867639
H	-3.20808687	2.56392072	-2.38822553
H	-4.68816344	2.17503886	-1.52555887
H	-3.26896216	1.05715196	0.07629976
N	-0.03939519	-3.22186390	-0.81068416
H	0.67459564	-2.52023168	-0.63280979
H	-0.36524033	-3.06399526	-1.76032937
C	0.51272339	-4.58228070	-0.69962813
H	1.34625229	-4.76218623	-1.39557711
H	0.91810415	-4.69809738	0.31119687
C	-0.57250618	-5.63274227	-0.93087902
H	-1.00429266	-5.49692846	-1.93009532
H	-1.38440611	-5.46427441	-0.21528309
C	-0.04941745	-7.07409905	-0.80520967
H	0.39577252	-7.19944130	0.19118602
H	0.75319047	-7.24444443	-1.53081765
C	-1.12711678	-8.10448420	-0.99540986
C	-1.14226230	-9.03298693	-1.94667738
H	-0.33896582	-9.11632784	-2.67287932
H	-1.95358044	-9.74682441	-2.03271192
H	-1.95498124	-8.05984042	-0.28872746

MP2 Electronic Energy(Ha): 1740.471093642258

B3LYP Electronic Energy(Ha): 1744.972285084795

M06-L Electronic Energy(Ha): 1744.745196367341

Zero point energy correction(kcal/mol): 474.734

Enthalpy correction(kcal/mol): 497.495

Entropy correction(cal/mol): 213.890

Imaginary Frequencies: -61.53 -60.68 -58.91 -56.34 -54.05 -44.37 -40.79 -34.01 -26.11

Deuterated zero point energy correction(kcal/mol): 465.657

Deuterated enthalpy correction(kcal/mol): 488.317

Deuterated entropy correction(cal/mol): 211.658

Deuterated imaginary Frequencies: -61.15 -60.42 -59.56 -55.23 -53.47 -44.43 -43.28 -35.09 -26.22

Equatorial Reaction C1-S

Reactant geometry

Zr	1.18265341	0.81429327	0.46522688
C	1.16708281	-1.55305749	1.18010294
C	2.28777553	-1.02772107	1.89370355
H	3.32388763	-1.25357702	1.68177607
C	0.01853072	-0.96111853	1.79471891
H	-1.00457324	-1.12757181	1.49174411
C	0.42696245	-0.03956764	2.78611588
H	-0.21703124	0.56309972	3.41030946
C	1.84682263	-0.08515641	2.84593517
H	2.46656512	0.49260769	3.51684186
B	1.21116335	-2.32571494	-0.26341769
C	1.24265223	-3.93843515	-0.22840075
C	-0.00433270	-1.65527320	-1.14316822
C	2.47928038	-1.61402182	-1.05280208
N	2.60499679	-0.32149175	-1.07891553
N	-0.29953335	-0.39559623	-1.05745438
O	-0.64090424	-2.33733393	-2.11055970
O	3.43882984	-2.29481197	-1.69743456
C	3.84930566	0.03107817	-1.78356217
C	4.32706626	-1.32780782	-2.33177880

C	-1.24941336	-0.05525485	-2.13847207
C	-1.56606944	-1.42329394	-2.76735139
N	2.80417531	2.10478665	0.83998359
H	3.65660805	0.75802542	-2.57564897
C	3.28534482	3.27276953	0.10681359
H	4.03074783	2.99413230	-0.65664691
H	2.44637601	3.71472373	-0.44254609
C	3.93201591	4.34231704	1.00349339
C	3.00514670	4.96044654	2.06586336
H	2.58110235	4.17101699	2.69262787
H	3.61839374	5.59295217	2.72140184
C	1.90003167	5.80349536	1.49352457
H	2.20813508	6.56563628	0.77749088
C	0.61001429	5.70468923	1.80643630
H	-0.13282974	6.36526630	1.37333780
C	1.19809575	-4.63737838	0.98708522
H	1.14326650	-4.07711827	1.91517800
C	1.31535319	-4.71362991	-1.39892221
H	1.34870633	-4.21957409	-2.36402505
C	1.34172444	-6.10519295	-1.35934823
H	1.39830018	-6.67143905	-2.28386185
C	1.22375619	-6.03151129	1.03972358
H	1.18826735	-6.53712756	1.99970279
C	1.29614865	-6.77277351	-0.13599448
H	1.31758354	-7.85707225	-0.10167721
H	-0.77432735	0.63554163	-2.84163470
H	-2.15188842	0.41142752	-1.74489689
H	-1.38616532	-1.48188676	-3.84092761
H	-2.58044600	-1.76093542	-2.54902748
H	4.55760212	0.47958269	-1.08138880
H	4.20200924	-1.42607460	-3.41181439
H	5.35000643	-1.58725658	-2.06136627
H	4.79692941	3.89496781	1.50953667

H	4.33327881	5.13786026	0.36290537
H	3.49304049	1.83012721	1.53296354
H	0.25437501	4.96645587	2.51914865
N	-0.09388915	2.44734867	0.17967459
H	0.36328880	3.30829762	0.47638576
C	-1.50609610	2.72320709	-0.04812159
H	-2.04246803	1.77786780	-0.16356174
H	-1.94912299	3.21525385	0.83254614
C	-1.77188727	3.60628702	-1.27777810
H	-1.33562135	3.12359467	-2.15912279
H	-1.24900678	4.56171726	-1.15726573
C	-3.27085123	3.86715040	-1.51140081
H	-3.70381913	4.35977441	-0.63336411
H	-3.77497026	2.89638796	-1.61184365
C	-3.54272908	4.69361379	-2.73585849
H	-3.19427207	4.27069114	-3.67777059
C	-4.14834567	5.87758402	-2.75025304
H	-4.51049671	6.34132736	-1.83717255
H	-4.30596435	6.42669018	-3.67183069
N	-4.73279801	0.05215755	-0.96839570
H	-5.22235558	0.93549716	-0.85250280
H	-5.25348695	-0.46794380	-1.66963766
C	-4.72309993	-0.68877766	0.30192271
H	-4.17624056	-1.62205481	0.14251974
H	-4.13285155	-0.10933161	1.02015753
C	-6.10178388	-0.99303592	0.90403262
H	-6.69767357	-1.55400812	0.17218531
H	-6.63309112	-0.04913258	1.07596077
C	-6.04018105	-1.78366701	2.22701334
H	-5.42394935	-1.24224985	2.95359390
H	-7.05248154	-1.82748098	2.64764588
C	-5.51895333	-3.18550891	2.06570154
H	-6.08592560	-3.82259537	1.38693056

C	-4.44836382	-3.68834977	2.67350600
H	-3.85011480	-3.09350438	3.35734918
H	-4.12933591	-4.71164087	2.51213288

MP2 Electronic Energy(Ha): 1740.444998455733

B3LYP Electronic Energy(Ha): 1744.973716318828

M06-L Electronic Energy(Ha): 1744.730088716376

Zero point energy correction(kcal/mol): 474.545

Enthalpy correction(kcal/mol): 504.138

Entropy correction(cal/mol): 274.310

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 466.139

Deuterated enthalpy correction(kcal/mol): 496.137

Deuterated entropy correction(cal/mol): 277.006

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	1.22881080	-0.64371337	0.88195842
C	-0.02931601	-2.78411425	1.23523149
C	1.33722738	-3.20316981	1.33604946
H	1.87710946	-3.77491596	0.59552144
C	-0.30084772	-2.08820944	2.44827213
H	-1.24073416	-1.61987201	2.70220466
C	0.86697449	-2.03824047	3.23944206
H	0.96358533	-1.56274292	4.20583923
C	1.88256798	-2.74295105	2.54917087
H	2.89480630	-2.91140119	2.89176230
B	-0.97508356	-2.85854775	-0.09696700
C	-1.99194120	-4.10706243	-0.20852375
C	-1.67774894	-1.37662762	-0.17184587
C	0.12062597	-2.73235094	-1.31043280
N	1.10975260	-1.90651037	-1.19533698
N	-1.02765658	-0.30624634	0.16296260
O	-2.93010155	-1.17131442	-0.61738157

O	0.09194122	-3.44717785	-2.44870897
C	2.00093262	-2.05539437	-2.35773818
C	1.20372488	-2.99971889	-3.27864683
C	-1.92677783	0.85831783	0.03969041
C	-3.13223694	0.26993793	-0.70895857
N	3.10137265	0.01266294	1.93346164
H	2.21165288	-1.09112526	-2.81836856
C	4.30097484	0.83739955	1.99640307
H	5.20133220	0.21704958	1.94377432
H	4.32936779	1.50195263	1.12864972
C	4.25511464	1.65336717	3.32462678
C	2.77117177	1.71894283	3.76583915
H	2.53898478	0.98162678	4.53955508
H	2.52679689	2.70008706	4.18756419
C	1.90509695	1.49410624	2.54870172
H	2.19864080	2.15067815	1.73348904
C	0.53797324	1.13284823	2.48727593
H	-0.07697192	1.74826296	1.84170664
C	-2.08969113	-5.06195929	0.81416154
H	-1.46618071	-4.95467082	1.69620369
C	-2.82056778	-4.29490058	-1.32835963
H	-2.78130669	-3.58229683	-2.14560601
C	-3.69662450	-5.37304844	-1.42302213
H	-4.32156225	-5.48655804	-2.30349421
C	-2.96410015	-6.14629092	0.73135107
H	-3.01227026	-6.86541021	1.54322279
C	-3.77285793	-6.30662682	-0.39004617
H	-4.45450281	-7.14796314	-0.46029170
H	-1.45858787	1.68804378	-0.49032746
H	-2.19991129	1.21242289	1.03954543
H	-3.14525827	0.53351171	-1.76944667
H	-4.09957346	0.50212797	-0.26565876
H	2.95598729	-2.48752720	-2.04062476

H	0.78228308	-2.49574030	-4.15116974
H	1.75498649	-3.88167044	-3.60319056
H	4.86309552	1.16967748	4.09336200
H	4.67001861	2.65426675	3.17917311
H	3.12819822	-0.59022622	2.75119646
H	0.05104432	0.76471673	3.38375585
N	1.82992362	0.84011179	-0.50790735
H	2.57097947	1.46373096	-0.20392902
C	1.28091506	1.33239543	-1.76361892
H	0.67703836	0.53832466	-2.21628399
H	0.58784132	2.17527519	-1.60332076
C	2.35380837	1.79191506	-2.76306590
H	3.06439156	0.97528833	-2.93562341
H	2.93441243	2.60944344	-2.31661578
C	1.76873791	2.26977461	-4.10431833
H	1.06126461	3.08803731	-3.93076762
H	1.18993213	1.44672886	-4.54578992
C	2.81970844	2.71132816	-5.08297052
H	3.55326831	1.95534275	-5.36187068
C	2.92373027	3.92882930	-5.60765533
H	2.21711051	4.71600955	-5.36066702
H	3.71355051	4.18400571	-6.30524128
N	-1.21258094	4.39778074	-0.86525160
H	-0.24451648	4.60916278	-0.64001017
H	-1.37426437	4.75889793	-1.80116845
C	-2.11371140	5.04880458	0.09429767
H	-3.14050255	4.79923042	-0.18774897
H	-1.94660925	4.58883424	1.07462867
C	-1.96709930	6.57209897	0.21958778
H	-2.11665187	7.03099518	-0.76641301
H	-0.93780573	6.80737310	0.51627224
C	-2.93866133	7.20820677	1.23460876
H	-2.81982525	6.72754774	2.21219039

H -2.65632056 8.25991989 1.36764544

C -4.38029938 7.14490927 0.81052220

H -4.61240087 7.62804409 -0.13855519

C -5.36364661 6.56347499 1.49135180

H -5.18293755 6.07008869 2.44184779

H -6.38533624 6.56408637 1.12851168

MP2 Electronic Energy(Ha): 1740.413353727074

B3LYP Electronic Energy(Ha): 1744.921904154265

M06-L Electronic Energy(Ha): 1744.691465629990

Zero point energy correction(kcal/mol): 473.984

Enthalpy correction(kcal/mol): 498.674

Entropy correction(cal/mol): 231.143

Imaginary Frequencies: -375.16 -37.02 -36.03 -34.31 -32.80 -22.20 -18.69

Deuterated zero point energy correction(kcal/mol): 465.495

Deuterated enthalpy correction(kcal/mol): 490.564

Deuterated entropy correction(cal/mol): 233.620

Deuterated imaginary Frequencies: -371.39 -36.98 -35.94 -33.57 -32.51 -21.89 -18.63

Product geometry

Zr -0.19275703 2.17335326 0.34873865

C 2.27817599 1.99791239 -0.08301749

C 1.80494407 3.01514658 -0.97501998

H 1.70537622 2.91934236 -2.04635397

C 2.27152580 2.59427003 1.20967966

H 2.54163566 2.09301269 2.12812843

C 1.75098984 3.89912640 1.12882227

H 1.61830190 4.58074280 1.95831295

C 1.45843993 4.16602041 -0.23623892

H 1.08183193 5.09534319 -0.64203248

B 2.48056207 0.40996162 -0.41761876

C 3.99462592 -0.11247713 -0.61700851

C 1.61866681 -0.36449277 0.74367463

C 1.48661409 0.19739369 -1.70361517

N	0.28373087	0.67008111	-1.68547987
N	0.50305834	0.12535791	1.19775552
O	1.93832597	-1.57716202	1.20912721
O	1.87890893	-0.37401093	-2.86029080
C	-0.28779100	0.53364310	-3.03846302
C	0.73401508	-0.36551087	-3.75736050
C	-0.13643957	-0.86410290	2.08520713
C	0.92844111	-1.96943858	2.19466460
N	-1.44620713	4.22954811	1.08898294
H	-1.28324547	0.09193379	-3.01218760
C	-2.49372598	5.24099019	0.83341812
H	-2.08891500	6.07549793	0.25890960
H	-3.28746832	4.78378507	0.23786363
C	-3.01606677	5.65603258	2.24944584
C	-2.37638979	4.63657769	3.23475313
H	-1.50778072	5.06893119	3.74275074
H	-3.07376471	4.30037923	4.00456714
C	-1.92225481	3.49221089	2.31037267
H	-2.82424298	2.95747945	1.99151744
C	-0.85121813	2.46512592	2.62264473
H	-1.27569761	1.58417344	3.10669288
C	5.09046124	0.75334818	-0.48775744
H	4.91215681	1.79683672	-0.24781289
C	4.28414496	-1.45156964	-0.93181871
H	3.46941649	-2.15997765	-1.04132507
C	5.59008384	-1.90171961	-1.10642333
H	5.77594673	-2.94340669	-1.34975957
C	6.40398325	0.31469833	-0.66002649
H	7.22648398	1.01499302	-0.55215727
C	6.65988566	-1.01762499	-0.97053133
H	7.67902926	-1.36456971	-1.10611161
H	-1.06687671	-1.22249061	1.63420236
H	-0.37988776	-0.41616310	3.04897530

H	0.57410640	-2.96485429	1.92598068
H	1.42300571	-1.99192408	3.16795761
H	-0.37774149	1.52183989	-3.50342044
H	0.38998774	-1.39703660	-3.86862281
H	1.06614435	0.00933267	-4.72499412
H	-2.73181664	6.68254634	2.48967717
H	-4.10665143	5.61002406	2.28187271
H	-0.61922482	4.74164047	1.38945592
H	-0.06798402	2.86870470	3.27223888
N	-2.14955370	1.71927126	-0.28959103
H	-2.83178133	2.42534498	-0.02717913
C	-2.86597245	0.53571279	-0.74298683
H	-2.13579398	-0.21613284	-1.05610681
H	-3.42929320	0.07751733	0.08789046
C	-3.85550319	0.81102180	-1.88572483
H	-3.31659772	1.26011288	-2.72732281
H	-4.58454223	1.56083337	-1.55480737
C	-4.60927949	-0.44786688	-2.35083054
H	-5.15437299	-0.88632655	-1.50774747
H	-3.87390573	-1.19934469	-2.67105290
C	-5.56163555	-0.18000666	-3.48176086
H	-5.11329291	0.20726644	-4.39630980
C	-6.87825658	-0.36200588	-3.44046178
H	-7.37116314	-0.74374836	-2.55101445
H	-7.51165644	-0.13953427	-4.29188353
N	0.16059189	-5.06367815	0.77330584
H	0.13603412	-4.76528701	-0.19782564
H	1.10564426	-5.39626185	0.94377820
C	-0.81056280	-6.14007148	1.00610052
H	-0.75144747	-6.42203199	2.06100030
H	-1.81314682	-5.72343539	0.85836585
C	-0.64407444	-7.38619995	0.12480954
H	0.36610703	-7.79253032	0.26356424

H -0.71433880 -7.08911350 -0.92847463

C -1.68400251 -8.49017121 0.40419993

H -2.69560640 -8.08245158 0.29758488

H -1.57710997 -9.26461979 -0.36549960

C -1.53578481 -9.13030668 1.75705028

H -0.56874200 -9.59270072 1.95450673

C -2.47248108 -9.17550710 2.69992141

H -3.45144598 -8.72952444 2.55067111

H -2.29877549 -9.66371617 3.65226711

MP2 Electronic Energy(Ha): 1740.437185884256

B3LYP Electronic Energy(Ha): 1744.947893602483

M06-L Electronic Energy(Ha): 1744.712725949649

Zero point energy correction(kcal/mol): 477.003

Enthalpy correction(kcal/mol): 505.462

Entropy correction(cal/mol): 262.333

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.360

Deuterated enthalpy correction(kcal/mol): 497.187

Deuterated entropy correction(cal/mol): 264.760

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction C2-S

Reactant geometry

Zr 1.19763028 -0.97906482 0.01478324

C 1.72616843 1.45765956 -0.24037355

C 2.60899310 0.98142182 0.78888948

H 2.52251543 1.20358480 1.84314627

C 2.23521317 0.91338402 -1.44636036

H 1.80427956 1.05043525 -2.42783463

C 3.36914971 0.10094146 -1.16450193

H 3.96671655 -0.43421045 -1.89040311

C 3.61418455 0.16879255 0.22082285

H	4.39643339	-0.34709819	0.75792092
B	0.25433185	2.13795004	-0.01858463
C	0.19923781	3.75427753	0.00280974
C	-0.69091530	1.44231678	-1.17526920
C	-0.28946413	1.43643725	1.36862694
N	-0.08523980	0.17880310	1.62347448
N	-0.63483632	0.18271637	-1.46367989
O	-1.54104498	2.17767440	-1.92888800
O	-0.93422639	2.11244861	2.33400033
C	-0.55709735	-0.12445524	2.98557346
C	-1.27143344	1.17705887	3.39689416
C	-1.47973798	-0.05999572	-2.64731207
C	-2.23678680	1.26857545	-2.82157931
N	-0.84263365	-2.44634158	0.33372801
N	1.98332441	-2.41342228	0.98950324
C	2.89062487	-3.45919881	1.30579212
H	2.91058044	-3.66335964	2.38695349
H	-1.22847362	-0.98707982	2.99456839
H	-0.84660489	-0.29464041	-3.51080102
C	-2.27322216	-2.08107007	0.33429000
H	-2.36734490	-1.11321980	0.83157848
H	-2.58005881	-1.92374601	-0.69974123
C	-3.18641869	-3.11516926	1.00047046
C	2.51150059	-4.77202215	0.57230651
C	1.94295908	-4.52207307	-0.85291792
H	0.86624526	-4.71648641	-0.88120687
H	3.93002462	-3.18923000	1.03790530
C	2.20990674	-3.16314378	-1.43944430
C	1.35745191	-2.46088759	-2.23349048
H	2.38428731	-5.25154812	-1.54484868
H	-0.52750864	-2.72170678	1.26275860
C	-1.00064904	4.46199044	0.19027566
H	-1.92809251	3.91370662	0.32083733

C	1.36146842	4.52131872	-0.16403269
H	2.30900475	4.01345731	-0.31291904
C	-1.04024124	5.85356122	0.21095135
H	-1.98602663	6.36623908	0.35759732
C	1.33531457	5.91653878	-0.14576155
H	2.25601677	6.47618252	-0.27884437
C	0.13197465	6.58994432	0.04259338
H	0.10534183	7.67464055	0.05784890
C	-4.67631958	-2.71794208	0.97679851
H	-4.80592379	-1.73472534	1.44241695
H	-5.22980557	-3.43292757	1.59763280
C	-5.27623158	-2.70918646	-0.40258798
H	-5.22901799	-3.65508423	-0.94200274
C	-5.85311724	-1.66382431	-0.98893102
H	-5.93057844	-0.70242297	-0.48977909
H	-6.28097841	-1.73367304	-1.98265265
H	-0.92256794	1.60036417	4.33808371
H	0.29648730	-0.36310995	3.62670363
H	-2.35919156	1.08389713	3.42423505
H	-3.27925575	1.21146349	-2.49792842
H	-2.19448049	1.68354355	-3.82821960
H	-2.15469190	-0.90550466	-2.49665313
H	3.38534653	-5.43081209	0.52528582
H	1.75289526	-5.30493469	1.15319608
H	-3.06186292	-4.08668513	0.50525148
H	-2.87261329	-3.25821122	2.04129377
H	-0.69712784	-3.27580297	-0.23624527
H	3.24011300	-2.82434343	-1.37817563
H	0.35455780	-2.82397722	-2.43616545
H	1.70727997	-1.63490638	-2.83847305

MP2 Electronic Energy(Ha): 1489.145184129850

B3LYP Electronic Energy(Ha): 1492.972141430490

M06-L Electronic Energy(Ha): 1492.794690725459

Zero point energy correction(kcal/mol): 377.548

Enthalpy correction(kcal/mol): 400.897

Entropy correction(cal/mol): 223.965

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 373.508

Deuterated enthalpy correction(kcal/mol): 397.053

Deuterated entropy correction(cal/mol): 225.093

Deuterated imaginary Frequencies: -0.00

Transition State geometry

Zr	-1.18390322	0.98117361	-0.10549057
C	-1.72167107	-1.45626090	-0.26537261
C	-2.61859039	-0.93934417	0.72989509
H	-2.54918545	-1.12296326	1.79286558
C	-2.20538730	-0.94944016	-1.50035248
H	-1.75555187	-1.11707871	-2.46829903
C	-3.33116161	-0.11658507	-1.26780645
H	-3.90137541	0.41009672	-2.02071784
C	-3.60110259	-0.13338748	0.11675658
H	-4.38692360	0.40965644	0.62097068
B	-0.26263139	-2.15144708	0.00116755
C	-0.22345545	-3.76623171	0.05075047
C	0.69786495	-1.47781381	-1.15313587
C	0.26213291	-1.42461678	1.37994208
N	0.08014089	-0.15705778	1.59265827
N	0.65644388	-0.21468596	-1.42815979
O	1.51789241	-2.21866879	-1.93111456
O	0.87144197	-2.08869632	2.37802516
C	0.53713604	0.17551981	2.95331084
C	1.20493037	-1.13218519	3.42157333
C	1.47013738	0.02661477	-2.63283383
C	2.20880150	-1.30908451	-2.82960864
N	0.85460164	2.42909537	0.31510886

N	-2.01304706	2.50451206	0.79581233
C	-2.84411824	3.53000505	1.33043071
H	-2.74927398	3.56161930	2.42294277
H	1.23513117	1.01719030	2.94802590
H	0.81340148	0.27157712	-3.47491513
C	2.28105562	2.04704265	0.31145613
H	2.36477919	1.07246721	0.79691523
H	2.58429905	1.89910868	-0.72469578
C	3.20634804	3.06418295	0.98697162
C	-2.43183926	4.88919347	0.70879262
C	-1.88253949	4.59873172	-0.70926241
H	-0.80582829	4.78612388	-0.76366682
H	-3.91398364	3.34395757	1.12023859
C	-2.16811706	3.17547718	-1.13847414
C	-1.35008341	2.44146086	-2.03842049
H	-2.33912851	5.26385621	-1.45186001
H	0.55567868	2.71546392	1.24531546
C	0.97041146	-4.47914417	0.25553179
H	1.90146586	-3.93534873	0.38071174
C	-1.39065957	-4.52719713	-0.10829626
H	-2.33363582	-4.01508473	-0.27123389
C	0.99967749	-5.87040653	0.30031993
H	1.94097525	-6.38752177	0.45951748
C	-1.37493365	-5.92200692	-0.06568565
H	-2.29902096	-6.47722832	-0.19358907
C	-0.17735392	-6.60079132	0.13960526
H	-0.15882944	-7.68521600	0.17330882
C	4.69091267	2.64749697	0.96182779
H	4.80737040	1.66085088	1.42363842
H	5.25375360	3.35280664	1.58534151
C	5.29059362	2.63552724	-0.41764453
H	5.25449129	3.58319152	-0.95473681
C	5.85472292	1.58465618	-1.00649779

H	5.92031162	0.62117140	-0.50965584
H	6.28307999	1.65158722	-2.00018347
H	0.81910091	-1.51689740	4.36503953
H	-0.31849203	0.45901412	3.57394062
H	2.29356186	-1.06619147	3.47738866
H	3.25686510	-1.26624176	-2.52238153
H	2.14498190	-1.71695483	-3.83789049
H	2.15707571	0.86458386	-2.49825771
H	-3.28021951	5.57946376	0.68105108
H	-1.65596126	5.36261950	1.31668856
H	3.09476139	4.04112858	0.49958587
H	2.89410509	3.20292733	2.02907776
H	0.71720194	3.25483222	-0.26167898
H	-3.23174426	2.95485943	-1.19079083
H	-0.39308351	2.87146961	-2.32475772
H	-1.83479071	1.86279167	-2.81532911

MP2 Electronic Energy(Ha): 1489.145066320835

B3LYP Electronic Energy(Ha): 1492.968523051414

M06-L Electronic Energy(Ha): 1492.789594785566

Zero point energy correction(kcal/mol): 377.540

Enthalpy correction(kcal/mol): 400.242

Entropy correction(cal/mol): 218.954

Imaginary Frequencies: -262.31

Deuterated zero point energy correction(kcal/mol): 372.921

Deuterated enthalpy correction(kcal/mol): 396.040

Deuterated entropy correction(cal/mol): 223.095

Deuterated imaginary Frequencies: -186.42

Product geometry

Zr	1.10939546	-0.99113209	-0.19498354
C	1.80201780	1.38454678	-0.25357430
C	2.65645397	0.78044323	0.72687143
H	2.58870900	0.93104593	1.79521575

C	2.26734766	0.88811923	-1.50439372
H	1.83736103	1.11486644	-2.46913783
C	3.32110321	-0.03303313	-1.29588202
H	3.84984611	-0.58277972	-2.06070654
C	3.57435852	-0.08564186	0.09520145
H	4.31821184	-0.69753656	0.58397127
B	0.37165266	2.14080549	0.01836072
C	0.39661893	3.75479006	0.06939615
C	-0.61176635	1.50908395	-1.14518709
C	-0.18586135	1.43086332	1.39674968
N	-0.06512419	0.15522723	1.60881000
N	-0.57416695	0.25155084	-1.45909145
O	-1.45239650	2.26055173	-1.88064553
O	-0.76441954	2.12362200	2.39284206
C	-0.54179588	-0.15402372	2.96922150
C	-1.14432423	1.18525737	3.43739941
C	-1.40561714	0.03657146	-2.65605194
C	-2.16124216	1.36981437	-2.78952980
N	-0.99196920	-2.33608568	0.23592356
N	1.89938411	-2.78469835	0.50953071
C	2.57249985	-3.68444369	1.41472854
H	2.23173904	-3.55050109	2.44587984
H	-1.27805335	-0.96207525	2.96237095
H	-0.75862558	-0.17222016	-3.51400624
C	-2.39218014	-1.87465114	0.32251119
H	-2.41892920	-1.00191016	0.97827909
H	-2.68909690	-1.52107964	-0.66422367
C	-3.37658177	-2.93982650	0.81557851
C	2.27556588	-5.11819338	0.86455923
C	1.79615917	-4.88501281	-0.59287188
H	0.72057278	-5.06829647	-0.68599311
H	3.66496094	-3.51620552	1.41314044
C	2.09126699	-3.38993985	-0.85019131

C	1.27655210	-2.58391144	-1.87613065
H	2.30085944	-5.53052082	-1.31714776
H	-0.70321870	-2.78606540	1.10211036
C	-0.76911249	4.51457240	0.26726598
H	-1.72208721	4.00881205	0.38581743
C	1.59492527	4.46747499	-0.08140972
H	2.51768778	3.91810261	-0.23860716
C	-0.74207045	5.90579872	0.31338207
H	-1.66253120	6.46047253	0.46717001
C	1.63526153	5.86164381	-0.03712571
H	2.58172714	6.37917915	-0.15830760
C	0.46465673	6.58784165	0.16116750
H	0.48979722	7.67200648	0.19601614
C	-4.83363440	-2.43849355	0.87908657
H	-4.89235802	-1.54522619	1.51086485
H	-5.43815182	-3.20961568	1.37185396
C	-5.42997896	-2.14512078	-0.47039409
H	-5.45111120	-2.98261657	-1.16744486
C	-5.92930168	-0.97444310	-0.85748300
H	-5.93747754	-0.11246196	-0.19689553
H	-6.36109241	-0.83820317	-1.84257246
H	-0.73885657	1.55080444	4.38012044
H	0.29723631	-0.47695281	3.59360806
H	-2.23471767	1.17398464	3.49386832
H	-3.19872388	1.30859179	-2.45236733
H	-2.12829930	1.81104617	-3.78468911
H	-2.07694445	-0.81560559	-2.53726037
H	3.16754746	-5.74824615	0.90633900
H	1.50437360	-5.61294532	1.46049770
H	-3.32218332	-3.81838304	0.16067867
H	-3.07388963	-3.28022909	1.81310748
H	-0.90833243	-3.06313282	-0.47009921
H	3.16231598	-3.30783406	-1.11116723

H 0.34468135 -3.09291843 -2.15069125

H 1.83270983 -2.38996091 -2.79320025

MP2 Electronic Energy(Ha): 1489.156065077347

B3LYP Electronic Energy(Ha): 1492.983715239100

M06-L Electronic Energy(Ha): 1492.801620081460

Zero point energy correction(kcal/mol): 378.330

Enthalpy correction(kcal/mol): 401.163

Entropy correction(cal/mol): 221.121

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 374.320

Deuterated enthalpy correction(kcal/mol): 397.350

Deuterated entropy correction(cal/mol): 222.248

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H3-S

Reactant geometry

Zr -0.66894648 0.39310324 -0.90948339

C 0.11454176 2.72977445 -1.11334302

C 0.99508187 1.97937903 -1.95593690

H 2.02976753 1.75900247 -1.73617976

C -1.13743285 2.74599891 -1.79784873

H -2.04278974 3.21406996 -1.43786382

C -1.04654798 1.96855676 -2.97508759

H -1.83322347 1.80287143 -3.69522309

C 0.28653090 1.49214592 -3.07535184

H 0.68556184 0.88666438 -3.87540401

B 0.37665784 3.12900163 0.45559860

C 0.94743300 4.60860848 0.74775338

C -1.05480639 2.76794313 1.18869436

C 1.28513851 1.89491889 1.04740938

N 1.07023250 0.66811838 0.68189605

N -1.65421062 1.63806380 0.97205547

O	-1.69382146	3.61539373	2.01153710
O	2.22395065	2.05555889	1.99073694
C	2.00398425	-0.22286209	1.40231262
C	2.65620607	0.72843008	2.41993423
C	-2.95683018	1.65408833	1.66407052
C	-2.88218470	2.93742989	2.51132142
N	0.28863727	-1.42943970	-1.39254176
N	-2.60652220	-0.42577301	-1.17167973
C	-3.59218937	-0.22505885	-2.23916547
H	-3.12726078	0.13241099	-3.15619943
H	1.48377752	-1.06059941	1.86791935
H	-3.76602644	1.68072671	0.92856895
C	1.64648282	-1.80167166	-1.77481650
H	2.30151980	-0.93316193	-1.64118623
H	2.05061612	-2.58544351	-1.11588172
C	1.76546260	-2.29045402	-3.22549238
C	-4.28868758	-1.59490306	-2.43222845
C	-4.06852196	-2.31711760	-1.08248033
H	-3.44481924	-3.20629850	-1.21302424
H	-4.34267181	0.52546281	-1.93637393
C	-3.32206116	-1.28025160	-0.20716347
C	-2.44292873	-1.91745916	0.86474492
H	-5.00191126	-2.63970494	-0.61343505
H	-4.08984094	-0.66925299	0.30178775
C	1.23094184	5.49925762	-0.29796917
H	1.05827935	5.18309652	-1.32193070
C	1.18816028	5.07069939	2.05324691
H	0.98599214	4.41784598	2.89596461
C	1.72782019	6.78155155	-0.06169534
H	1.93533903	7.44329285	-0.89672645
C	1.68361639	6.34783020	2.30179768
H	1.85750300	6.67123618	3.32334095
C	1.95663958	7.21182056	1.24191945

H	2.34272620	8.20780307	1.43198837
C	3.20138759	-2.66553460	-3.64271348
H	3.86654369	-1.80584847	-3.50318005
H	3.19755425	-2.88385989	-4.71833943
C	3.75757294	-3.85853504	-2.91559109
H	3.16489148	-4.77057872	-2.98819231
C	4.89295680	-3.88641670	-2.22273226
H	5.52037479	-3.00531921	-2.12445017
H	5.24221072	-4.79097254	-1.73733729
H	3.74527306	0.71538061	2.41689852
H	2.73216634	-0.63606788	0.69869581
H	2.29388749	0.58149840	3.43961280
H	-2.72814442	2.74258964	3.57478800
H	-3.72955630	3.61043750	2.38620650
H	-3.08997499	0.75977636	2.27550235
H	-5.34644153	-1.47647678	-2.67948941
H	-3.82305571	-2.14907189	-3.25014267
H	1.10951888	-3.16044536	-3.36291528
H	1.38583290	-1.51169318	-3.89421588
H	-0.36128415	-2.15594926	-1.67792199
N	1.02578046	-3.50749181	1.53466529
H	1.99609915	-3.69200450	1.29476901
C	0.33333311	-4.77273774	1.81708524
H	0.61857590	-3.03870129	0.72859008
H	-0.72767247	-4.54644859	1.96821603
H	0.38617672	-5.49486198	0.98889817
C	0.88895157	-5.41612948	3.08752091
H	0.82141059	-4.68719220	3.90077512
H	1.95796039	-5.62583225	2.94811755
C	0.16815927	-6.71473674	3.49622081
H	0.55113320	-7.02047066	4.47808794
H	-0.90227056	-6.52024801	3.62762080
C	0.36094757	-7.85180652	2.53083048

H	1.39640986	-8.12815935	2.33159187
C	-0.61056373	-8.53117384	1.92809824
H	-1.65734017	-8.29419701	2.09448501
H	-0.39752584	-9.35103396	1.25132221
H	-1.71418440	-2.59583594	0.41669511
H	-1.89823117	-1.17494437	1.45626718
H	-3.05832775	-2.49410031	1.56121882

MP2 Electronic Energy(Ha): 1740.474353633673

B3LYP Electronic Energy(Ha): 1744.983179876966

M06-L Electronic Energy(Ha): 1744.750462011633

Zero point energy correction(kcal/mol): 475.328

Enthalpy correction(kcal/mol): 503.590

Entropy correction(cal/mol): 271.542

Imaginary Frequencies: -12.17 -9.42

Deuterated zero point energy correction(kcal/mol): 466.577

Deuterated enthalpy correction(kcal/mol): 494.758

Deuterated entropy correction(cal/mol): 268.413

Deuterated imaginary Frequencies: -13.06 -11.66 -2.86

Transition State geometry

Zr	-1.05689469	-0.38398583	-0.17120915
C	-1.24712493	-2.82037940	0.18498832
C	-1.99471207	-2.21186370	1.24580705
H	-1.69177258	-2.17273346	2.28240615
C	-2.03447386	-2.62398095	-0.98577313
H	-1.75740760	-2.93330222	-1.98387727
C	-3.17388550	-1.84688417	-0.67471457
H	-3.94013416	-1.52881318	-1.36630697
C	-3.15523312	-1.59553334	0.72372794
H	-3.90661086	-1.05944999	1.28424144
B	0.34341470	-3.22616660	0.22175161
C	0.69494948	-4.78195755	0.45978757
C	0.96315010	-2.57749510	-1.16855888

C	0.99887061	-2.17950489	1.31264788
N	0.62756250	-0.93500149	1.33301020
N	0.64855190	-1.38775504	-1.59060727
O	1.86113336	-3.23468978	-1.91623088
O	1.95333706	-2.50223532	2.19240303
C	1.34222705	-0.22473184	2.41285611
C	2.37273326	-1.27335893	2.86777452
C	1.37800732	-1.12040180	-2.84643958
C	2.28546747	-2.35578431	-2.99650822
N	-1.34946283	1.39927420	0.60382628
N	-1.64857363	1.12176308	-1.92077775
C	-3.04063196	1.18387685	-2.37788534
H	-3.72762484	1.12635513	-1.52808407
H	1.79732657	0.69669589	2.04564258
H	0.67349645	-1.01854042	-3.67551938
C	-1.72280498	2.46057214	1.50561164
H	-1.05437116	2.46267780	2.38142226
H	-1.59437922	3.44509112	1.03034384
C	-3.16856848	2.35016278	2.01853938
C	-3.13681627	2.51579867	-3.13480257
C	-1.77239164	2.59968159	-3.84345406
H	-1.39441707	3.62399775	-3.89050640
H	-3.29038906	0.35027757	-3.05575920
C	-0.82346886	1.67347826	-3.01282590
C	0.41059543	2.40942939	-2.48815673
H	-1.84660023	2.23715118	-4.87224852
H	-0.48205774	0.86490495	-3.67625587
C	-0.32002388	-5.74083519	0.59280323
H	-1.35631220	-5.42334346	0.53381389
C	2.01854129	-5.24697776	0.54691050
H	2.83887384	-4.54327211	0.45290898
C	-0.03749525	-7.09139358	0.79993740
H	-0.84969507	-7.80470126	0.89837248

C	2.31300721	-6.59192558	0.75377084
H	3.34719892	-6.91567158	0.81644318
C	1.28303673	-7.52316814	0.88116498
H	1.50911475	-8.57193883	1.04263386
C	-3.56347960	3.45805269	3.01450537
H	-2.87686290	3.45389659	3.86889782
H	-4.55752158	3.21825712	3.41384487
C	-3.61002518	4.83462301	2.41155872
H	-4.26460701	4.94673442	1.54719676
C	-2.93950041	5.89710019	2.84855762
H	-2.27663675	5.83661617	3.70691722
H	-3.03202318	6.86595477	2.37062587
H	2.37791196	-1.47022168	3.93880703
H	0.63435624	0.03527702	3.20633796
H	3.38786335	-1.05071466	2.53312390
H	3.34476503	-2.13879921	-2.84826783
H	2.15510004	-2.89341900	-3.93523967
H	1.94620329	-0.19144362	-2.77531336
H	-3.98129785	2.55731492	-3.82763405
H	-3.25044271	3.33431795	-2.41836050
H	-3.85168459	2.36351588	1.16097491
H	-3.29132788	1.37409697	2.49883029
H	-1.52387943	1.62833810	-0.66451661
N	1.92789197	2.96411260	1.18114779
H	1.59122704	3.44084101	2.01348793
C	2.72059777	3.89488990	0.36430059
H	1.09637312	2.65708755	0.68162592
H	2.99310715	3.37848204	-0.56252156
H	2.16468276	4.79657478	0.06920682
C	3.99652327	4.30357088	1.09998989
H	4.54170488	3.39666494	1.37917496
H	3.72672252	4.80381551	2.03978389
C	4.91928149	5.22775684	0.28283180

H	5.85271820	5.35770329	0.84501075
H	5.19085052	4.74177153	-0.66110362
C	4.33470713	6.58493892	0.00272013
H	4.03015127	7.15558997	0.88008844
C	4.17602131	7.12747610	-1.20102926
H	4.46410548	6.59879842	-2.10497523
H	3.75749872	8.11951463	-1.32839695
H	0.11385032	3.28027936	-1.89630393
H	1.02788461	1.76768086	-1.85335571
H	1.03364424	2.75761147	-3.31744040

MP2 Electronic Energy(Ha): 1740.430539616951

B3LYP Electronic Energy(Ha): 1744.937736960209

M06-L Electronic Energy(Ha): 1744.698595789203

Zero point energy correction(kcal/mol): 472.901

Enthalpy correction(kcal/mol): 501.697

Entropy correction(cal/mol): 271.633

Imaginary Frequencies: -1595.65

Deuterated zero point energy correction(kcal/mol): 464.983

Deuterated enthalpy correction(kcal/mol): 494.188

Deuterated entropy correction(cal/mol): 275.576

Deuterated imaginary Frequencies: -1149.28

Product geometry

Zr	-0.95680972	-0.10647335	-0.37950202
C	-1.32738319	-2.57297003	-0.45118793
C	-2.46664427	-2.02167092	0.22758626
H	-2.67048023	-2.10991465	1.28484225
C	-1.49403472	-2.21074823	-1.81368224
H	-0.79828279	-2.44574458	-2.60692040
C	-2.65088036	-1.39981637	-1.95827272
H	-3.04121882	-0.98800328	-2.87924957
C	-3.26487160	-1.29625359	-0.68517356
H	-4.18508303	-0.77693321	-0.46228538

B	0.06038304	-3.08482714	0.25782966
C	0.25431646	-4.68077498	0.40815406
C	1.30026002	-2.31379992	-0.53046525
C	0.12661939	-2.22406754	1.66426634
N	-0.16918711	-0.96330820	1.66409066
N	1.25968819	-1.06419758	-0.88959578
O	2.48995794	-2.91944437	-0.70369395
O	0.50281322	-2.72475582	2.85138273
C	-0.06966384	-0.43395739	3.03687535
C	0.55876377	-1.61395102	3.80113245
C	2.61517390	-0.64857666	-1.29775760
C	3.38632286	-1.97832330	-1.35301485
N	-1.54983232	1.51753097	0.38242360
N	-0.47758936	1.05898076	-2.51849322
C	-0.15275563	0.30391371	-3.76377617
H	-1.04307902	-0.20542135	-4.13049495
H	0.54103658	0.47015187	3.05613241
H	2.60528627	-0.13507713	-2.26119903
C	-2.28242127	2.56606598	1.02894288
H	-2.03245206	2.60553256	2.10428572
H	-2.00001646	3.55655336	0.63314514
C	-3.80899386	2.41893383	0.90907766
C	0.41859075	1.34458119	-4.72781579
C	1.25603060	2.23023565	-3.79348919
H	1.39218788	3.24367549	-4.17555472
H	0.59021283	-0.45882620	-3.52251108
C	0.48541389	2.22986136	-2.44464494
C	-0.26447990	3.52816225	-2.16648382
H	2.25194592	1.79775583	-3.66338775
H	1.17440147	2.04138183	-1.61911628
C	-0.67108320	-5.57633716	-0.14838749
H	-1.53072626	-5.18127408	-0.68036403
C	1.34385210	-5.24601253	1.09364648

H	2.08368504	-4.59527908	1.54704390
C	-0.52224064	-6.95910567	-0.03501487
H	-1.26005813	-7.62042954	-0.47859399
C	1.50268065	-6.62398903	1.21461443
H	2.35594762	-7.02464212	1.75315649
C	0.56804124	-7.48986283	0.64804884
H	0.68844713	-8.56420119	0.74124294
C	-4.60547929	3.52758329	1.62492701
H	-4.32436809	3.56531135	2.68368038
H	-5.66930432	3.25753287	1.59544120
C	-4.44372035	4.89061392	1.01161524
H	-4.69216927	4.96021558	-0.04769011
C	-4.04322443	5.98848605	1.64736144
H	-3.78525275	5.97122235	2.70227845
H	-3.96298187	6.94392356	1.14075982
H	0.01580596	-1.91555055	4.69602251
H	-1.06974224	-0.18126619	3.40314608
H	1.60965464	-1.45258003	4.05090292
H	4.32809522	-1.97622133	-0.80553658
H	3.56054177	-2.33277867	-2.37160809
H	3.02773562	0.04276279	-0.55471556
H	1.00305916	0.89897060	-5.53529973
H	-0.39251223	1.92041215	-5.18510048
H	-4.07739626	2.39708248	-0.15417370
H	-4.09521001	1.44584064	1.32057893
H	-1.40420364	1.46318571	-2.64222355
N	1.16520510	2.69338295	2.09379619
H	0.69200570	3.34448298	2.71450949
C	2.23470388	3.38952153	1.36993749
H	0.45297290	2.34737389	1.44921636
H	2.68068039	2.67789282	0.66416726
H	1.87822211	4.24166260	0.77111986
C	3.31953296	3.87074688	2.33351122

H	3.65454000	3.01726296	2.93079632
H	2.87966347	4.58779139	3.03945268
C	4.53138245	4.52180088	1.64088655
H	5.28733963	4.73264343	2.40805673
H	4.98841458	3.81038848	0.94345218
C	4.21249590	5.80189350	0.91886808
H	3.73304841	6.57398273	1.52061884
C	4.47737020	6.05869206	-0.35908590
H	4.95743153	5.32330688	-0.99836298
H	4.23380414	7.01369893	-0.81103919
H	-0.91054256	3.79604997	-3.01008841
H	-0.87533313	3.42406512	-1.26935244
H	0.44251322	4.34672947	-2.01250525

MP2 Electronic Energy(Ha): 1740.470183037761

B3LYP Electronic Energy(Ha): 1744.971029553140

M06-L Electronic Energy(Ha): 1744.738175355309

Zero point energy correction(kcal/mol): 477.216

Enthalpy correction(kcal/mol): 505.748

Entropy correction(cal/mol): 262.781

Imaginary Frequencies: -0.00

Deuterated zero point energy correction(kcal/mol): 468.191

Deuterated enthalpy correction(kcal/mol): 497.143

Deuterated entropy correction(cal/mol): 266.353

Deuterated imaginary Frequencies: -0.00

Equatorial Reaction H6-S

Reactant geometry

Zr	0.35093357	-1.85729363	-0.59769935
C	-2.04144734	-1.16683626	-0.57044947
C	-1.82183653	-1.70605549	-1.86837053
H	-1.83532002	-1.13508759	-2.78373871
C	-1.93932063	-2.28001509	0.32572397

H	-2.05053177	-2.22682910	1.39985004
C	-1.65986067	-3.45660969	-0.40767472
H	-1.54796767	-4.44955413	-0.00012997
C	-1.56542411	-3.09909450	-1.77368291
H	-1.35633713	-3.76841070	-2.59586358
B	-2.16540538	0.39652174	-0.11734410
C	-3.58437728	0.77543996	0.59531004
C	-0.89222461	0.62492312	0.88982698
C	-1.91533921	1.36659957	-1.40098508
N	-0.93368656	2.16444823	-1.62522929
N	0.15700309	-0.15887411	0.91336929
O	-0.85089127	1.62298660	1.77225262
O	-2.88136861	1.31525915	-2.37240714
C	-1.16746491	2.82466644	-2.92545139
C	-2.54393374	2.29770103	-3.37980956
C	1.04091760	0.25259288	2.02713002
C	0.44509676	1.60148125	2.44543983
N	1.41143865	-3.46292710	0.18394163
N	2.62743497	-0.82578143	-0.90211702
C	3.60484053	0.21634226	-0.50622693
H	4.28741557	-0.16295345	0.25641708
H	-1.15519566	3.91155619	-2.80467978
H	0.99266436	-0.49826707	2.82241249
C	1.30505557	-4.86566733	0.57595240
H	0.44490943	-5.30772895	0.06644599
H	2.18137117	-5.42500397	0.22434426
C	1.15140923	-5.07118900	2.09048633
C	4.32147342	0.63204651	-1.82675079
C	3.41312808	0.09118996	-2.96731977
H	3.87063442	-0.77296306	-3.45905576
H	3.05476364	1.06279283	-0.09126689
C	2.12664488	-0.35741478	-2.24366642
H	1.53008757	0.54076330	-2.03018948

H	3.21106582	0.83715139	-3.73815804
C	1.21002253	-1.45634923	-2.73727902
H	1.78279688	-2.31134580	-3.11979033
H	3.15759167	-1.67599384	-1.10253361
H	0.52838684	-1.12097787	-3.51871793
C	-3.82414966	2.06586172	1.10016240
H	-3.04075873	2.81384780	1.03873222
C	-4.63732334	-0.14487030	0.69948969
H	-4.50597325	-1.14910436	0.31092874
C	-5.03980119	2.41532317	1.68299484
H	-5.18764767	3.42179960	2.06232094
C	-5.86033804	0.19440217	1.27994266
H	-6.65257815	-0.54542658	1.33978620
C	-6.06707888	1.47751592	1.77751971
H	-7.01605668	1.74581840	2.22995762
C	1.04922985	-6.55198021	2.50771340
H	0.22228404	-7.03316576	1.97320718
H	0.79318639	-6.58897686	3.57407378
C	2.31513335	-7.33389709	2.28958219
H	3.19797017	-6.94991735	2.80100420
C	2.43190608	-8.43106345	1.54693896
H	1.58174142	-8.85306406	1.01908189
H	3.37766585	-8.95105174	1.44332589
H	-2.53199871	1.80267452	-4.35254577
H	-0.36585829	2.56477637	-3.62539102
H	-3.32215142	3.06438765	-3.37964966
H	1.02228869	2.44139097	2.05944220
H	0.26338195	1.70414656	3.51402771
H	2.07534486	0.34013461	1.70105414
H	4.43692821	1.71671303	-1.87281508
H	5.32391178	0.20210255	-1.88291492
H	2.00199329	-4.60467811	2.60400618
H	0.25774946	-4.53546676	2.42657113

H	2.33738903	-3.12361907	0.44520350
N	1.55999618	3.47635063	-0.18067262
H	0.73319810	3.02506246	-0.58365162
H	2.23963812	3.55183031	-0.93321087
C	1.21945939	4.82354945	0.29671206
H	0.82622504	5.47722057	-0.49913749
H	0.41541997	4.72239012	1.03390220
C	2.42368370	5.50482622	0.94762537
H	3.23850984	5.58151672	0.21680419
H	2.79581251	4.86701160	1.75737498
C	2.10407827	6.90923179	1.48850480
H	1.27703763	6.82657352	2.20675915
H	1.74806291	7.55013248	0.67460750
C	3.27843026	7.55920312	2.16405533
C	3.85042020	8.69889295	1.78735778
H	3.48395450	9.26379801	0.93509193
H	4.70133546	9.11220496	2.31720893
H	3.68205999	7.02796429	3.02557193

MP2 Electronic Energy(Ha): 1740.442934009213

B3LYP Electronic Energy(Ha): 1744.959780414762

M06-L Electronic Energy(Ha): 1744.720124090789

Zero point energy correction(kcal/mol): 475.471

Enthalpy correction(kcal/mol): 499.242

Entropy correction(cal/mol): 226.345

Imaginary Frequencies: -44.01 -43.72 -41.81 -36.28 -34.70 -26.26 -12.36 -3.05

Deuterated zero point energy correction(kcal/mol): 466.427

Deuterated enthalpy correction(kcal/mol): 490.672

Deuterated entropy correction(cal/mol): 231.047

Deuterated imaginary Frequencies: -43.88 -43.67 -42.26 -36.30 -34.97 -27.54 -25.16 -9.63

Transition State geometry

Zr	-0.47805655	-2.24746619	-0.31377959
C	-2.40944346	-0.57348928	-0.18889322

C	-2.52174245	-1.16829095	-1.47489113
H	-2.42073001	-0.63949232	-2.41246041
C	-2.64888310	-1.63440688	0.74621900
H	-2.64933724	-1.52462412	1.82216792
C	-2.90248047	-2.84213588	0.04725717
H	-3.13681137	-3.80172841	0.48499670
C	-2.80315746	-2.55593051	-1.33846586
H	-2.96514944	-3.25997791	-2.14267328
B	-1.92068541	0.93560509	0.18469076
C	-2.90969810	1.71946641	1.22754437
C	-0.40411537	0.75228180	0.77465198
C	-1.78668549	1.82331627	-1.17505095
N	-0.74795188	2.37738549	-1.68691584
N	0.29214417	-0.35383806	0.67052352
O	0.23536234	1.74422635	1.38987176
O	-2.96457200	2.00878271	-1.85702510
C	-1.16784203	3.09959869	-2.90457207
C	-2.69828262	2.91235614	-2.95330047
C	1.62380000	-0.15563364	1.28466059
C	1.59294832	1.31835443	1.71954056
N	0.36593154	-3.66740904	0.67433017
N	1.26052796	-1.78142469	-1.94494822
C	1.80986234	-0.69256962	-2.78591045
H	2.54208933	-0.11244219	-2.22437962
H	-0.87793196	4.15205758	-2.83816844
H	1.75657729	-0.85055205	2.11707628
C	0.85145019	-4.78713566	1.43965390
H	0.01989331	-5.43972813	1.74612857
H	1.51866959	-5.41012092	0.82472001
C	1.61303026	-4.33953343	2.69540009
C	2.40377180	-1.40925525	-4.03848109
C	1.84531470	-2.86021464	-3.98557806
H	2.61600918	-3.56636594	-3.65962521

H	0.99344901	-0.01933878	-3.04987887
C	0.73510498	-2.79390070	-2.92082855
H	-0.14301562	-2.31866900	-3.37671543
H	1.47191777	-3.20683680	-4.95065389
C	0.27935903	-4.01163307	-2.12536148
H	1.07535951	-4.76588021	-2.08561446
H	2.04962990	-2.22849899	-1.47430923
H	-0.59897390	-4.48973728	-2.55816414
C	-2.53785010	2.93835127	1.82307131
H	-1.55652772	3.35060357	1.61973264
C	-4.19884670	1.24863957	1.52174846
H	-4.54284566	0.32360070	1.07232265
C	-3.39357259	3.63706974	2.67221128
H	-3.06822711	4.57429689	3.11341202
C	-5.06444910	1.94068747	2.36952894
H	-6.05415101	1.54250816	2.57103396
C	-4.66437791	3.13926437	2.95329288
H	-5.33340854	3.68026177	3.61436312
C	2.26763816	-5.50429179	3.46385954
H	1.51855584	-6.26937335	3.69639650
H	2.62855674	-5.11895906	4.42566575
C	3.42355808	-6.12827985	2.73154015
H	4.23978564	-5.44991858	2.48224800
C	3.52392685	-7.40643146	2.37737490
H	2.73896740	-8.12228391	2.60263595
H	4.39556056	-7.78577291	1.85568381
H	-3.06227665	2.45352944	-3.87480011
H	-0.66384557	2.67872606	-3.78196458
H	-3.25204640	3.83720453	-2.77441861
H	2.26359421	1.95489720	1.14162635
H	1.73033127	1.46567223	2.79072096
H	2.41362085	-0.34941601	0.55431973
H	2.10615908	-0.89317469	-4.95294510

H	3.49538165	-1.40757755	-4.01163794
H	2.38166181	-3.61711192	2.39779759
H	0.92073356	-3.80659414	3.35475569
H	0.33039593	-4.01029222	-0.62580312
N	2.14822145	3.38018573	-0.80568385
H	1.23210665	2.99163632	-1.04662280
H	2.68130027	3.43196985	-1.66990428
C	1.98018636	4.73135173	-0.25596568
H	1.50424851	5.43159603	-0.96312865
H	1.30428514	4.65628287	0.60218148
C	3.31483168	5.32249599	0.20000063
H	4.00656347	5.36584025	-0.65066737
H	3.76885943	4.64564304	0.93239808
C	3.17396710	6.73165361	0.80189435
H	2.46006175	6.68427831	1.63547773
H	2.74274651	7.41265756	0.06002031
C	4.47556776	7.29123343	1.30206713
C	5.05833573	8.40203655	0.86082009
H	4.60700665	9.00911450	0.08133785
H	6.00362205	8.74869224	1.26329806
H	4.96747370	6.71550261	2.08560398

MP2 Electronic Energy(Ha): 1740.401397800469

B3LYP Electronic Energy(Ha): 1744.912325598568

M06-L Electronic Energy(Ha): 1744.668451224491

Zero point energy correction(kcal/mol): 474.387

Enthalpy correction(kcal/mol): 502.378

Entropy correction(cal/mol): 256.354

Imaginary Frequencies: -1474.81

Product geometry

Zr	-0.22086664	-2.14238732	-0.21712572
C	-2.30997947	-0.66300356	-0.24563998
C	-2.24689900	-1.21384539	-1.55303185

H	-2.09226902	-0.64389022	-2.45950193
C	-2.54753744	-1.77679834	0.62601737
H	-2.66202528	-1.71305685	1.69987217
C	-2.61600379	-2.97523451	-0.12981879
H	-2.80736003	-3.96688451	0.25336123
C	-2.40826835	-2.62800503	-1.48901822
H	-2.44401533	-3.31199093	-2.32652009
B	-1.95052878	0.85668375	0.22722061
C	-3.08456711	1.52659303	1.20062441
C	-0.47942903	0.76416441	0.96180641
C	-1.74719549	1.79128989	-1.09356148
N	-0.65824742	2.25491153	-1.59761288
N	0.30968963	-0.28951604	0.94241831
O	0.01317730	1.79199928	1.64693337
O	-2.89729453	2.09658029	-1.77032625
C	-1.00739986	3.02544867	-2.80884088
C	-2.54830107	2.98659489	-2.85471359
C	1.50229928	-0.02136834	1.78179146
C	1.36912109	1.47407902	2.09503333
N	0.64711520	-3.57057283	0.61616584
N	1.16183136	-1.96749583	-2.18001169
C	1.56485231	-0.55388049	-2.53353078
H	2.49184551	-0.31865686	-2.00876931
H	-0.61596687	4.04407593	-2.73628158
H	1.46926243	-0.65628997	2.67064592
C	1.08117097	-4.75032951	1.30630398
H	0.26339515	-5.48744610	1.36336797
H	1.89089103	-5.24502943	0.74887699
C	1.57229759	-4.46517457	2.73596373
C	1.72781705	-0.51359210	-4.07396831
C	1.68734796	-1.98570403	-4.50897974
H	2.68402947	-2.43873048	-4.45462180
H	0.80616743	0.15145047	-2.19074205

C	0.77241941	-2.64166737	-3.46767665
H	-0.26304039	-2.35243206	-3.67127095
H	1.31761013	-2.12010865	-5.52744520
C	0.87151299	-4.15687700	-3.36693768
H	1.89800980	-4.46820870	-3.14761978
H	1.99462431	-2.45509846	-1.85208208
H	0.57884950	-4.61320651	-4.31538364
C	-2.86077300	2.72012568	1.91017473
H	-1.88980262	3.19775974	1.85591824
C	-4.36885177	0.96940325	1.30775469
H	-4.59871753	0.05902896	0.76565430
C	-3.85229171	3.31348869	2.68951978
H	-3.63840315	4.23420260	3.22379564
C	-5.36936146	1.55603226	2.08264583
H	-6.34973067	1.09279139	2.13687874
C	-5.11495643	2.73207384	2.78247563
H	-5.88909571	3.19089607	3.38868426
C	2.03743701	-5.72179170	3.49771786
H	1.22963957	-6.46190602	3.52512922
H	2.23388707	-5.43694532	4.53958354
C	3.28030335	-6.35123482	2.93249297
H	4.14862272	-5.69538845	2.86498542
C	3.39900153	-7.61285852	2.52785003
H	2.56321545	-8.30488034	2.57415545
H	4.33413586	-8.00196822	2.14041049
H	-2.95748568	2.57819862	-3.78061452
H	-0.54874976	2.56513736	-3.69168773
H	-3.01033194	3.95738556	-2.65977651
H	2.04290516	2.09631969	1.50397153
H	1.42823333	1.71816219	3.15476328
H	2.42048076	-0.24992327	1.23832606
H	0.89631771	0.03629155	-4.52069471
H	2.64821980	-0.01054582	-4.37397993

H	2.39060301	-3.73678193	2.68751697
H	0.75992512	-3.98532163	3.29147145
H	0.22443272	-4.55464762	-2.58270009
N	2.15405485	3.33866914	-0.55172680
H	1.25210290	2.94926730	-0.83788779
H	2.75799160	3.31118776	-1.36901445
C	1.98733036	4.72996358	-0.11416261
H	1.57952252	5.38769510	-0.90036282
H	1.25526914	4.73525612	0.70034196
C	3.30746981	5.31828380	0.38512454
H	4.05019853	5.28590380	-0.42194758
H	3.69625599	4.68138815	1.18745310
C	3.17251201	6.76804646	0.88205387
H	2.41608342	6.79447549	1.67815823
H	2.79818634	7.40606809	0.07402888
C	4.46205842	7.32984448	1.41044196
C	5.09626847	8.39280167	0.92468564
H	4.70088507	8.95467619	0.08337602
H	6.02961594	8.74384474	1.35044229
H	4.89829372	6.79813102	2.25558849

MP2 Electronic Energy(Ha): 1740.452573269315

B3LYP Electronic Energy(Ha): 1744.968988374876

M06-L Electronic Energy(Ha): 1744.722522484656

Zero point energy correction(kcal/mol): 476.711

Enthalpy correction(kcal/mol): 505.751

Entropy correction(cal/mol): 272.875

Imaginary Frequencies: -0.00