ABSTRACT

Title of Dissertation:	MECHANISMS AND RATIONAL CATALYST DESIGN OF ORGANIC TRANSFORMATIONS FOR THE SYNTHESIS OF NEW C-C AND C-X BONDS
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The creation of new C-C or C-X bonds, where X can be oxygen, nitrogen or fluorine, is vital to organic synthesis and the discovery of new methods for complex molecule synthesis. In many cases, the mechanism of these transformations is not investigated, although an understanding of the underlying mechanism would allow for rational design of new catalysts and would lead to the development of novel reactivity. Computational studies probing the mechanisms of valuable synthetic methods including C-H oxidation, organocatalysis, nickel photocatalysis, alkyne metathesis and multicomponent reactions are presented. Specifically, computational methods were used in the development of a novel tetradentate amine iron (II) catalyst for the promotion of C(sp^3)-H oxidation (**Chapter 1**). Next, the mechanism of an organocatalyzed amination was studied thoroughly with density functional theory

(DFT) calculations in combination with molecular dynamics simulations to develop a predictive model for reactivity for use in the creation of new catalysts in the field of amination chemistry (**Chapter 2**). Additionally, the mechanism of a regio- and enantioselective iridium-catalyzed asymmetric fluorination was studied, with an emphasis on determining the role of the trichloroacetimidate group in the reaction (**Chapter 3**). Further, the mechanisms of various transition metal-catalyzed C-C bond formations were studied through computationally. First, a photoredox/nickel-dual catalyzed Tsuji-Trost reaction was studied through DFT and DLPNO-CCSD(T) calculations to investigate the stereoselectivity of the reaction as well as the order of reaction events. Next, a photoredox/nickel-dual catalyzed C-C bond formation using oxanorbornadienes as electrophilic coupling partners was investigated computationally (**Chapter 4**). Additionally, the mechanism of tungsten- and molybdenum-catalyzed alkyne metathesis as well as the difference in reactivity between the two metals was explored (**Chapter 5**). A nickel-catalyzed diarylation of alkenes was studied computationally, with particular emphasis on the role of the phosphine ligand in controlling regioselectivity (**Chapter 6**). Finally, an iron-catalyzed dicarbofunctionalization of vinyl ethers with aryl Grignard reagents and alkyl halides or (fluoro)alkyl halides was developed experimentally (**Chapter 7**).

MECHANISMS AND RATIONAL CATALYST DESIGN OF ORGANIC TRANSFORMATIONS FOR THE SYNTHESIS OF NEW C-C AND C-X BONDS

by

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Dedication

To my mom and dad
for raising me to be curious about the world and to pursue knowledge for its own sake.

To my husband
for making this pursuit of knowledge worthwhile.

To my daughter
may you follow your dreams and never stop learning.

I love you all.

And to those who lost the battle with depression while on their academic journey,

this is for you.

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Ad Majorem Dei Gloriam

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Chapter 1: Rational Design of Chiral Iron Catalysts for Asymmetric C(sp^3)-H Oxidations

1.1 Abstract

Iron is one of the most attractive targets in the search for inexpensive and nontoxic metals for catalytic organic transformations (e.g., C(sp^3)-H oxidation). Que, White, Costas and others have used tetradentate amine ligand scaffolds capable of binding to iron to promote site-selective aliphatic C-H oxidations. However, the role of spin state in these reactions and the ability to tune the spin state of the iron center is not well-defined. Herein, I report a computational method for the prediction of geometry and spin state of a series of known N_4-tetradentate ligand iron complexes is described. Specifically, quantum-mechanical calculations were undertaken on this library of compounds to identify a predictive method for determining spin state and geometry of such iron complexes. The ability of this model to predict the geometry and spin state of a series of new chiral diamine tetradentate iron complexes was tested. Finally, applications to C-H oxidation chemistry were explored.

1.2 Introduction

Homogenous iron catalysis is an attractive area of research for several reasons, including the ability of iron complexes to catalyze a wide range of transformations (**Figure 1.1**) from organic textbook classics such as Friedel-Crafts alkylation and acylation to, more recently, aliphatic C-H oxidations.[1] It is iron's ability to adopt a variety of oxidation states, from -2 to +5, from which the versatility of iron in catalysis stems.[2] On the one hand, iron in low oxidation states can act as a nucleophile and promote substitutions at sp^3 carbon

centers, additions to aromatic rings, and hydrogenations of alkenes while iron in a +2 or +3 oxidation state can promote electrophilic aromatic substitutions.[3] In addition, iron can act as a one electron transfer agent which is important for promoting transformations that proceed via radical intermediates and can participate in 2-electron chemistry such as traditional cross-coupling reactions.[4] Iron is also an attractive target for catalysis because of its natural abundance, cost, low toxicity, and biological relevance. For example, iron is the second most abundant metal on earth, existing in both the earth's core and crust.[5]

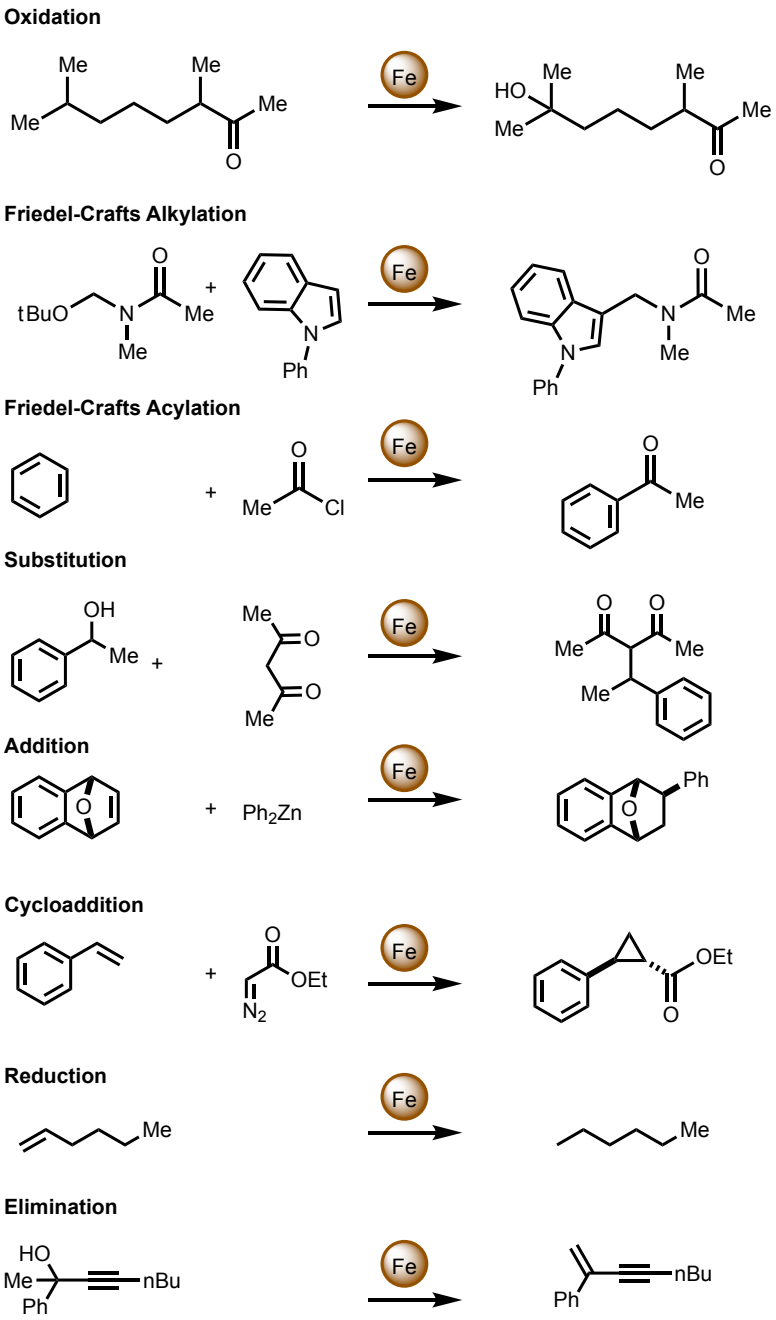


Figure 1.1 Versatility of homogenous iron catalysis for promoting a wide range of transformations. This work focuses on iron as a catalyst in aliphatic C-H oxidation reactions.

Iron is also a cheaper transition metal compared to precious metals traditionally used to promote organic transformations such as palladium, platinum, and ruthenium. For a price comparison of their chloride salts used commonly as precatalysts in carbonylations

of alkynes[6] (**Figure 1.2**), iron (II) chloride costs approximately $3/g while palladium (II) chloride is $65/g.[6]

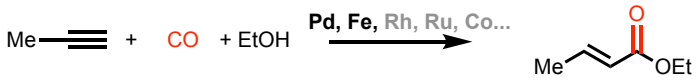


Figure 1.2 Carbonylation of alkynes catalyzed by palladium, iron, rhodium, ruthenium, and cobalt.[6]

Furthermore, iron is involved in many metabolic processes including safe disposal pathways leading to its low toxicity. For this reason, there is a greater tolerance (up to 1200 ppm) for iron as an impurity in pharmaceuticals in contrast to palladium or platinum which has a tolerance of 3 ppm.[7] In the body, iron is present in heme which is involved in oxygen transport in the blood. Cytochrome P450, which contains heme as a cofactor at the active site, is part of the major group of enzymes involved in drug metabolism.[8] Nature's ability to selectively and efficiently oxidize aliphatic C-H bonds at the active site of cytochrome P450 serves as inspiration to the synthetic chemistry community in the search of iron enzymes, which can replicate this selectivity.[9]

In addition to iron being a versatile, cost effective, and less toxic alternative catalyst to other precious transition metals, iron can also adopt various geometries and spin states which, although a challenge to characterization of the complexes, also provides new opportunities to promote new reactions. For example, octahedral iron with a tetradentate ligand is well-known to adapt any of the three different geometries (**Figure 1.3**: cis-α, cis-β, and *trans*).[10]

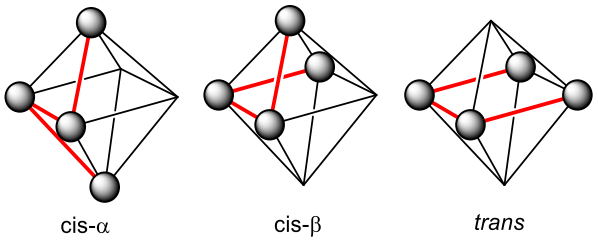


Figure 1.3 Possible geometries that a tetradentate ligand can adopt in an iron complex.

In general, the degenerate d-orbitals in octahedral complexes split into two energy levels in the presence of a ligand field such that the d_{xy}, d_{xz}, and d_{yz} orbitals are lower in energy while the $d_{x^2-y^2}$ and d_{z^2} are higher in energy.[11] The magnitude of this d orbital splitting (Δo) (**Figure 1.4**) is sensitive or dependent on the nature of the ligands.[11]

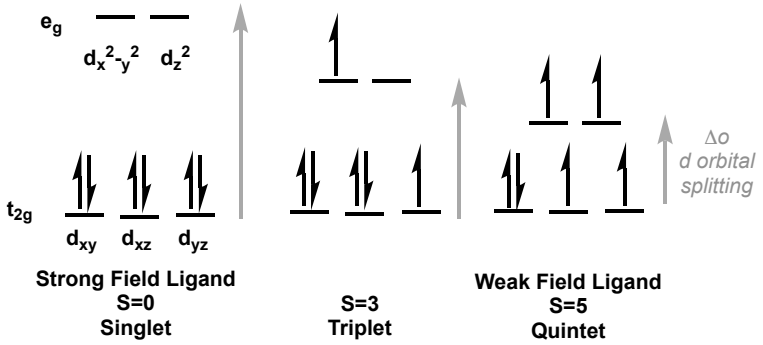


Figure 1.4 The three possible spin states that iron (II) can adopt in an octahedral complex and the varying magnitude of the d orbital splitting.

For example, a strong field ligand such as the π-acceptor CO ligand will result in a large d orbital splitting while a weak field ligand such as the π-donor Cl ligand will result in a small d orbital splitting. In the case of iron (II), a strong field ligand, in an octahedral environment, will cause the electrons to occupy the lower energy levels, resulting in a low spin octahedral complex (singlet). This complex is "low spin" as the electrons, which each have a spin of ±1/2 lead to an overall spin of zero. On the other hand, iron (II) in the presence of a weak field ligand is likely to adapt a high spin state (quintet) in which the electrons can populate the higher energy levels. Iron (II) can also occupy a medium spin

state (triplet). The overall spin state or spin multiplicity is determined by the formula 2S + 1 where S is the electronic spin quantum number. *The ability to access multiple spin states on the iron center is therefore controlled by changing the ligand properties*. By tuning the electronic (and steric) properties of the ligand, in principle the spin state of the iron complex can be controlled as well.

The ability to tune the spin state can affect the reactivity and selectivity in organic transformations.[12] For example, a high spin iron catalyst would be useful in an oxidation reaction in which we seek to destabilize the competing β-elimination.[12] β-Hydride elimination requires an empty orbital at the metal center to accept the electrons from the C-H bond that is broken.[13] In the case of a high spin iron species, the metal does not have an empty d orbital in which to accept these electrons and as a result this pathway is avoided.[14] The sensitivity of the spin state at the iron center to the electronic environment of the ligand provides an opportunity to tune the catalyst to the desired spin. However, our understanding of the molecular-level factors controlling spin state is rudimentary and our ability to characterize, tune, and predict spin states in iron-catalysis remains challenging.

At the start, the goal of this work was to develop new chiral N_4-tetradentate ligands and, using a combination of experiment and computation, to rationally design chiral iron (II) catalysts to promote C(sp^3)-H oxidation.[15] Fe-catalyzed C(sp^3)-H oxidation has been studied by Que, White, Costas, Britovsek and others but there is still a lack of understanding of the mechanism of iron-catalyzed oxidation reactions.[16,17,18] The study of selective and catalytic C(sp^3)-H oxidation is of interest as a greater understanding of the reaction could streamline drug synthesis. For example, two of the highest grossing drugs in 2017, Lipitor and Seroquel (**Figure 1.5**) contain aliphatic C-O bonds, which could in

principle be installed directly via Fe-catalyzed C(sp^3)-H oxidation, that are vital to the drugs' activity.[19]

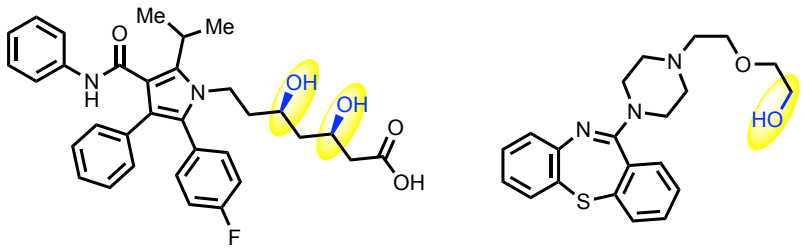


Figure 1.5 Two of the highest grossing drugs in 2017, both of which contain C(sp^3)-OH bonds.

A change from a C(sp^3)-H bond to a C(sp^3)-OH bond can change a molecule's physical or chemical properties such as its solubility and polarity.[19] Moreover, the C(sp^3)-OH bond can act as a hydrogen bond donor and acceptor to interact differently with protein sites and vary the physiological response of the body. For example, drugs such as Taxol and erythromycin A (**Figure 1.6**) have a vital oxygen functionality which, if removed, will cause a loss of all or some of the drug's activity.[20]

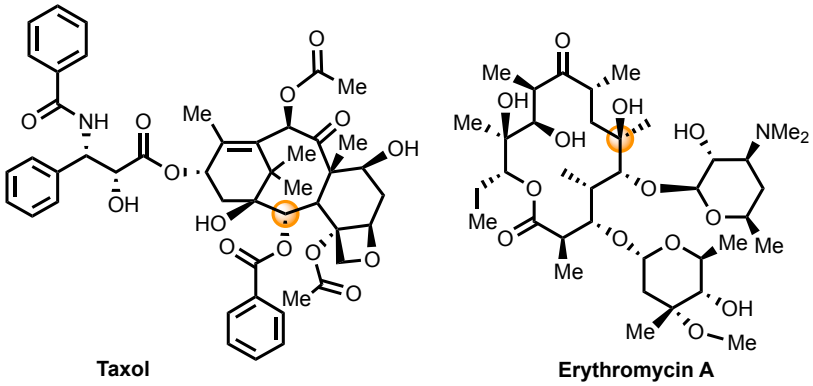


Figure 1.6 Two small molecule drugs with oxygen functionalities that are vital to the drug's activity.

In addition, the introduction of a hydroxyl group is important for metabolic processes.[21] As a result, selective C(sp^3)-H oxidation is vital to drug discovery.[22] Directing groups are often used in late-stage functionalization of complex molecules (**Figure 1.7**).

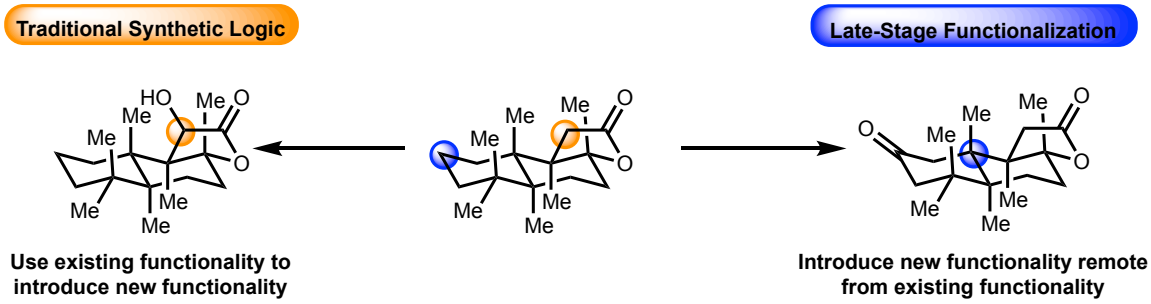


Figure 1.7 Directing groups are traditionally used to insert new functionality into a molecule while late-stage functionalization can be used to insert new functionality without the aid of such a group.

However, due to the few differences between neighboring aliphatic C(sp^3)-H bonds in complex molecules, selective oxidation of aliphatic C-H bonds without the use of a directing group remains a grand challenge.[23] In addition, bond dissociation energies and pKa's of neighboring C(sp^3)-H bonds can be similar, preventing oxidation in a controlled manner.[24] On the other hand, enzymes such as cytochrome P450 and non-heme enzymes such as α-ketoglutarate-dependent oxygenase alike perform late-stage functionalization to perform site selective C-H hydroxylation reactions (**Figure 1.8**).[25]

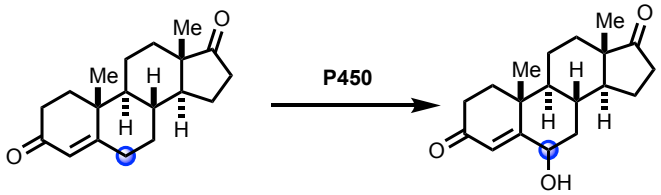
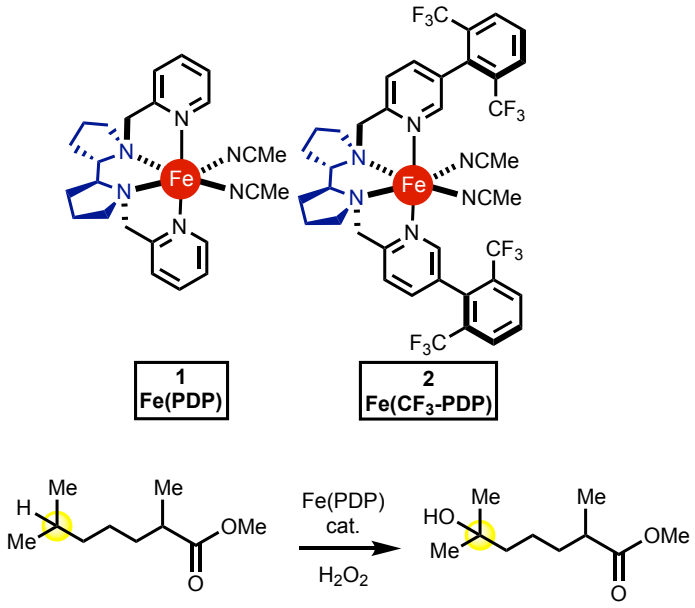


Figure 1.8 Example of selective oxidation of C(sp^3)-H bond by cytochrome P450.

By mimicking this late-stage functionalization done by nature, site selective oxidation of C(sp^3)-H bonds can be achieved. White et al. utilized this approach in her work on oxidation of C-H bonds by non-heme iron catalysts (**Figure 1.9**).[26] Specifically, the Fe(PDP) catalyst **1** (see **Figure 1.9** for definition of PDP ligand) used in her work is capable of site selective C-H oxidation of tertiary and secondary carbons based on subtle electronic and steric differences of the C(sp^3)-H bonds.[26] Notably, by modifying the Fe(PDP) **1** to a more sterically hindered Fe(CF_3-PDP) **2** (**Figure 1.9**), different sites on the same molecule can be selectively oxidized.[27] However, there is still a lack of understanding of the steric and electronic factors (i.e., spin, oxidation state, ligand coordination, etc.) that control this selectivity. Characterization and understanding of the spin state of the precatalyst iron species in both systems would be beneficial to the development of future catalysts.



PDP = 2-({(S)-2-[(S)-1-(pyridin-2-ylmethyl)pyrrolidin-2-yl]pyrrolidin-1-yl}methyl)pyridine
CF_3-PDP = (2S,2'S)-1,1'-bis((5-(2,6-bis(trifluoromethyl)phenyl)pyridin-2-yl)methyl)-2,2'-bipyrrolidine

Figure 1.9 Ligand scaffolds used by White and coworkers to perform selective C-H oxidation, with a representative example shown.

Notably, Que used non-heme iron catalyst scaffold[28] **3** (**Figure 1.10**) to catalyze *cis*-dihydroxylation of aromatic double bonds using hydrogen peroxide as the oxidant in a similar manner to the site-selective Rieske dioxygenases developed by nature.[29] This result highlights the potential of diamine iron (II) catalysts to promote challenging transformations.

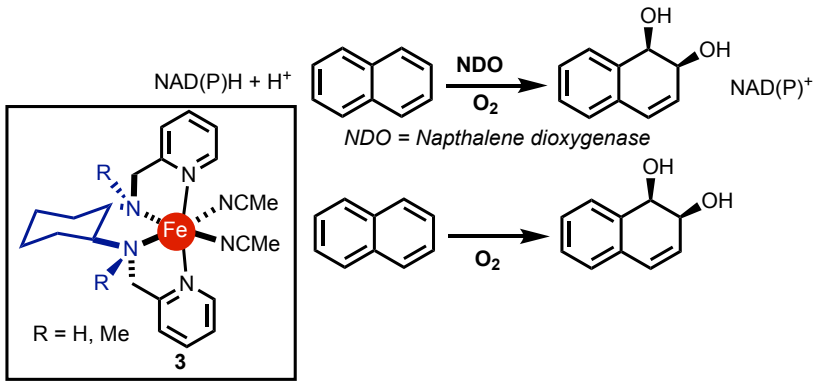


Figure 1.10 Rieske dioxygenase-catalyzed *cis*-dihydroxylation of aromatic double bonds using hydrogen peroxide as the oxidant with the small-molecule catalyzed version shown below.

Britovsek and coworkers hypothesized that a scaffold with a biphenyl bridge (**Figure 1.11**) would constrain the iron complex to a *cis*-*α* geometry.[30] They found that the bis(imine) **4** results in a cis-*α* geometry while the bis(amine) ligand **5** forces a *trans* geometry. Both the bis(imine) **4** and bis(amine) **5** complexes show moderate catalytic activity for the oxidation of cyclohexane. However, selectively remained a problem with these catalysts.[31]

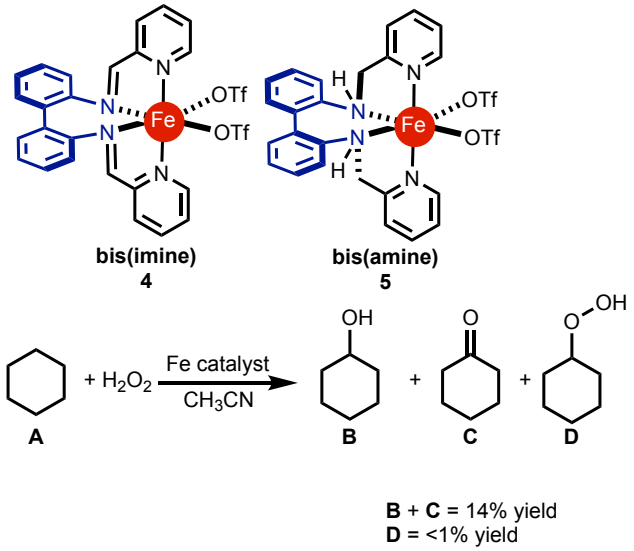


Figure 1.11 Iron (II) complexes utilized by Britovsek.

Inspired by these reports, Maimone sought to utilize a tetradentate chiral diamine iron (II) catalyst to perform selective late-stage C(sp^3)-H oxidation (**Figure 1.12**).[32] After screening of related catalysts, it was found that only **6** formed the desired oxidation product albeit low yield. Further, complex **6** also decomposes unprotected material without promoting the C-H oxidation. *This work exemplifies the potential of using homogenous tetradentate chiral iron (II) catalysts for late-stage C-H oxidation while revealing its limitations and the need for more efficient and active iron catalysts.*

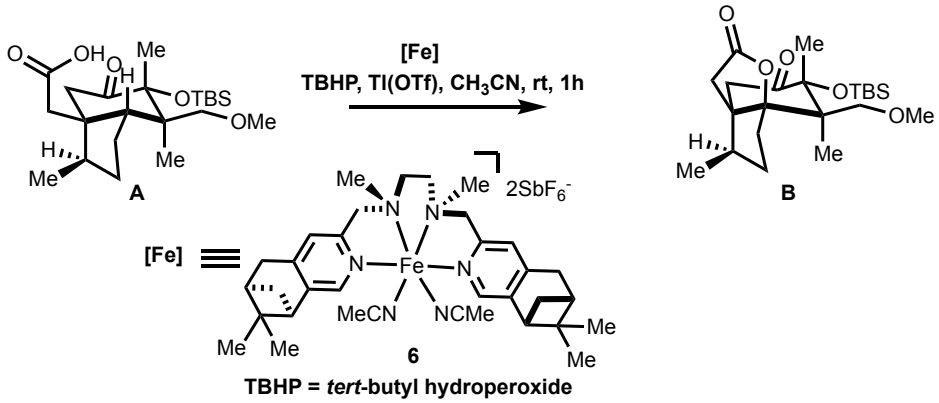


Figure 1.12 Formation of a lactone by iron catalysis as a step in Maimone's synthesis of a sesquiterpene.

1.3 Results and Discussion

1.3.1 Computational Studies

To gain a greater understanding of selective C(sp^3)-H oxidation catalyzed by non-heme iron catalysts, a combination of experimental and computational tools was used. Based on past non-heme ligand scaffolds prepared by Que, Costas, White and Britovsek (**Figure 1.13**), a new chiral diamine scaffold was targeted, which can be prepared from the condensation and subsequent reduction of (*R*)-[1,1'-Binaphthalene]-2,2'-diamine and varying derivatives of pyridine carboxyaldehdye.

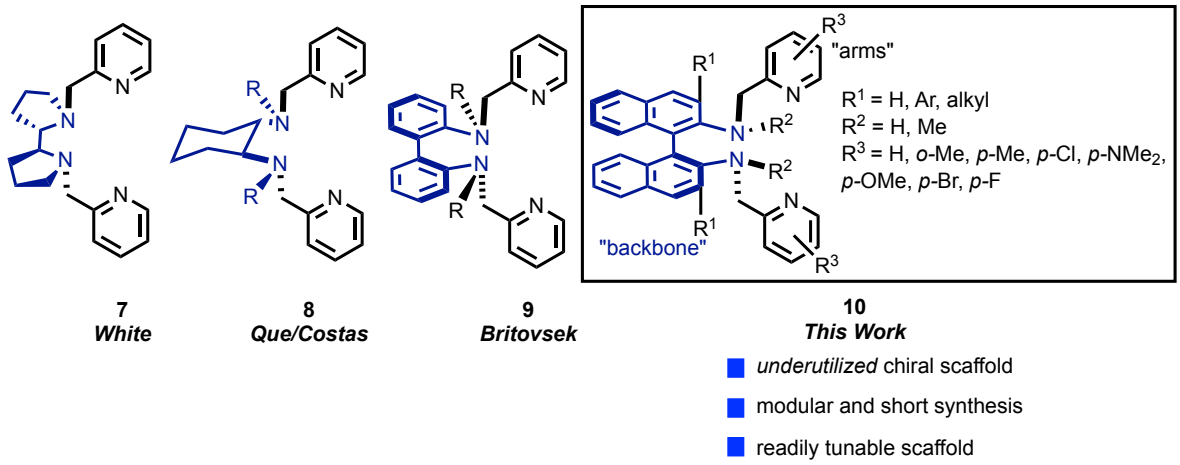


Figure 1.13 Traditional ligand scaffolds used in iron (II)-catalyzed C-H oxidations. The focus of the experimental work is this chiral scaffold as a ligand library can be easily prepared and modulated from the biphenyl diamine and a pyridine carboxyaldehyde derivative.

A hallmark of this work is the use of *axial* chiral ligand scaffold and the ability to tune the electronic and steric environment by substituting various functional groups at different positions of the ligand. For example, both the chiral diamine backbone (blue) and the pyridine carboxyaldehyde "arms" (black) can be modified (**Figure 1.13**). The chiral

binaphthalene backbone can be modified at the R^1 position with aryl or alkyl derivatives.[33] The arms of the chiral diamine ligand can also readily be adjusted to afford different electronic and steric environments in the complex by substituting the pyridine ring with various groups R^3 such as Cl, Br, NMe_2, Me and others. The unique tunability of this chiral diamine scaffold makes it an attractive candidate for our research in the field of iron catalysis. For example, a highly electron-donating substituent on the pyridine group of the ligand may decrease the d orbital splitting of the iron center as the ligand serves as a π donor of electron density to the iron metal center while an electron-withdrawing substituent would increase the d orbital splitting. Further, the stereochemistry of the ligand has potential to afford stereocontrol in C-H oxidation. This work could have implications for regio- and enantioselective C-H oxidations.

To begin, computational studies were used to develop a model for the rational design of iron catalysts. To develop a predictive computational method for geometry and spin state of the iron catalyst, examples of N_4-tetradentate non-heme iron catalysts were identified in the literature that adhere to the following criteria: 1) the geometry of the complex is characterized via x-ray crystallography, 2) the spin state of the iron complex has been probed experimentally, 3) the iron complex has been used in C-H oxidations and 4) the complex is chiral. Nine examples from the literature (**Figure 1.14**) meet these specific criteria and were used to develop a predictive model for geometry and spin state based on relative energies of the iron complexes.

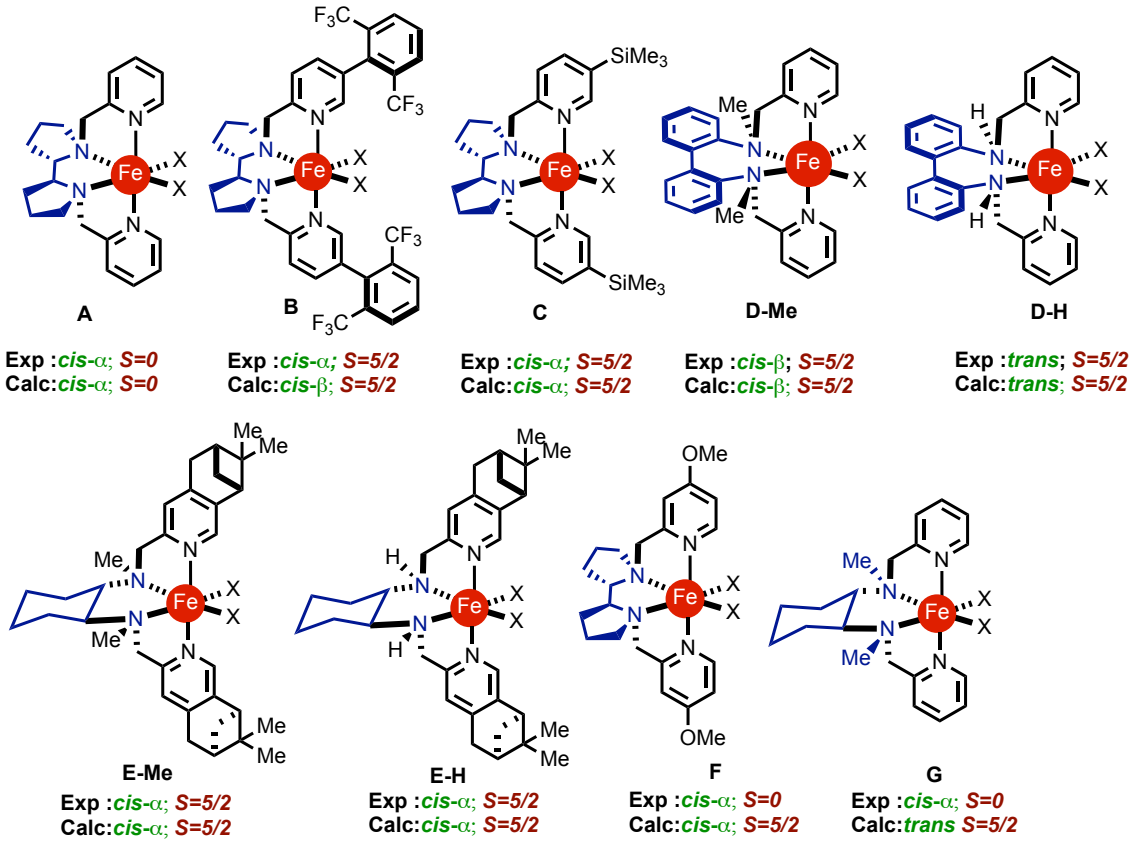


Figure 1.14 Training set of tetradentate amine iron catalysts (X=NCMe) with known geometry and spin state for use in the identification of a predictive model. The computational model matches with the experimental results for the compounds **A, C, D-Me, D-H, E-Me, E-H,** and **F**.[34]

These nine catalysts were optimized to the lowest energy structure using density functional theory (UB3LYP/6-31G(d)-gas) for the three possible geometries and three spin states, leading to 81 distinct structures studied.[35] After optimizing the structures, the energies were further refined by taking single point energy calculations with four different functionals (UPBEPBE, UB3LYP-D3, UM06, UM06L) and the 6-311+G(d,p) basis set in dichloromethane. The first two functionals were chosen as they take dispersion interactions into account while the latter two are suitable for organometallic complexes, with M06L being widely used for transition metals.[36] The resulting lowest energy structures were compared with reported geometry and spin state. One method (UM06L/6-311+G(d,p)-

CPCM(dichloromethane)//UB3LYP-6-31G(d)-gas) accurately predicted the lowest energy complex (same geometry and spin state with that reported in the literature) for 7 of the 9 structures. For example, complex **A** (**Figure 1.14**) was reported experimentally to be a cis-α singlet complex and the lowest energy structure of complex A computed (at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP-6-31G(d)-gas level of theory) was also the cis-α singlet structure. Thus, this method can be used in the rational design of iron catalysts as the probable geometry and spin state of the iron complex can be predicted prior to synthesizing the catalyst.

In addition, key Fe-N bond lengths in the lowest energy structure of each catalyst were compared in the computational model to the x-ray crystal structure. Iron-nitrogen bond lengths are especially important to analyze as they are indicators of spin state.[37] Typically, longer iron-nitrogen bond lengths are indicative of a high spin metal center while shorter bond lengths are indicative of a lower spin complex.[38] Bond lengths and angles in the computed structures are in agreement with the experimental result. As shown for one example in **Figure 1.15**, the computational model can be used to predict structural and geometric parameters.

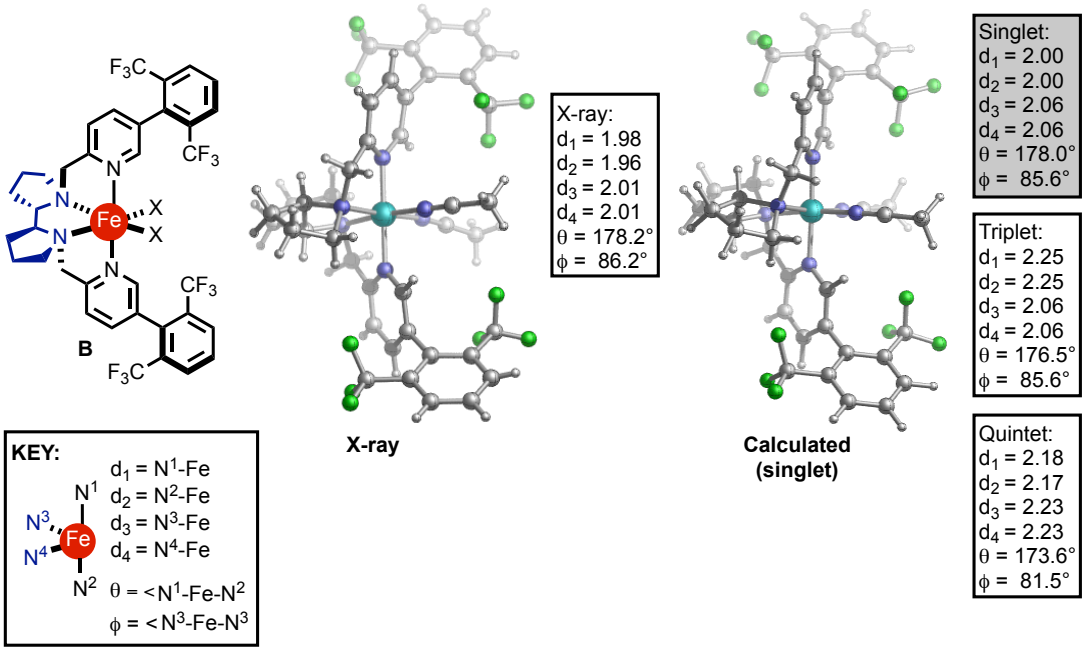
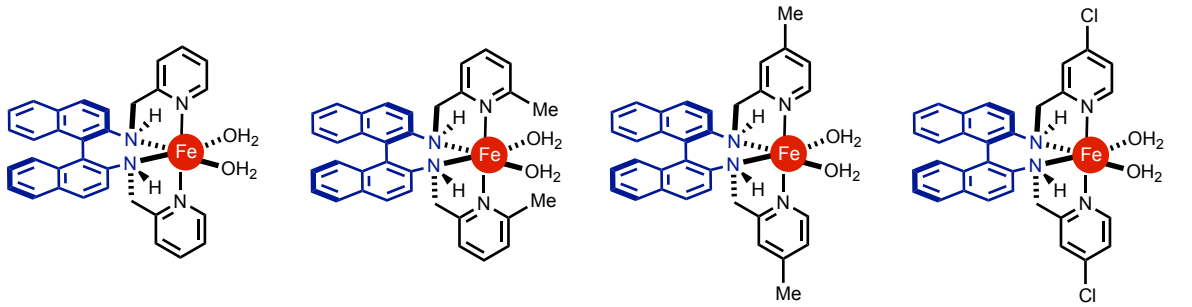


Figure 1.15 Key bond lengths (Å) and angles (º) of x-ray crystal structure (left) compared to computed structure in the singlet state (right) showing the agreement of the computational model (UB3LYP-6-31G(d)-gas) with experimental results.

A series of tetradentate amine iron complexes were chosen for synthesis and prior to their preparation, were also optimized and compared using UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP-6-31G(d)-gas for predicting the most stable geometry and spin state. This series of complexes shown in **Figure 1.16** were found to be lowest energy in the cis-β geometry at the high spin state.



1-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	12.0	12.2	16.8
S=3/2	14.0	14.3	14.8
S=5/2	0.0	-2.9	2.6

2-OH$_2$

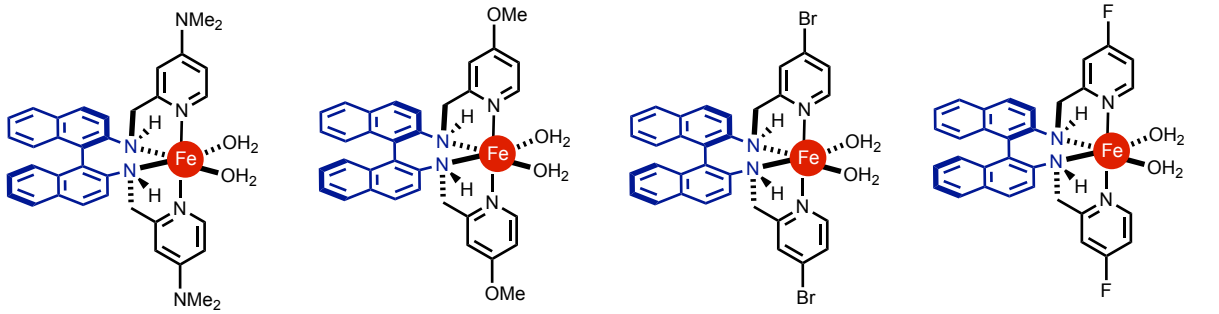
	cis-α	*cis*-β	*trans*
S=0	18.5	22.3	29.4
S=3/2	16.8	19.6	14.9
S=5/2	0.0	-0.7	1.9

3-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	9.5	20.0	18.5
S=3/2	11.0	11.6	13.9
S=5/2	0.0	-6.2	-0.1

4-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	9.1	9.6	19.9
S=3/2	11.2	12.0	14.2
S=5/2	0.0	-5.7	0.6



5-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	14.7	14.0	23.3
S=3/2	16.7	14.0	15.6
S=5/2	0.0	-2.6	1.3

6-OH$_2$

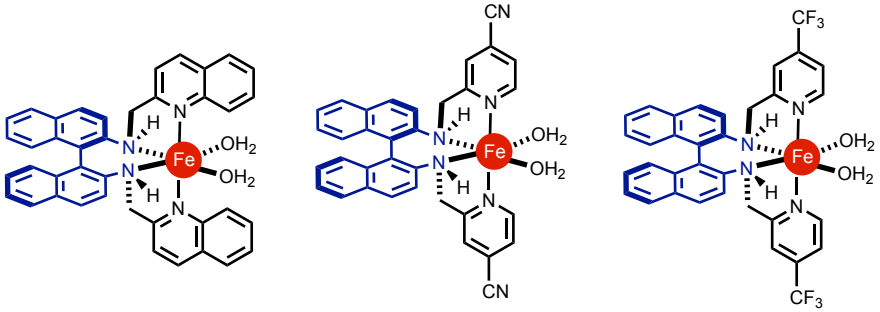
	cis-α	*cis*-β	*trans*
S=0	11.8	11.4	21.1
S=3/2	13.4	12.7	14.4
S=5/2	0.0	-4.2	-0.2

7-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	12.6	12.5	23.2
S=3/2	14.4	15.3	17.1
S=5/2	0.0	-2.9	3.6

8-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	13.0	13.2	23.5
S=3/2	14.8	15.7	17.6
S=5/2	0.0	-2.7	3.6



9-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	21.0	19.7	24.5
S=3/2	12.6	18.2	13.7
S=5/2	0.0	-2.4	-0.5

CN-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	19.7	12.3	23.0
S=3/2	11.1	15.7	18.1
S=5/2	0.0	-2.5	4.3

CF$_3$-OH$_2$

	cis-α	*cis*-β	*trans*
S=0	19.9	11.8	23.6
S=3/2	11.7	15.8	17.8
S=5/2	0.0	-3.3	3.5

Figure 1.16 Relative free energies for the cis-α, cis-β, and trans geometries of complexes **1-OH$_2$** through **9-OH$_2$** as well as **CN-OH$_2$ and CF$_3$-OH$_2$** computed at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level.[34]

1.3.2 Synthesis of Diamine Ligands and Iron Catalysts

Having studied the complexes computationally to predict their geometry and spin state, I moved on to synthesize the iron complexes. First, a library of chiral diamine ligands was synthesized in a one-pot procedure involving a condensation followed by a reduction as shown in **Figure 1.17**.

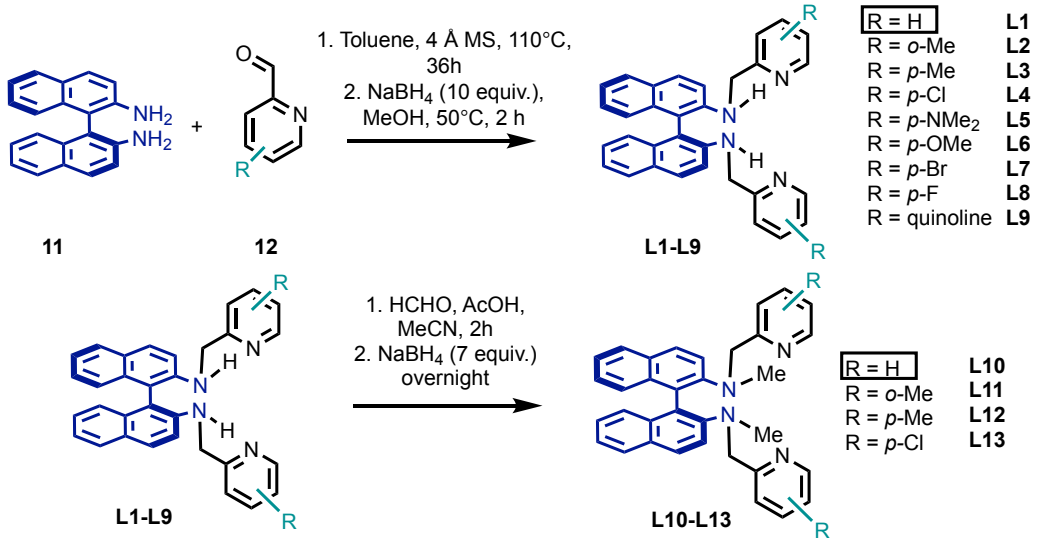


Figure 1.17 General procedure for the synthesis of a series of chiral diamine tetradentate nitrogen ligands (**L1** through **L9**) from condensation of (R)-[1,1'-binaphthalene]-2,2'-diamine with 2-pyridinecarboxaldehyde and its derivatives. Subsequent N-alkylation of **L1-L4** corresponding to **L10-L13** ligands.

Commercially available (*R*)-[1,1'-Binaphthalene]-2,2'-diamine and pyridine carboxyaldehyde **12** react to form an imine intermediate which is subsequently reduced with sodium borohydride. The resulting ligand must be carefully purified by silica gel column chromatography to remove any mono-substituted or imine byproducts. By using different substituted pyridine carboxyaldehyde derivatives, a library of ligands with varied steric and electronic properties can be prepared. This ligand library can be further expanded by N-alkylation. The ligands were characterized by ^{1}H and ^{13}C NMR as well as

mass spectrometry and infrared spectroscopy (See **Appendix 1** for full characterization data).

Following the ligand synthesis, iron complexes can be prepared, as shown in **Figure 1.18,** by reaction of ligand with iron (II) chloride in anhydrous acetonitrile. Successive reaction of the complex with silver triflate or silver hexafluoroantimonate leads to the desired tetracoordinated iron (II) diamine complex balanced with triflate or hexafluoroantimonate counterion. Precipitated silver chloride byproduct is removed by filtration.

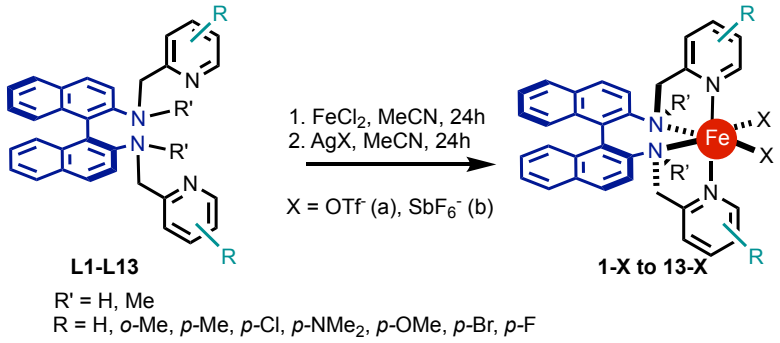


Figure 1.18 Synthesis of a series of chiral diamine tetradentate iron (II) catalysts (**1-X** to **13-X**) with triflate or hexafluoroantimonate counterions (X).

In contrast to the chiral diamine ligands which can be characterized by conventional techniques such as NMR, characterization of the iron complexes, if paramagnetic (**Figure 1.19**), by NMR is challenging, necessitating the need for other analytical techniques such as UV-visible and infrared spectroscopy, and x-ray crystallography.

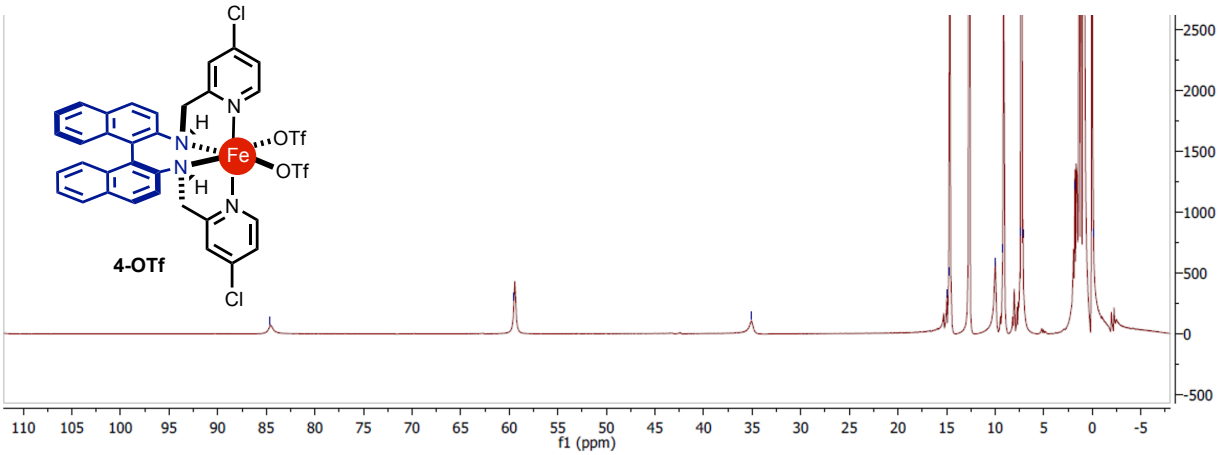
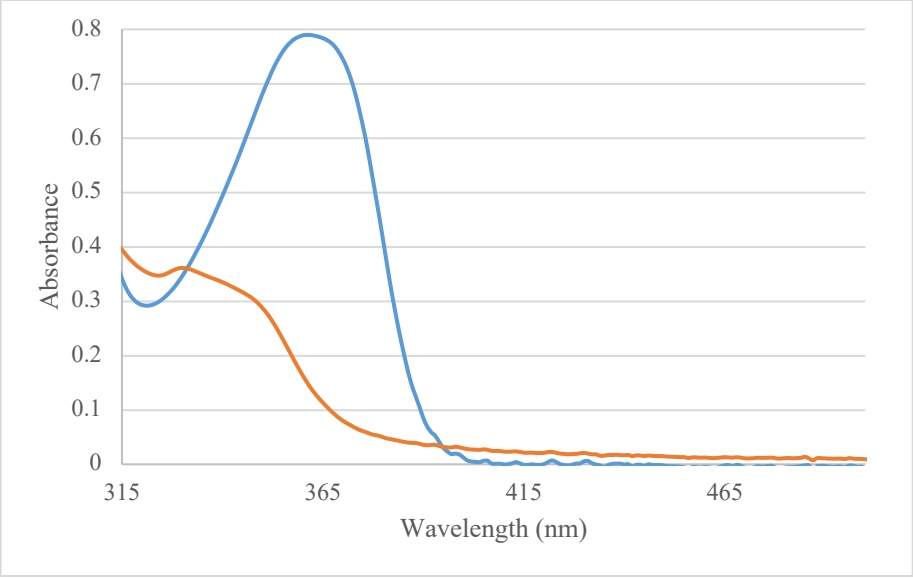
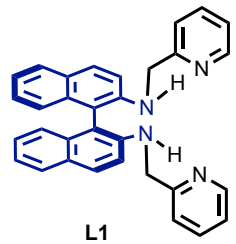


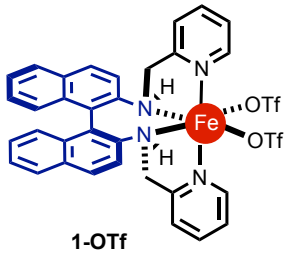
Figure 1.19 ^{1}H NMR spectrum of compound **4-OTf** in $CDCl_3$ showing the effect of paramagnetism on the chemical shifts.

In addition to characterizing the iron complexes by NMR, UV-visible spectroscopy was used for analysis of the compounds. The recorded UV-visible spectrum of the ligand and corresponding iron complex were compared for differences in maximum absorption wavelengths. In the spectrum of the iron complex, there is a clear shift in maximum absorbance wavelength as compared to the ligand, theoretically indicating that iron is bound to the ligand, thereby changing the maximum absorbance wavelength. In the case of the unsubstituted ligand **L1**, there is a hypsochromic shift from a λ_{max} of 362 nm to 332 nm in the iron complex **1-OTf** (**Figure 1.20**) providing support that the iron center was covalently bound to the ligand.





L1



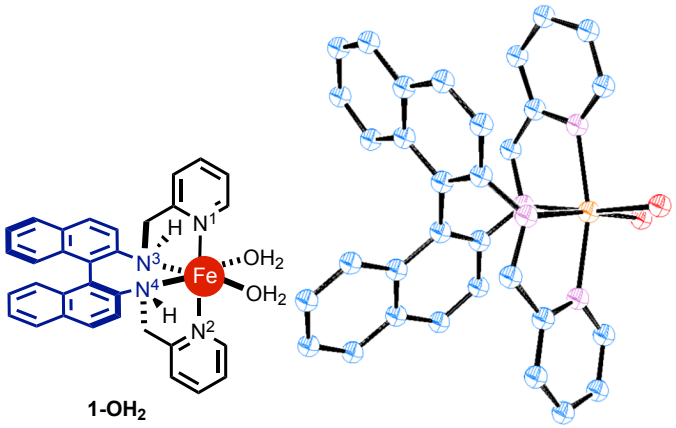
1-OTf

Figure 1.20 UV-vis spectrum (in dichloromethane) of ligand **L1** (blue) and complex **1-OTf** (orange). The maximum absorbance for each complex is labeled.

Inspired by the UV-vis results, I attempted to grow single crystals of the iron complexes to show that the iron atom is coordinated with the given ligand scaffold, which was previously not known.[39] Crystals of the iron complexes were prepared by the solvent-layering technique in which the powder form of the complex is dissolved in dichloromethane and placed in an NMR tube. Hexanes were carefully layered on top of the dichloromethane and crystals of the complex form at the interface between the two

liquids.[40] Three crystal structures (**Tables 1.1-1.3**) were obtained by x-ray crystallographic analysis from suitable crystals. The first of these complexes **1-OH$_2$** results from the reaction of the ligand **L1** with iron (II) chloride and silver triflate and adopted a cis-α geometry. Further, iron-nitrogen bond lengths in the range of 2.1 to 2.2 Å indicated that **1-OH$_2$** is likely a high spin complex. This result is supported by computationally predicted bond lengths for the same structure in the high spin state (**Table 1.1**).

Bond Length	***X-ray***	***Singlet***	***Triplet***	***Quintet***
Fe-N^1 (Å)	2.145	1.99	1.96	2.16
Fe-N^2 (Å)	2.131	1.99	1.97	2.14
Fe-N^3 (Å)	2.241	2.05	2.13	2.16
Fe-N^4 (Å)	2.293	2.05	2.05	2.16



1-OH$_2$

Table 1.1 Selected bond length (Å) data from X-ray crystal structure for iron (II) complex **1-OH$_2$** compared to the computed values (B3LYP/6-31G(d)-gas) of the complex in different spin states. Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, orange, and red ellipsoids represent C, N, Fe, and O atoms respectively.

Next the crystal structure of the unsubstituted iron (II) complex **1-μ-oxo** prepared with silver hexafluoroantimonate was obtained (**Table 1.2**). Following with the observation that the silver salt (AgOTf vs. $AgSbF_6$) influences the geometry of the structure, the hexafluoroantimonate complex afforded the cis-β iron complex as a μ-oxo dimer. Similar bridged oxo-iron dimers have been reported with cis-α geometries and have been shown to have catalytic properties for olefin epoxidation.[41] Iron-nitrogen bond lengths in **1-μ-oxo** are also indicative of a high spin iron complex.

Bond Length and Angle	***X-ray***	***Singlet***	***Triplet***	***Quintet***
$Fe\text{-}N^1$ (Å)	2.169	1.981	1.974	2.156
$Fe\text{-}N^2$ (Å)	2.158	1.976	2.044	2.149
$Fe\text{-}N^3$ (Å)	2.247	2.047	2.042	2.233
$Fe\text{-}N^4$ (Å)	2.233	2.035	2.062	2.198
$N^1\text{-}Fe\text{-}N^2$ (deg)	93.7(6)	98.9(4)	102.2(6)	103.5(0)
$N^3\text{-}Fe\text{-}N^4$ (deg)	82.0(6)	94.1(3)	96.0(8)	92.9(9)

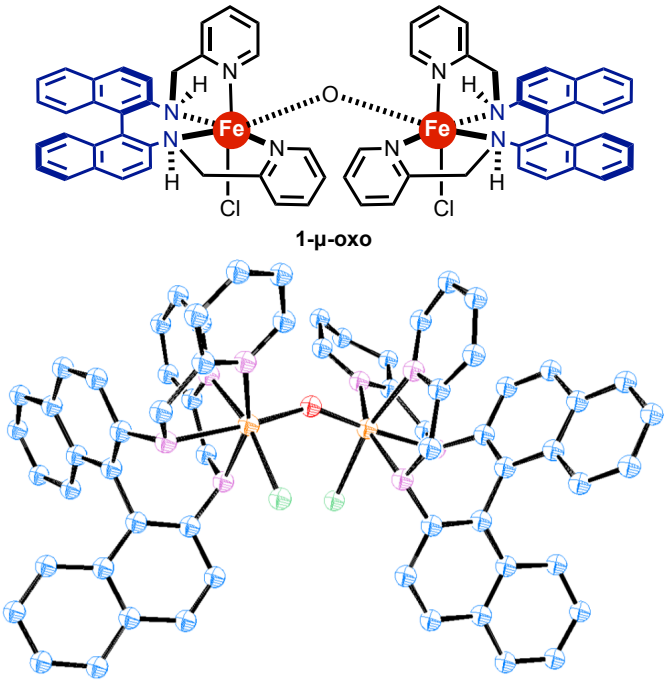


Table 1.2 Selected bond length (Å) and angle (deg) data from X-ray crystal structure for iron (II) complex **1-μ-oxo** compared to the computed values (B3LYP/6-31G(d)-gas) of the complex in different spin states. Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, orange, red and green ellipsoids represent C, N, Fe, O, and Cl atoms respectively.

Finally, **4-OH$_2$**, prepared from p-chloro-substituted ligand **L4**, iron(II) chloride and silver triflate, was crystallized and analyzed for its geometrical properties. A cis-α complex in a high spin state was obtained, as shown by the computed bond length data given in **Table 1.3**. It displays π-π stacking interactions between the aromatic rings in which the tetradentate ligand bends slightly out of the plane of a true octahedral geometry to optimize this stabilizing noncovalent interaction.

Bond Length and Angle	*X-ray*	*Singlet*	*Triplet*	*Quintet*
Fe-N^1 (Å)	2.168	1.989	1.965	2.176
Fe-N^2 (Å)	2.141	1.987	1.973	2.177
Fe-N^3 (Å)	2.278	2.047	2.129	2.186
Fe-N^4 (Å)	2.247	2.046	2.052	2.186
N^1-Fe-N^2 (deg)	164.8(7)	178.1(8)	176.9(9)	159.2(8)
N^3-Fe-N^4 (deg)	91.7(7)	98.0(3)	106.0(8)	91.6(8)

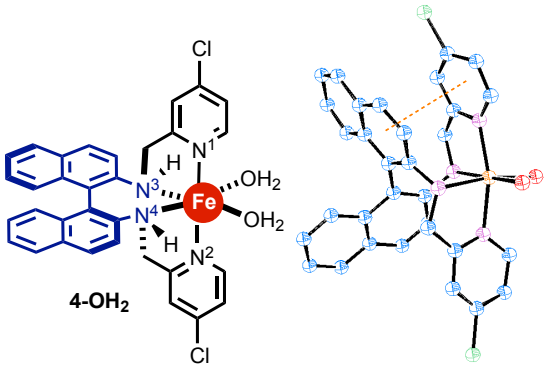


Table 1.3 Selected bond length (Å) and angle (deg) data from X-ray crystal structure for iron (II) complex **4-OH$_2$** compared to the computed values (B3LYP/6-31G(d)-gas) of the complex in different spin states. Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, orange, red and green ellipsoids represent C, N, Fe, O, and Cl atoms respectively.

The effect of using silver triflate or silver hexafluoroantimonate in the reaction on catalyst geometry was further probed by synthesizing and obtaining single crystals of manganese complexes with the **L1**. The synthetic scheme for the preparation of the manganese complexes is given in the supporting information as it is identical to the iron complex scheme apart from manganese (II) chloride having been substituted for iron (II) chloride. Like iron, the complex resulting from the unsubstituted ligand **L1** and manganese with silver triflate yielded a cis-α complex **Mn-1'-OTf** (**Figure 1.21**).

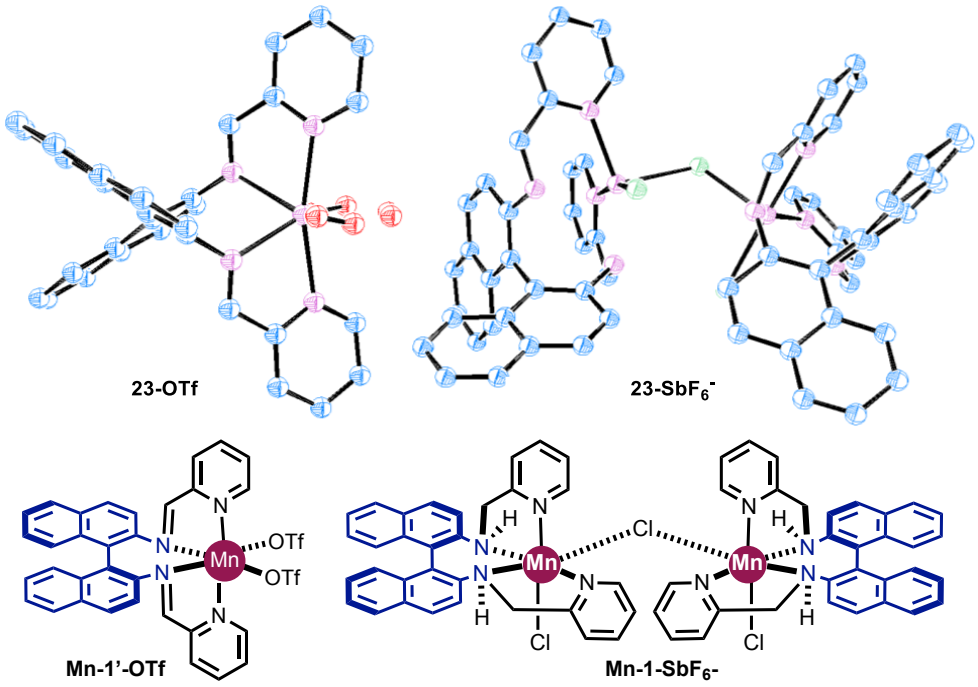


Figure 1.21 Solid-state structures of chiral diamine manganese catalysts **Mn-1'-OTf** and **Mn-1-SbF_6^-.** Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, brown, red and green ellipsoids represent C, N, Mn, O, and Cl atoms respectively.

Also similar to iron, the manganese complex prepared with silver hexafluoroantimonate in place of silver triflate afforded the cis-β dimer **Mn-1-SbF_6^-** where the two manganese atoms are linked by a bridging chlorine. Dimers of manganese complexes have been reported in the literature yet mainly in the cis-α geometry.[42] A few key differences between the iron and manganese complexes should be noted. In structure **Mn-1'-OTf**, the unsubstituted ligand **L1** has been oxidized to the imine, presumably by exposure to air showing the manganese complexes may be more sensitive to these conditions. Additionally, in both **Mn-1'-OTf** and **Mn-1-SbF_6^-**, there is no π-π stacking interaction as was observed in the iron complexes **1-OH_2** and **4-OH_2**. These notable differences make iron an attractive target for further research to understand the subtleties of the role this metal plays in affected ligand electronic and steric properties.

Further, two crystals of ligand scaffolds were obtained and analyzed by x-ray crystallography. The unsubstituted **L1** ligand showed the lack of noncovalent interactions between the aryl rings in the ligand alone, further supporting the claim that it is the iron center which restricts the geometry of the complex, causing the observed $\pi - \pi$ stacking. Additionally, a crystal structure of a possible byproduct in the ligand synthesis was obtained. The monosubstituted methoxy-functionalized ligand, a byproduct in the synthesis, crystallized as well (**Figure 1.22**).

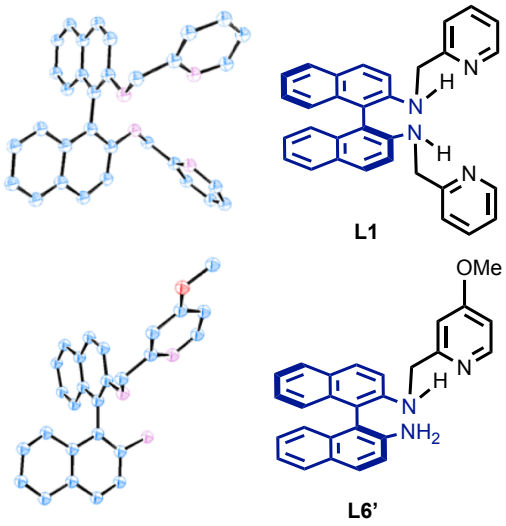


Figure 1.22 X-ray crystal structures of unsubstituted ligand **L1** (top) and monosubstituted ligand **L6'** (bottom). Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, and red ellipsoids represent C, N and O atoms respectively.

1.3.3 Variable Temperature (vt) NMR Studies

Having obtained data on the geometry of the select iron complexes, the spin state of the iron complexes was characterized. Thus far, x-ray crystallographic analysis of the three iron complexes supported a high spin (quintet) iron center in the solid state. However, the spin state in solution of the complexes also could be investigated using an NMR

technique known as Evans' method.[43] The magnetic moment of the iron complexes was evaluated by Evans' method at room temperature and the results, showing the complexes to range from intermediate to high spin are summarized in **Figure 1.23**.

Entry	[Fe]	R	μ_{eff}
1	**1-SbF_6^-**	H	3.74
2	**1-OTf**	H	0.95
3	**2-OTf**	o-Me	3.75
4	**3-OTf**	p-Me	4.42
5	**4-OTf**	p-Cl	3.09
6	**5-OTf**	p-NMe2	3.64
7	**6-OTf**	p-OMe	2.70
8	**7-OTf**	p-Br	4.47
9	**9-OTf**	quinoline	4.40

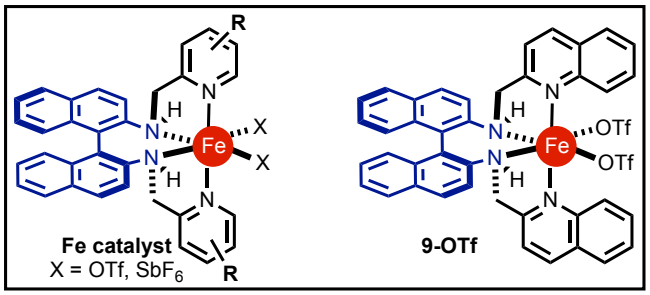


Figure 1.23 Magnetic moment of the iron complexes determined from ^{1}H NMR in CD_3CN at room temperature. With the exception of entry 2 (intermediate spin, triplet), the complexes all in the high spin (quintet) states.

After obtaining the spin state of **1-OTf** at room temperature by Evans' method (μ_{eff} = 0.99), the effect of temperature on spin state was probed by variable temperature NMR analysis of iron complex **1-OTf**, of which there was a crystal structure (**Table 1.1**). ^{1}H NMR spectra of compound **1-OTf** were recorded in d_3-acetonitrile at temperatures ranging from 233 K to 343 K (**Figure 1.24**). These experiments are done over the course of two days due to limitations with temperature changes in the instrument. First, the spectra were recorded every 10K from 298 K to 343 K. During this period, the CH_2Br_2 peak is shifted

from the unpaired electrons in compound **1-OTf** with an increasing spin state as the temperature increases from an effective magnetic moment of 0.99 to 2.13. Compound **1-OTf** retains the increased spin state at room temperature which may be a result of ineffective cooling of the sample. When cooled to -40 °C, the spin state of compound **1-OTf** decreases again to an effective magnetic moment of 0.81. This experiment was replicated with the same trend observed.

T(K)	μ_{eff}
303	0.99
313	0.80
323	1.13
333	2.02
343	2.13
302	1.78
233	0.98
243	0.95
253	0.91
263	0.82
273	0.81
283	0.85
293	0.95

Figure 1.24 Magnetic moment determined from variable temperature ^{1}H NMR of compound **1-OTf** in CD_3CN at temperatures from 233 K to 343 K. The magnetic moment steadily increases from 0.99 to 2.13 as the temperature increases.

Further, geometry changes in the solid state were studied to understand the effect of temperature on the geometry of these iron complexes. Preliminary experiments during the vt NMR studies show that the iron complex **1-SbF_6**$^{-}$ changes color upon heating and the UV-vis spectrum has an additional peak at 557 nm, leading to suspicions of a geometry change with temperature (**Figure 1.25**).

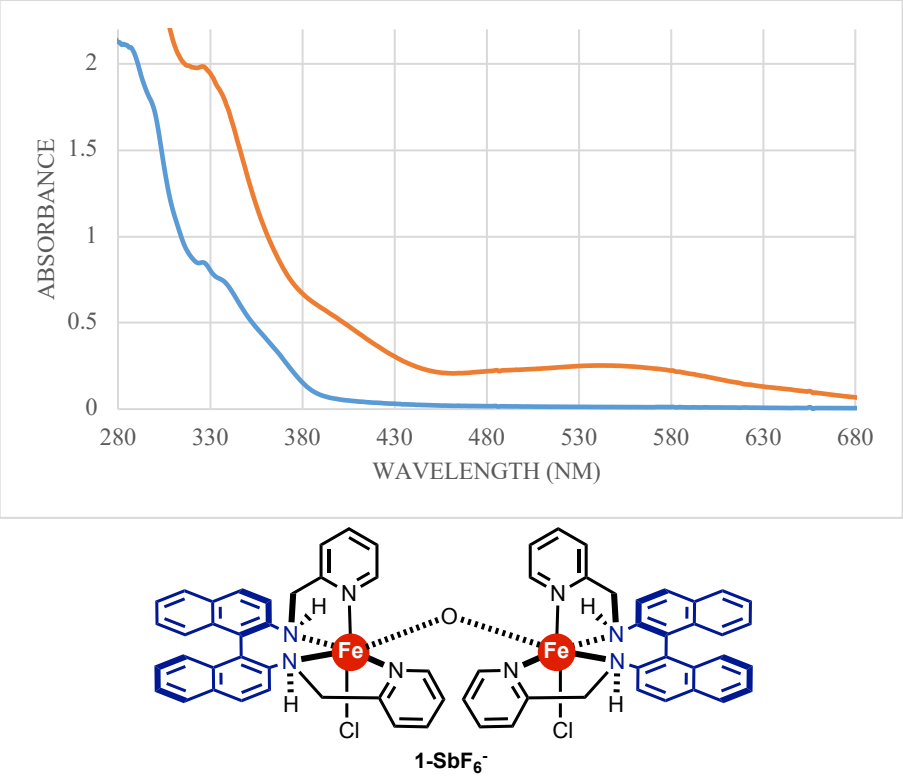
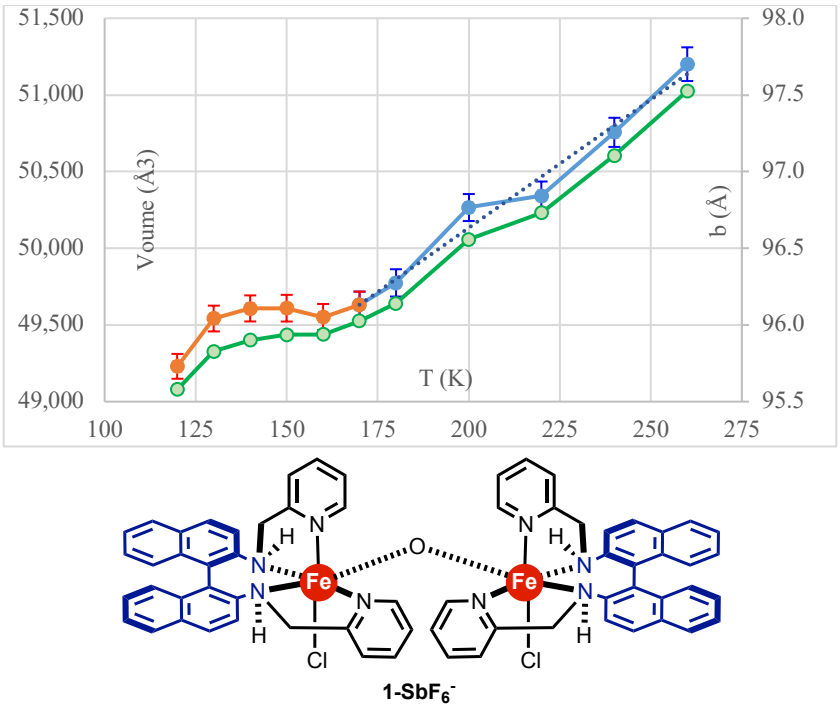


Figure 1.25 UV-vis spectrum of Complex **1-SbF$_6$**$^-$ before heating in the vt NMR experiment (blue) and after heating (orange). There is an additional λ_{max} peak at 557 nm after heating.

Studies by Garcia and coworkers reveal that temperature changes may cause geometry changes in iron (II) complexes.[44] To ensure that only the spin state was affected by temperature rather than the geometry, temperature-dependent x-ray crystallographic analysis was performed on **1-SbF$_6$**$^-$ The unit cell was analyzed every 10 K from 260 K to 120 K and **1-SbF$_6$**$^-$ was found to retain its cis-β geometry throughout the temperature range. The unit cell parameters (V, b) were plotted as a function of temperature (**Figure 1.26**) and it was shown that volume increases with increasing temperature, as expected due to the increased thermal energy at higher temperatures. This study verified that the geometry of the iron complexes is stable with low temperature as well as under air as this study was not performed in an inert environment. This result is very promising that the iron complexes will be stable for C-H oxidation reactions.

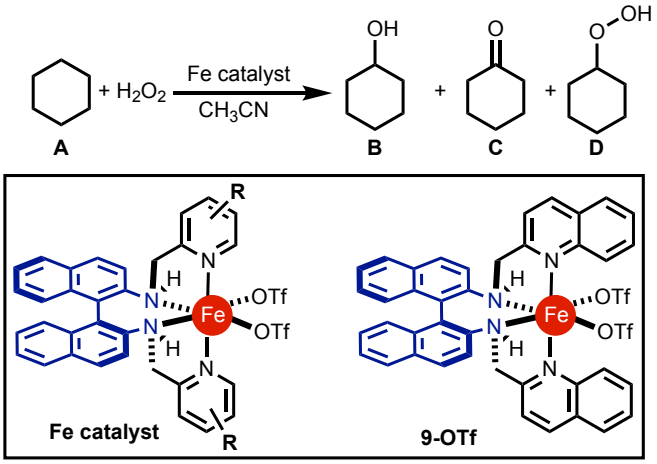


1-SbF$_6^-$

Figure 1.26 Unit cell parameters volume (Å^3) and b (Å) of **1-SbF$_6^-$** as a function of temperature from 120 K to 260 K. The unit cell parameters increase in volume and length with increasing temperature but the geometry of the molecules in the unit cell remains the same.

1.3.4 Fe-catalyzed C(sp^3)-H Oxidations

The complexes were tested for their ability to promote C(sp^3)-H oxidations, specifically the oxidation of cyclohexane. First, the iron complexes prepared were tested for their catalytic activity in the reaction, starting at the low catalyst loading of 0.5 mol% owing to the high molecular weight of the complexes. Iron complex **9-OTf** gave the highest yield of cyclohexanol (9%, **Table 1.4**, entry 8) at a loading of 0.5 mol%.

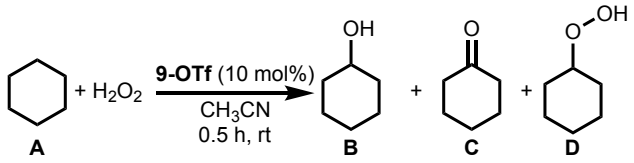


Entry	R	Catalyst Loading [mol%]	GC Yield (**B**) [%]	GC Yield (**C**) [%]	Presence of **D**
1	*p*-Cl	0.5 mol%	5%	trace	Y
2	*p*-OMe	0.5 mol%	3%	0%	Y
3	*p*-Br	0.5 mol%	3%	trace	Y
4	*p*-Me	0.5 mol%	5%	2%	Y
5	*o*-Me	0.5 mol%	0%	0%	N
6	*p*-NMe_2	0.5 mol%	1%	0%	Y
7	**9-OTf**	0.5 mol%	9%	trace	Y

Table 1.4 Evaluation of catalytic activity of iron complexes. The reaction was performed with cyclohexane **A** (0.1 mmol, 1.0 equiv.), iron catalyst (0.01 mmol, 0.1 equiv.), acetonitrile (1.0 mL), and hydrogen peroxide (0.36 mmol, 3.6 equiv.) which was added iteratively three times (every 10 minutes) as a solution in acetonitrile over 90 seconds as described by White.[34a] The yields of **B** and **C** were determined by GC/MS using biphenyl as internal standard using response factors determined using standards of cyclohexanol **B** and cyclohexanone **C** purchased from Sigma-Aldrich.

Following this result, the catalyst loading of **9-OTf** was increased to 10 mol%, giving a 58% yield of cyclohexanol (**Table 1.5**, entry 3). Further increasing the catalyst

loading to 20 mol% (**Table 1.5**, entry 4) saw a decrease in yield of cyclohexanol, so the loading was kept at 10 mol%. Other iron complexes, including **1-OTf** and **3-OTf**, gave a low yield of oxidation products (**B, C**) even at the higher loading of 10 mol% (**Table 1.5**, entries 1 and 2). Increasing the loading of hydrogen peroxide from 3.6 equiv. to 10 equiv. resulted in a decrease in yield of **B** (48%, **Table 1.5**, entry 5) as did decreasing the loading of H_2O_2 to 1.2 equiv. (31%, **Table 1.5**, entry 6). The addition of 0.5 equiv. of acetic acid as used in White's procedure[34a] resulted in a dramatic decrease in yield of cyclohexanol (12%, **Table 1.5**, entry 7). A control experiment using $FeCl_2$ in place of **9-OTf** resulted in a lower yield of cyclohexane (4%, **Table 1.5**, entry 9), showing that Fenton chemistry of iron does not contribute significantly to the oxidation reaction. Other control experiments showed that the ligand **L9** alone did not contribute to oxidation (**Table 1.5**, entry 10) nor did hydrogen peroxide alone (**Table 1.5**, entry 11).



Entry	Deviations from standard conditions	GC Yield (**B**) [%]	GC Yield (**C**) [%]	Presence of **D**
1	**1-OTf** (10 mol%)	8	2	Y
2	**3-OTf** (10 mol%)	7	2	Y
3	no deviations	58	13	Y
4	**9-OTf** (20 mol%)	52	0	N
5	10 equiv. of H_2O_2	48	13	Y
6	1.2 equiv. of H_2O_2	31	6	Y
7	0.5 equiv. of AcOH	12	8	Y
8	2 mL CH_3CN	20	8	Y
9	using $FeCl_2$ (10 mol%)	4	15	N
10	using **L9** (10 mol%)	0	0	N
11	No **9-OTf**	0	0	N

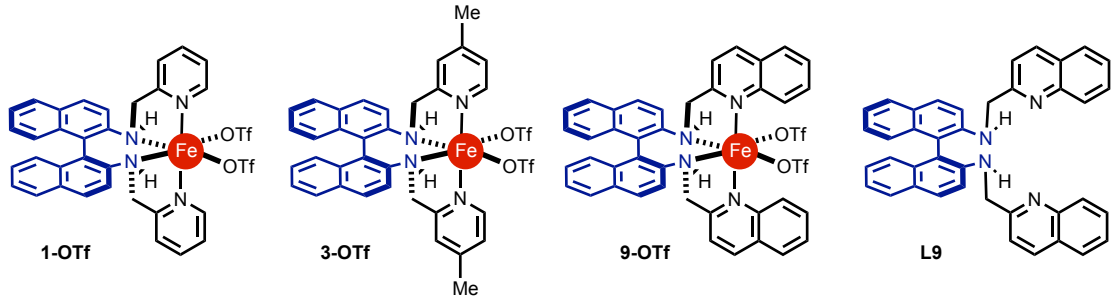


Table 1.5 Evaluation of reaction conditions. The reaction was performed with cyclohexane **A** (0.1 mmol, 1.0 equiv.), iron catalyst **9-OTf** (0.01 mmol, 0.1 equiv.), acetonitrile (1.0 mL), and hydrogen peroxide (0.36 mmol, 3.6 equiv.) which was added iteratively three times (every 10 minutes) as a solution in acetonitrile over 90 seconds as described by White.[34a] The yields of **B** and **C** were determined by GC/MS using biphenyl as internal standard using response factors determined using standards of cyclohexanol **B** and cyclohexanone **C** purchased from Sigma-Aldrich.

Additionally, *cis*-dimethylcyclohexane was oxidized using conditions described by Costas[45] (1.2 equivalents of peroxide, 0ºC). Since acetic acid was shown to have a detrimental effect on the yield (**Table 1.5**, entry 7), this additive was not used in the

reaction. GC/MS results revealed a mixture of alcohol and ketone isomers using these conditions. At room temperature, only one alcohol product *cis*-dimethylcyclohexanol **B** is formed based on GC/MS results and *cis*-dimethylcyclohexanone **C** (**Figure 1.27**).

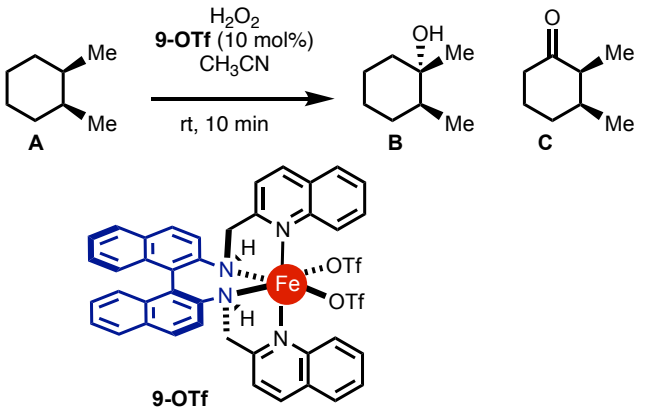


Figure 1.27 Oxidation of *cis*-dimethylcyclohexane **A** into *cis*-dimethylcyclohexanol **B** and dimethylcyclohexanone **C** catalyzed by **9-OTf.**

Finally, the oxidation of (R)-menthyl acetate was performed using conditions described by White.[34a] Initially, the oxidation was carried out in the absence of acetic acid but no oxidation product was observed by GC/MS. For comparison, the reaction was carried out again, this time in the presence of acetic acid. Surprisingly, oxidation product was observed in the GC/MS this time and was further confirmed by ^{1}H NMR analysis to be compound **B** (**Figure 1.28**).

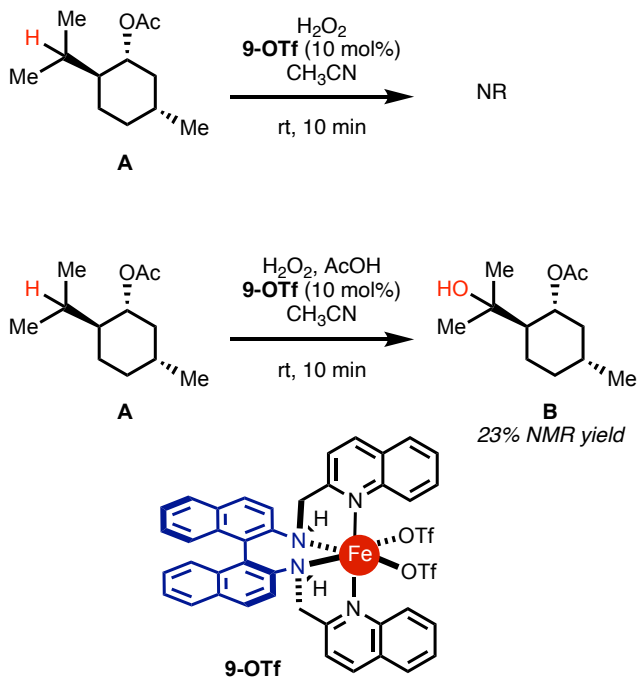


Figure 1.28 Oxidation of (R)-menthyl acetate catalyzed by **9-OTf.**

1.4 Conclusion

Site-selective iron-catalyzed oxidations of unactivated alkanes are challenging due to the strength and ubiquity of C(sp^3)-H bonds as well as the variation in key properties of the iron complexes (i.e. spin state, geometry). In effort to design new systems, first the geometry and spin state of known examples of tetradentate N_4-ligand scaffolds used for iron-catalyzed C-H oxidation reactions were studied to identify a computational model for the prediction of spin state and geometry. Using this method, iron complexes with a predicted spin state and geometry were prepared. Experimentally, the choice of silver salt used in the synthesis was shown to influence the resulting geometry of the iron complex. Specifically, silver triflate results in a monomer complex in the cis-α geometry while silver hexafluoroantimonate leads to a dimer, cis-β complex. As noted by White and Britovsek, the cis-α complex is known to be catalytically active. This catalytic activity was observed

in the promotion of cyclohexane oxidation for many of the catalysts prepared and can be delved further into to obtain a greater understanding of this reaction.

Chapter 2: Mechanism of Iminium Salt-Catalyzed C(sp^3)-H Amination: Factors Controlling Hydride Transfer versus H-atom Abstraction

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2.1 Abstract

Carbon−nitrogen bonds are prevalent in pharmaceuticals, natural products, and biologically relevant molecules such as nucleic acids and proteins. Intermolecular amination of C(sp^3)−H bonds by catalytic nitrene transfer is a promising method for forging C−N bonds. An organocatalytic approach to nitrene transfer by way of an iminium salt offers a site-selective method for C(sp^3)−H amination. Understanding of this amination mechanism including the nature of the relevant intermediates and the factors controlling the mechanism of the N−H bond formation step would aid in the rational design of catalysts and C(sp^3)−H amination methods. In this work, I used quantum mechanical methods and molecular dynamics simulations to study the mechanism of the iminium salt-catalyzed C(sp^3)−H amination via nitrene transfer.[46] Dispersion-corrected density functional theory calculations provide support for an open singlet biradical species which exists in equilibrium with the lower energy triplet species. Calculations further reveal that, while the singlet biradical species undergoes N−H bond formation by a hydride transfer process, the triplet species forms the N−H bond by H-atom abstraction. Molecular dynamics simulations show that fast rebound of the carbon substrate following N−H bond formation does not occur. A predictive model for mode of activation and site selectivity that is consistent with experimental observations is presented.

2.2 Introduction

Nitrogen is an abundant atom in pharmaceuticals, natural products, and molecules central to life such as nucleic acids and proteins and its prevalence has led to a need for the development of methods for the formation of C−N bonds.[47,48] In particular, intermolecular amination of C(sp^3)−H bonds via catalytic nitrene transfer holds great promise for streamlining synthesis, and applications of this reaction in the late-stage functionalization of bioactive compounds have captured widespread interest.[49,50] However, modulation of site- and stereoselectivity in these reactions via catalyst control is still a fundamental challenge.[51]

The discovery of different modes of catalytic nitrene transfer that are distinct from existing transition metal-catalyzed methods holds promise for the development of reactions exhibiting complementary selectivity.[52] Recently, the Hilinski laboratory disclosed the first example of organocatalytic nitrene transfer and demonstrated the method's capability to promote site-selective C(sp^3)−H amination[53] (**Figure 2.1**) and aziridination.[54] An iminium salt catalyst is proposed to react with an iminoiodinane nitrene precursor to produce the active oxidant, a diaziridinium salt,[55] which then reacts with the substrate to produce the observed product and regenerate the catalyst (**Figure 2.1**). This reaction extends organocatalytic atom-transfer oxidation reactions, which are well established for oxygen transfer via dioxirane and oxaziridinium intermediates, to nitrene transfer. Further, it shows the possibility of the development of sustainable strategies for atom-transfer C−H amination that are outside of the current transition metal-catalyzed methods.

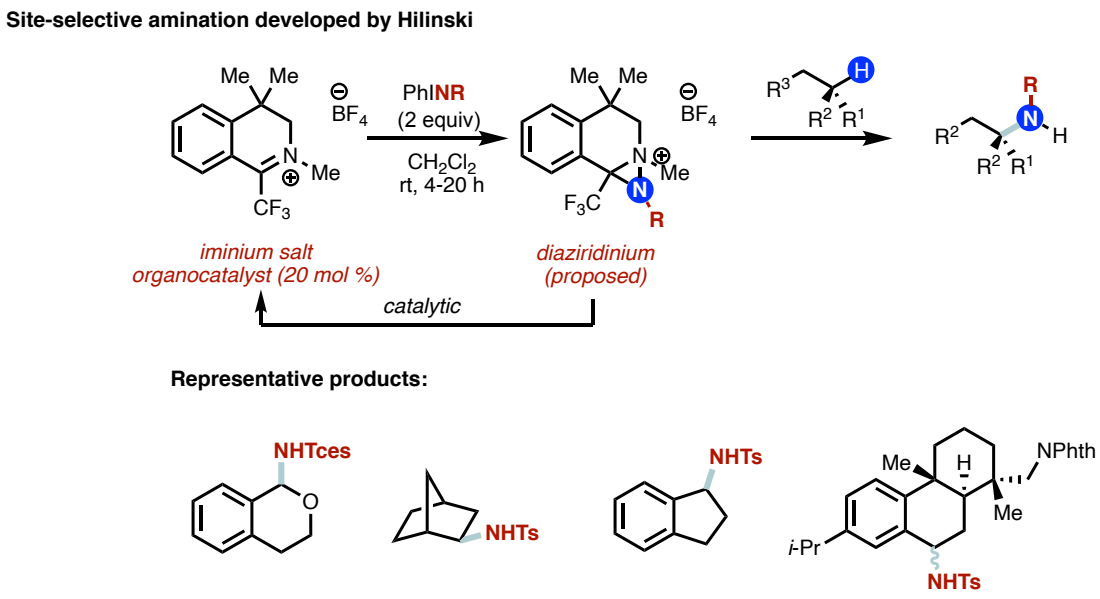


Figure 2.1 Iminium salt-catalyzed C–H amination developed by the Hilinski group and representative products. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

Initial investigations by Hilinski et al. into the scope of this iminium-catalyzed C−H amination revealed its ability to oxidize weak C(sp^3)−H bonds such as benzylic C−H bonds, α-positions of ethers and protected amines, and highly activated aliphatic substrates (**Figure 2.1**). Along with the work on the catalytic method and its scope, Hilinski reported preliminary mechanistic investigations which supported the initial hypothesis that the reaction of the iminoiodinane with the iminium catalyst produces an intermediate which resembles a nitrenoid species in reactivity. In addition, experiments revealed a dependence of yield on the iminium salt structure and a limited role of the tetrafluoroborate counterion in promoting the observed reactivity, supporting the hypothesis that the iminium ion is involved in the formation of an organic nitrenoid equivalent.[52] This initial conclusion was also supported by control experiments using tetrabutylammonium tetrafluoroborate as an organic-soluble source of the counterion (**Figure 2.2**). No reaction was observed either in the absence of a catalyst or with catalytic amounts of nBu$_4$NBF$_4$. In addition to providing

additional evidence of a limited role for tetrafluoroborate in initiating nitrenoid transfer from iminoiodinanes, this experiment also indicates that the iminium salt is not simply acting as a phase-transfer catalyst.

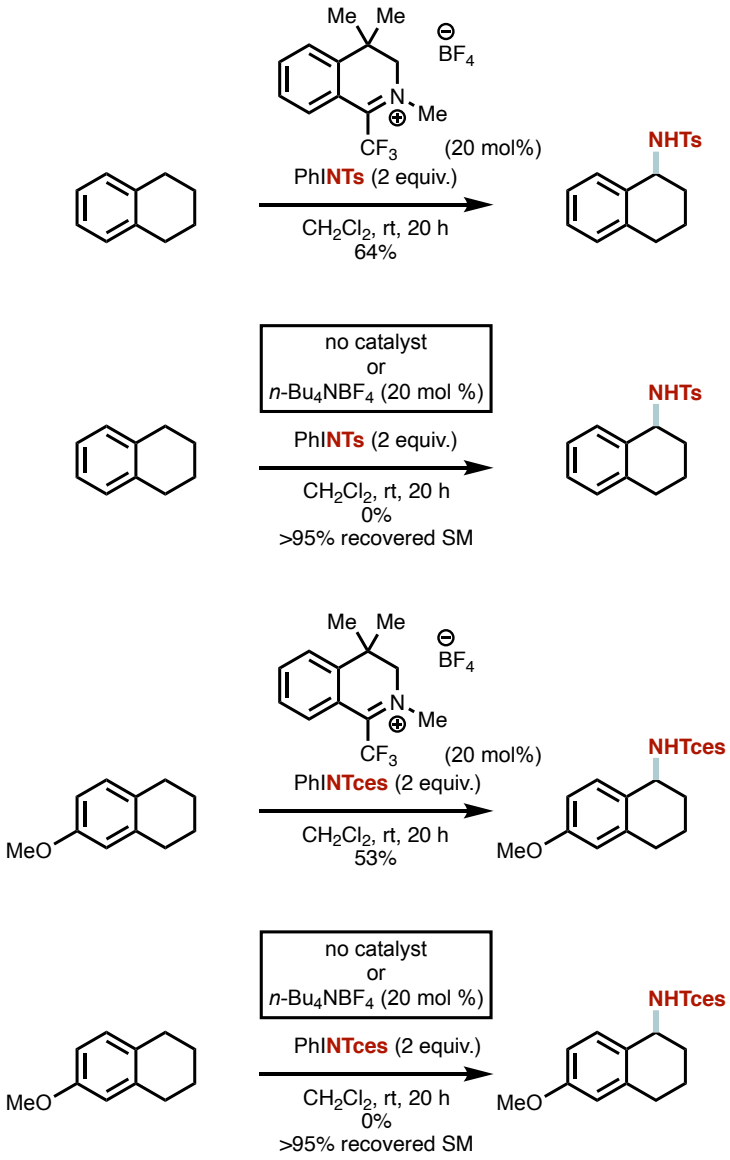


Figure 2.2 Control experiments by Hilinski confirming a key role for the iminium. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

Despite these initial experimental studies, substantial mechanistic questions remain, such as the potential existence and fate of the proposed diaziridinium intermediate.

For example, diaziridinium intermediate **1a** could undergo N−N homolysis to form **1b** or heterolysis to form **1c** (**Figure 2.3**). Further, **1b** and **1c** could interchange via an intramolecular single electron transfer (SET) and can undergo intersystem spin crossing to form singlet or triplet species. Moreover, contrary to the rich mechanistic literature of oxyfunctionalization of C(sp^3)−H bonds (i.e., dioxirane and Fe-oxo chemistry), there is a deficit of information on the mechanisms of azafunctionalization of C(sp^3)−H bonds.[56] A detailed understanding of the mechanism will allow for a broadened substrate scope and will help to address current challenges in C−H functionalization by rationally designing catalysts and methods. In this work, I used quantum mechanical calculations and quasi-classical direct-dynamics simulations to understand the nature of the active species, elucidate the mechanism for C−H activation, and gain insights into the origin of C−H site selectivity. Overall, a refined mechanistic proposal that is consistent with experimental observation and a predictive model for mode of activation and site selectivity is presented.

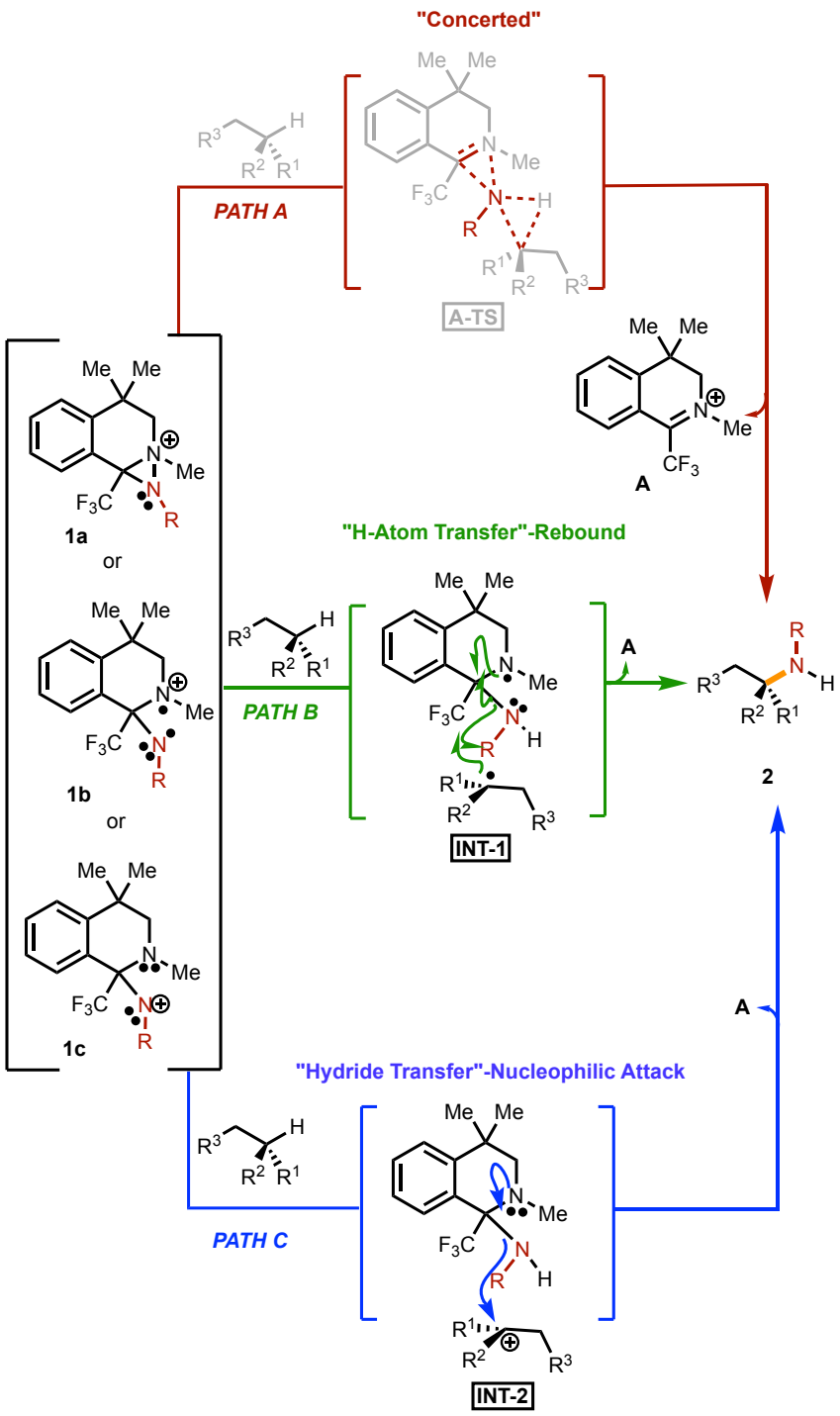


Figure 2.3 Possible mechanisms for iminium salt-catalyzed aliphatic C–H amination**.** Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

2.3 Results and Discussion

2.3.1 Reaction of Iminium Salt with Amination Reagent

The mechanistic analysis is broken down into five parts based on the computational findings: (1) mechanistic proposal leading to the production of four distinct amidyl-iminium and diazaridinium intermediates, (2) analysis of the nature of these intermediates, (3) mechanistic proposal for C−H activation from the lowest energy of these intermediates, (4) effect of carbon substrate on the mechanism of C−H activation, and (5) molecular dynamics simulations to investigate the time scale for C−H activation and approximate lifetime of the purported intermediates.

The mechanistic studies were started by constructing the potential energy surface using dispersion-corrected DFT (UB3LYP-D3/6-311+G(d,p)- SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)- LANL2DZ(I)-CPCM(dichloromethane)).[57,58,59,60] DFT methods were chosen for the computational analysis because DFT methods, and in particular the UM06-2X functional, correctly predict experimental trends for open-shell species with low computational cost compared with multireference methods (e.g., CASPT2).[61,62]

To initiate exploration of the mechanism, I started by studying the imininum organocatalyst. As shown in **Figure 2.4**, the iminium organocatalyst can adopt a downward (**A**) or an upward (**A'**) puckered 5-membered ring conformation. Since these two conformations are nearly isoenergetic, the computational studies were initiated from these two conformations.

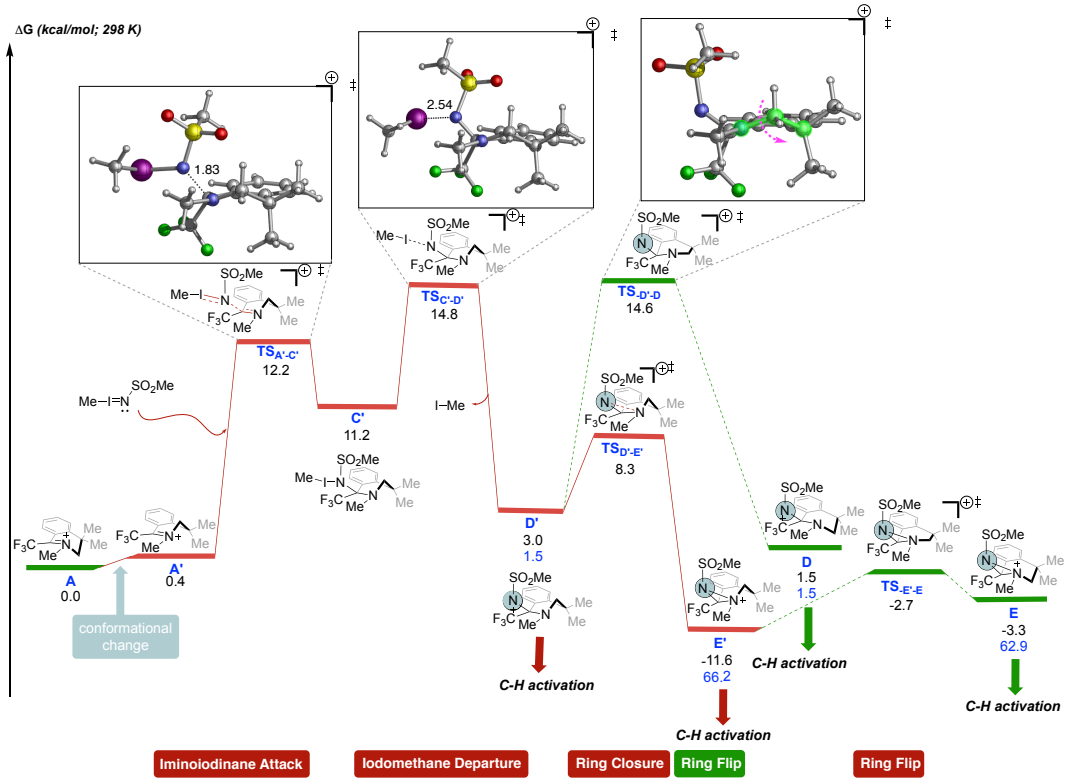


Figure 2.4 Energetics of reaction coordinate pathway leading to the formation of open-amidyl-iminium (**D** and **D'**) and closed-form (**E** and **E'**) diaziridinium intermediates. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level. Singlet energies are given in black and triplet energies are in blue. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

As shown in **Figure A2.1** in Appendix 2, the iminium ion organocatalyst **A** can undergo nucleophilic attack by the iminoiodinane MeINMs via $\mathbf{TS_{A\text{-}B}}$ (barrier of 19.7 kcal/mol) to form adduct **B**, uphill by 17.3 kcal/mol. In turn, complex **B** can then undergo 3-membered ring closure via $\mathbf{TS_{B\text{-}E}}$ (overall barrier of 26.1 kcal) with concomitant release of the iodomethane to form the "closed-form" diaziridinium **E** intermediate (see **Figure A2.1**), overall 3.3 kcal/mol downhill in energy.

This (singlet) intermediate **E** could promote C(sp^3)–H activation by engaging with the alkane substrate (vide infra) or can first undergo a homolytic ring opening via the

singlet spin state to form open intermediate **D** via $\mathbf{TS_{E\text{-}D}}$ (barrier of only 13.8 kcal/mol) and then promote C(sp^3)−H activation (vide infra). Notably, in contrast to the closed-formed amidyl-iminium species **E** (the singlet−triplet gap is >60 kcal/mol), the singlet and triplet "open-form" biradical species **D** are isoenergetic. Thus, both singlet and triplet "open-form" **D** intermediates were considered and only the singlet spin state of **E** for C−H activation. A heterolytic cleavage transition state, located using restricted DFT, leading to the closed-shell nitrenium intermediates is found to be much higher in energy (23.0 kcal/mol; see **Figure A2.2** in Appendix 2) and was not considered further.

Alternatively, **A** could undergo a conformational change to form **A'** (not calculated) followed by nucleophilic attack by MeINMs via the lower energy $\mathbf{TS_{A'\text{-}C'}}$ (**Figure 2.4**; barrier of 12.2 kcal/mol compared to barrier of 19.7 kcal/mol for $\mathbf{TS_{A\text{-}B}}$) to form adduct **C'**. Presumably, $\mathbf{TS_{A\text{-}B}}$ is higher in energy due to the negative steric interactions between the neighboring axial groups, which are not present in $\mathbf{TS_{A'\text{-}C'}}$ (See **Figure A2.3** in Appendix 2).

Intermediate **C'** can then undergo a concerted ring closure with simultaneous removal of the iodomethane via $\mathbf{TS_{D''\text{-}E''}}$ (barrier is 16.8 kcal/mol) to give the diaziridinium **E'**. Notably, calculations favor the stepwise process in which the MeI dissociation occurs first (via $\mathbf{TS_{C'\text{-}D'}}$) to form an amidyl-iminium intermediate **D'**, which can quickly undergo ring-closing (via $\mathbf{TS_{D'\text{-}E'}}$) leading to **E'** ($\mathbf{TS_{D''\text{-}E''}}$ versus $\mathbf{TS_{D'\text{-}E'}}$). Further, a conformational change transition state ($\mathbf{TS_{B\text{-}C'}}$) was found to have a low energy barrier that connects "down" and "up" I(II) intermediates, **B** and **C'**, respectively, as well as two other conformational change transition states ($\mathbf{TS_{D\text{-}D'}}$ and $\mathbf{TS_{E\text{-}E'}}$), which connect the down **D** and

E intermediates and the up **D'** and **E'** intermediates. Given that singlet and triplet "open" amidyl- iminium intermediates (**D** and **D'**) are nearly isoenergetic, in principle, C−H activation could occur from the singlet or triplet spin states. Thus, singlet and triplet open-(amidyl-iminium) and closed-form (diaziridinium) intermediates (**D, D', E,** and **E'**) were considered as potential species for C−H activation.

2.3.2 Nature of Amidyl-Iminium and Diaziridinium Intermediates

To better understand the mechanism of C−H activation, the electronic nature of the open- and closed-form intermediates was investigated. The singlet and triplet forms of both geometries were located (**Figure 2.4**). As shown in **Figure 2.5**, the singlet−triplet gap of these amidyl-iminium intermediates is small (<2 kcal/mol).

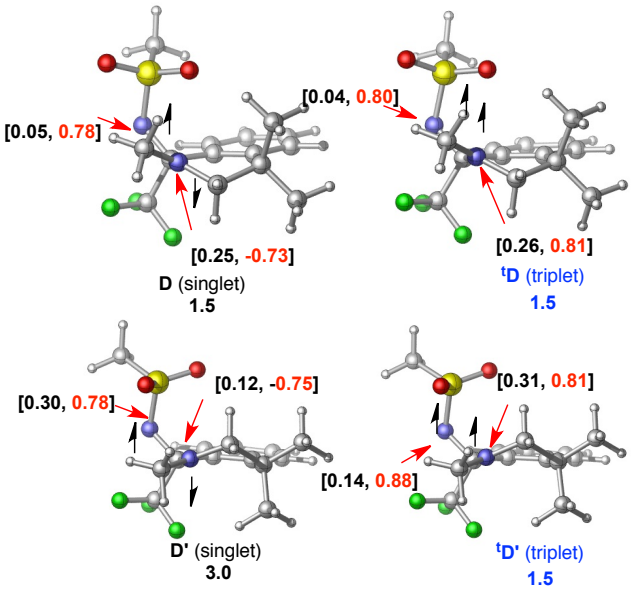


Figure 2.5 Closer inspection of the open-form singlet (**D**, **D'**) and triplet (**^{t}D**, **^{t}D'**) amidyl-iminium intermediates. Mulliken charges and spins of the nitrogen atoms are shown in black and red respectively. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane) level of theory. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

Further, closer inspection of the open-form amidyl-iminium intermediates revealed that the singlet nitrenium **D** and **D'** can be classified as biradical amidyl-iminium species (i.e., **1b** in **Figure 2.3**) as noted by the Mulliken spins at both nitrogen atoms of close to ±1.[63] The open triplet nitrenium intermediates **^{t}D** and **^{t}D'** are also biradicals resembling **1b** (**Figure 2.3**) with Mulliken spins on the nitrogen atoms of close to +1. As shown by Gassman, the singlet open nitrenium species could undergo spin inversion to produce the lower- energy triplet species, which can promote a distinct mode of C−H activation (vide infra).[64] On the other hand, the energy difference between the diaziridinium singlet and triplet spin states (**Figure 2.6**) was significantly higher in energy (>65 kcal/mol); thus, the triplet spin states from **^{t}E** and **^{t}E'** were not considered further.

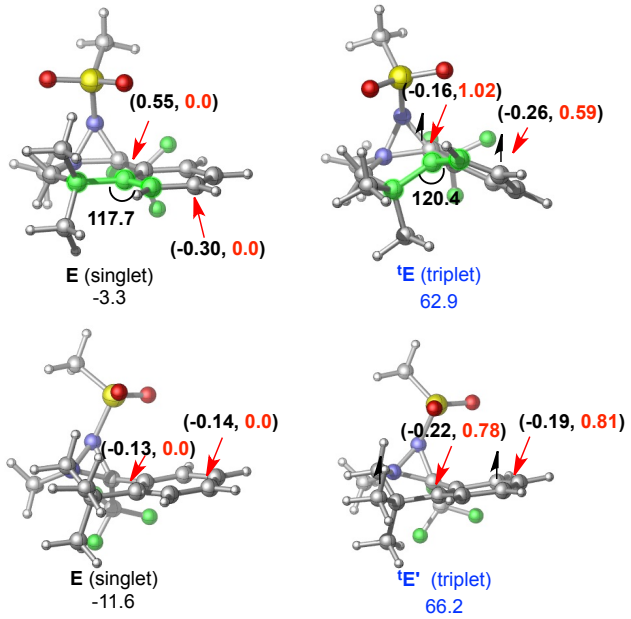


Figure 2.6 Comparison between the singlet and triplet states of the *diaziridinium* intermediates **E, E'** and **^{t}E, ^{t}E'**. Relevant Mulliken charges and spins are given in black and red respectively and relevant bond angles (º) in black. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

This large energy gap can be attributed to the disruption of aromaticity as evidenced by the localization of the electron spin in the aryl ring. For example, the free radical in the triplet form **^{t}E** is located at the phenyl carbon (indicated by Mulliken spin of 1.02; red). Overall, these results suggest that the closed-form diaziridinium **E** and **E'** exist only in the singlet state, which are significantly lower in energy than the triplet closed-form species. On the contrary, the singlet state (amidyl-iminium) of the open form is in equilibrium with the triplet biradical state. Electrostatic potential maps also support the nature of the intermediates as described above (See **Figures A2.4** and **A2.5** in Appendix 2).

2.3.3 Mechanism for C-H Activation

Having investigated the nature of the open and closed intermediates, the viable pathways for C−H activation by the amidyl-iminium and diaziridinium intermediates were explored. For simplicity, only the lowest-energy pathway from the open intermediates (**Figure 2.7**) is discussed, since the pathways for C−H activation from the thermodynamically favored closed-formed diaziridinium intermediates **E** and **E'** are higher in energy (See **Figures A2.6** and A**2.7** in Appendix 2 for the full pathway).

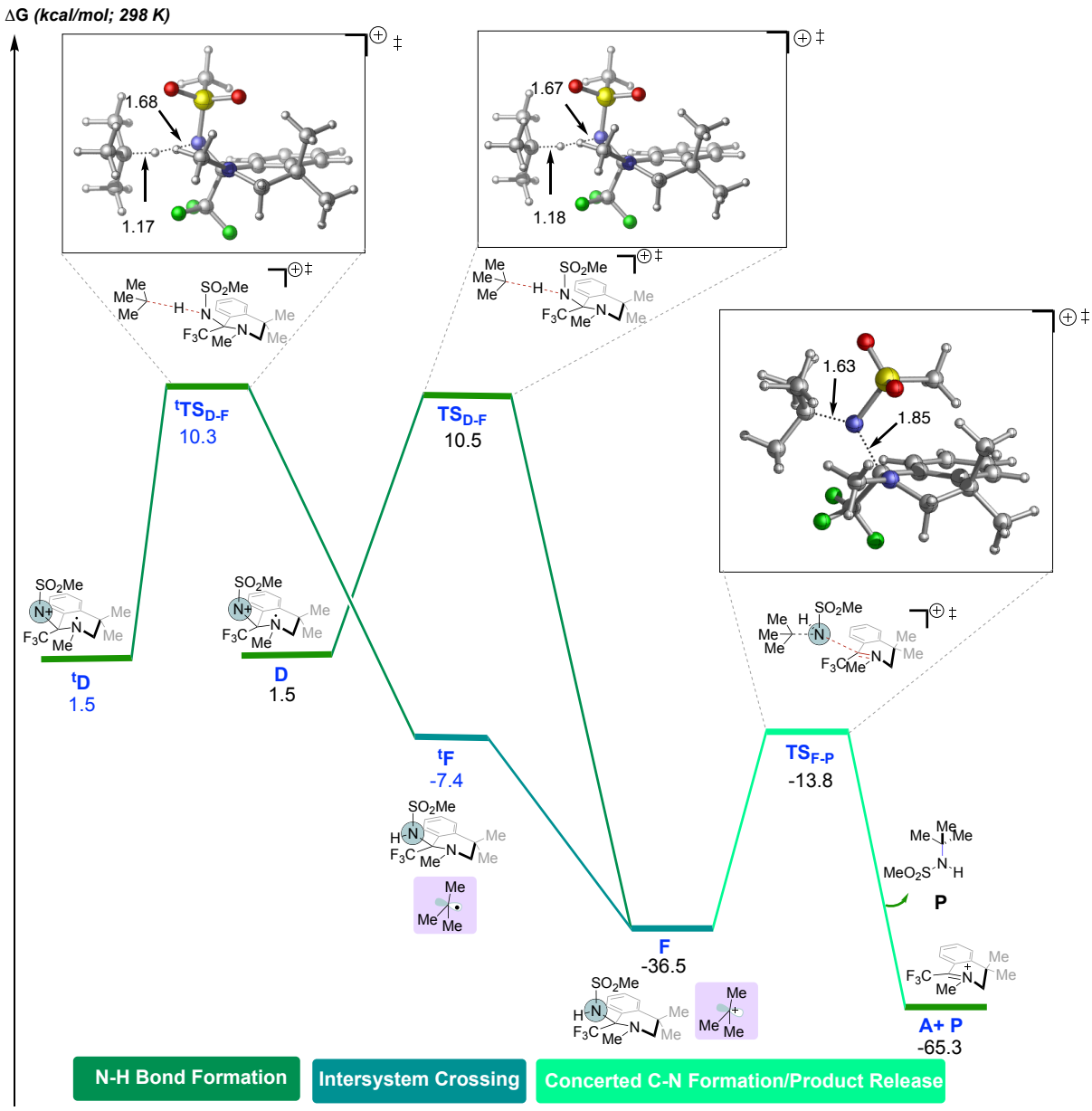


Figure 2.7 Lowest energy pathways leading to C-H activation via open diaminium species **D** which undergoes N-H bond formation to give **F**. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory. Singlet energies are given in black and triplet energies are in blue. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

Further, initially the investigation was started with the tertiary alkyl radical as the substrate although later the effects of other C−H bonds were also explored. It was

particularly interesting to investigate the possibility of a hydrogen-atom-transfer (HAT) mechanism (homolytic cleavage) as opposed to a hydride transfer mechanism (heterolytic cleavage) from the putative amidyl-iminium intermediates. Hydride transfer models have been proposed for oxidation reactions catalyzed by oxoammonium salts as well as for intramolecular C−H amination, which led to the hypothesis that this process was plausible for the nitrenium species.[65] To probe the nature of the C−H activation step, Mulliken charge and spin analysis was used. A HAT mechanism was identified if the spin on the resulting carbon is approximately +1 and the overall charge is ∼0. Alternatively, a hydride transfer mechanism is identified by the formation a carbocation species (spin ∼0 and a charge approximately +1). As shown in **Figure 2.7**, singlet amidyl-iminium **D** undergoes C−H activation through a hydride mechanism via $\mathbf{TS_{D\text{-}F}}$ (barrier of 10.5 kcal/mol), leading to the formation of **F**, a carbocation as determined by analysis of the spin and charge of the intermediate (**Figure 2.8**).

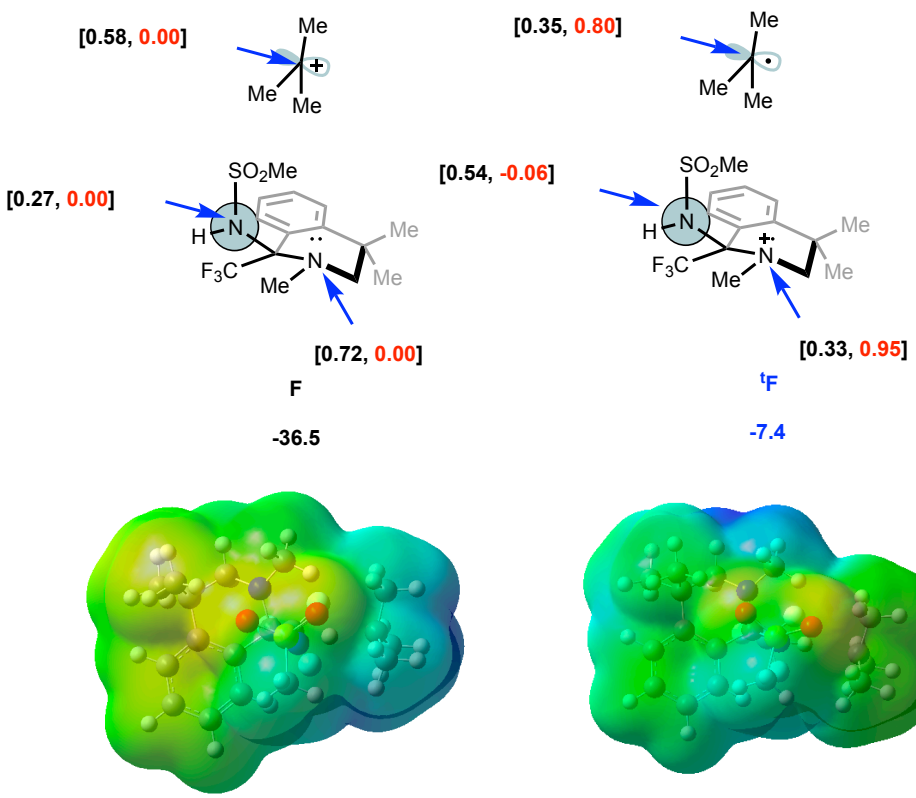


Figure 2.8 Comparison of singlet (left) and triplet (right) states of intermediate **F**. Mulliken charges and spins for select atoms are given in black and red respectively. Electrostatic potential maps (EPM) are given as well. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

Subsequently, **F** can undergo concerted N−C bond formation and C−N bond breaking via $\mathbf{TS_{F\text{-}P}}$ (barrier is 22.7 kcal/mol from **F**) to give the desired product **P** and regenerate the iminium ion organocatalyst **A**. Alternatively, the singlet open nitrenium species **D** can undergo spin inversion to give the energetically similar triplet species ^{t}**D.** This triplet species undergoes HAT via $\mathbf{TS_{D\text{-}F}}$ to form radical complex ^{t}**F** (barrier of 10.3 kcal/mol) as determined by the presence of the radical on the carbon substrate (**Figure 2.8**; see **Figure A2.8** in Appendix 2 for the other conformers **F'** and ^{t}**F'**). In principle, ^{t}**F** can undergo radical rebound but the relative barriers for this process were high (34.8 kcal/mol),

and quasi-classical dynamic calculations from ^{t}**TS$_{D\text{-}F}$** show that 64% of the trajectories led to ^{t}**F** and 36% led back to open-form ^{t}**D** without any trajectories leading to radical rebound (See **Figure A2.9** in Appendix 2 for details). Overall, these results support facile intersystem crossing from ^{t}**F** to form the carbocation F complex followed by C−N bond formation and subsequent product release.

The C−H activation pathway from the "up" conformational intermediates **D'** and ^{t}**D'**, (singlet and triplet, respectively) was also explored. As shown in **Figure A2.7** in Appendix 2 (red; left), the lowest-energy pathway (from **D'** or ^{t}**D'**) proceeds from ^{t}**D'** through a HAT mechanism (via ^{t}**TS$_{D'\text{-}F'}$** with overall barrier of 12.0 kcal/ mol) to form alkyl radical complex ^{t}**F'**. The triplet species ^{t}**F'** will then undergo an intersystem crossing to form the lower energy singlet carbocation species **F'** (downhill by 41.6 kcal/ mol). Finally, this intermediate **F'** will undergo a concerted C−N bond formation and product release via **TS$_{F'\text{-}P}$** (barrier is only 23.8 kcal/mol from **F'**). Analysis of the Mulliken spin of the **F'** and ^{t}**F'** intermediates supports this hypothesis that the triplet ^{t}**D'** undergoes HAT (radical process) to produce a radical carbon species while the singlet undergoes hydride transfer (anionic process) to produce a carbocation (see **Figure A2.8** in Appendix 2 for electrostatic potential maps of **F'** and ^{t}**F'**).

Overall, the open-form amidyl-iminium biradical intermediates **D** and **D'** are responsible for C−H activation. Moreover, akin to nitrenium chemistry, the mechanism is spin-controlled in which the singlet amidyl-iminium undergoes a "hydride" transfer, leading to a carbocation while the triplet amidyl-iminium biradical undergoes a HAT to form an alkyl radical. In the case of the triplet alkyl radical complexes ^{t}**F** or ^{t}**F'**, the species

then undergoes an intersystem crossing, leading to the singlet alkyl carbocation **F** or **F'**, respectively. Notably, for the tertiary substrate, both HAT and hydride mechanisms are competitive (within 0.2 kcal/mol).

2.3.4 Effect of Substrate on C-H Activation

The results show that both singlet and triplet amidyl-iminium biradical intermediates could be responsible for C−H activation. Moreover, for singlet species, the N−H bond formation step proceeds via a nucleophilic "hydride" mechanism, leading to the formation of a carbocation complex (**Figure A2.10** in Appendix 2). On the other hand, the triplet species proceeds via a HAT mechanism leading to the formation of an alkyl radical, which could then undergo intersystem crossing and single-electron transfer (SET) to form the energetically favored singlet carbocation complex (**Figure A2.11** in Appendix 2). With these intriguing results in hand, the effect of the substrate (e.g., methyl vs 1° vs 2° vs 3° vs benzyl) in the C−H activation step (e.g., from singlet and triplet amidyl- iminium intermediates) was explored. For simplicity, only the C−H activation step from the "down" conformation of the singlet and triplet amidyl-iminium intermediate is discussed since the barriers from the "up" conformation were found to be higher in energy (see **Figures A2.12−A2.15** in Appendix 2 for full details).

As shown in **Figures 2.9-2.10**, from this analysis we observe that (1) the overall barriers from C−H activation are correlated to the bond dissociation of the alkyl substrate; (2) independent of alkyl substrate the singlet and triplet C−H activation, barriers are nearly isoenergetic; and (3) highly unactivated alkyl substrates (e.g., methane and ethane) favor a HAT mechanism (from spin and charge analysis of the corresponding products)

independent of the spin while for activated (2°, 3°, and benzyl) substrates both hydride and the HAT mechanism are competitive. Overall, the mechanism for C−H activation from the singlet biradical is sensitive to substituent effects, while the hydride mechanism is operative from the triplet biradical independent of the nature of the substrate. That is, from a singlet biradical, the alkyl substrates capable of stabilizing positive charge (e.g., through inductive effects; secondary and tertiary) proceed via a hydride transfer step, leading to formation of a carbocationic **F** complex, while methyl and primary substrates proceed exclusively via the HAT mechanism.

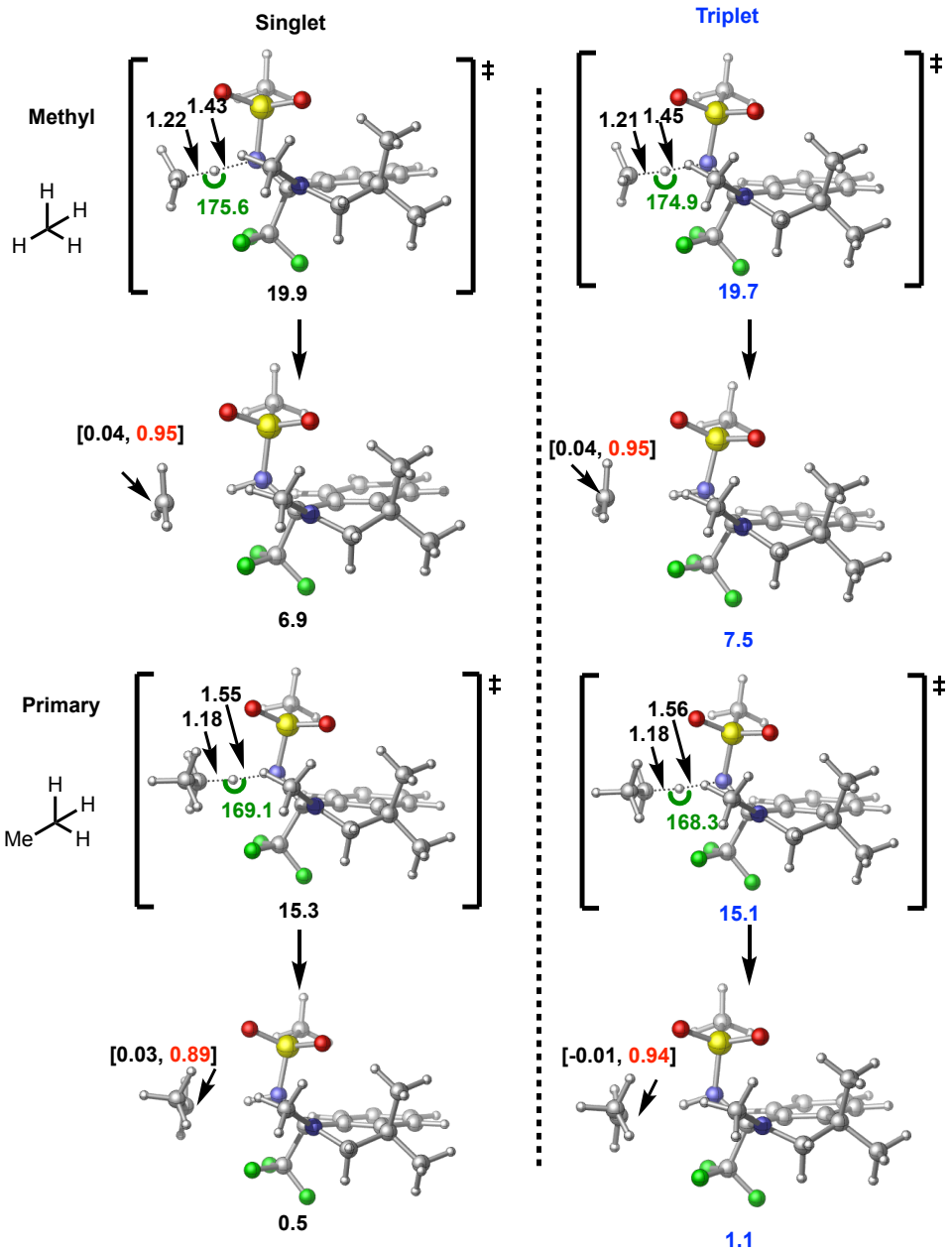


Figure 2.9 Effect of substrate (methyl, primary) and spin state on mechanism. Bond lengths (Å) are given as well as Mulliken charge (black) and spin (red) of the central carbon atom of the substrate. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory.

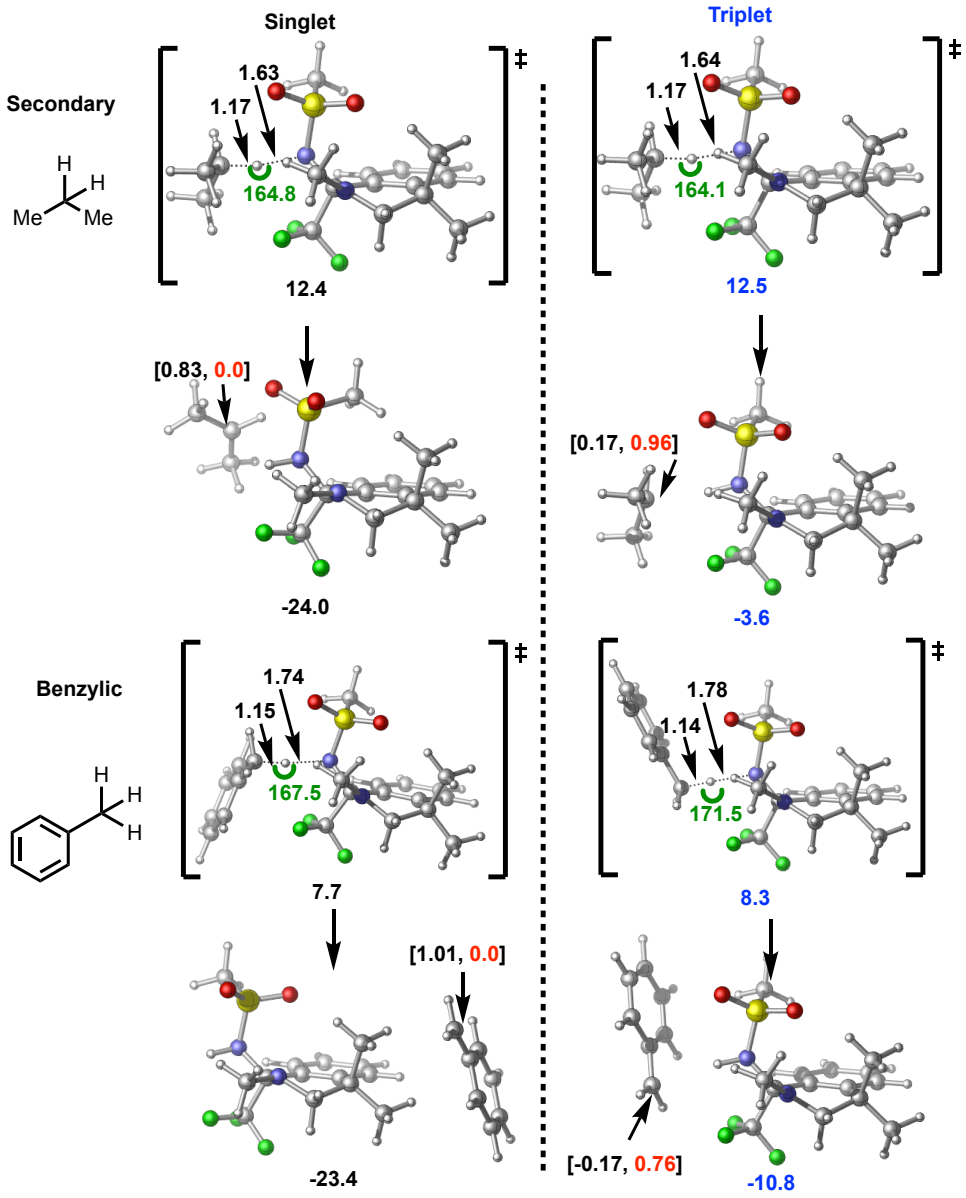


Figure 2.10 Effect of substrate (secondary, benzylic) and spin state on mechanism. Bond lengths (Å) are given as well as Mulliken charge (black) and spin (red) of the central carbon atom of the substrate. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory.

2.3.5 Molecular Dynamics Simulations

To further explore the timing and formation of the N−H bond formation step in more detail, molecular dynamics simulations (MD) on $\mathbf{TS_{D\text{-}F}}$ were performed using Singleton's Progdyn program.[66] To minimize the computational cost, a truncated system was studied in which the aryl and sulfonyl groups of the catalyst were replaced by an alkene and methyl, respectively (**Figure 2.11**). MD simulations were performed in the gas phase using UB3LYP/6-31G(d) from the open-shell singlet and triplet transition states located using UM06-2X/6-31+G(d,p)-CPCM(dichloromethane) in Gaussian 16. As shown in **Figure 2.11** the structural and energetic features (e.g., relative energetics between the singlet and triplet transition states) of the full system are preserved in the truncated system.

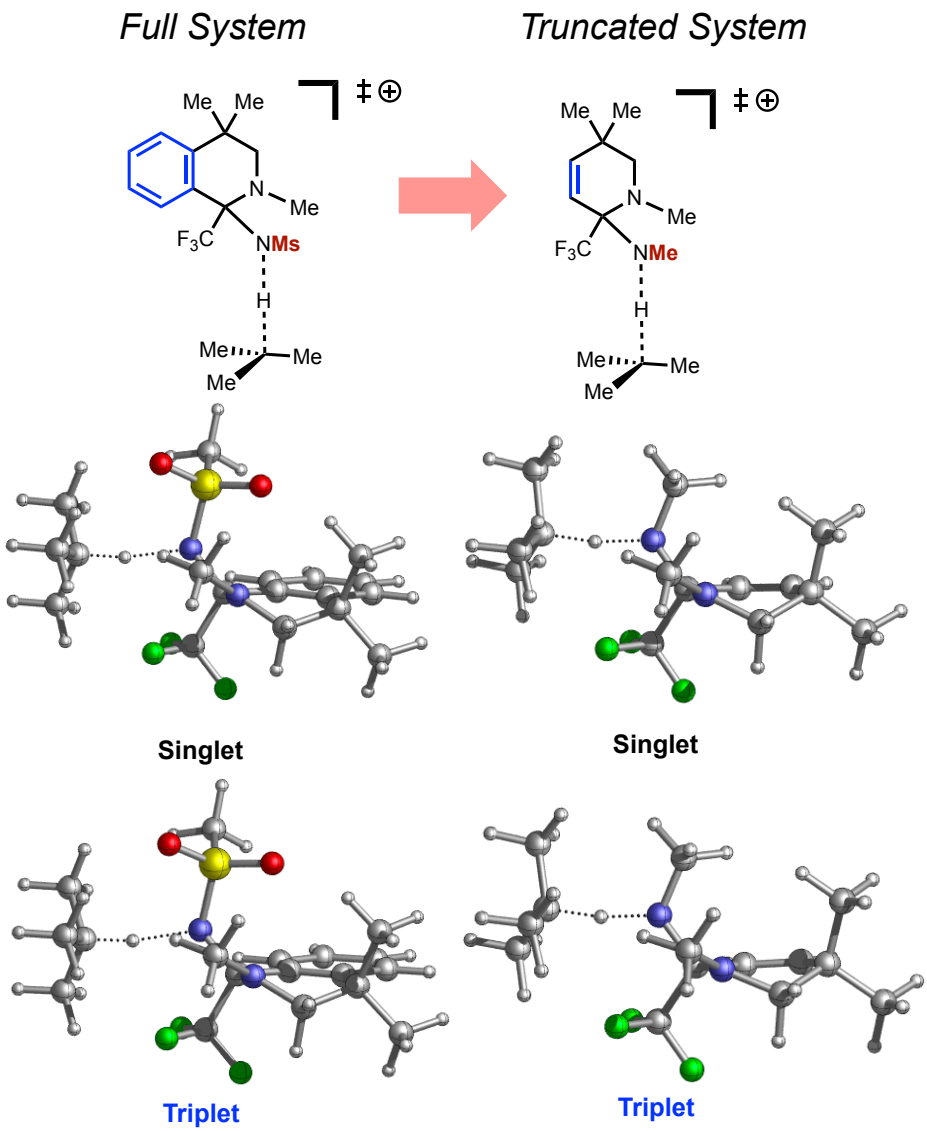


Figure 2.11 The singlet and triplet transition states for the full and truncated systems are shown. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory.

A typical trajectory involving N−H bond formation from the singlet biradical is shown in **Figure 2.12.** In this trajectory, the hydride (N−H bond of <1.0 Å) is transferred within 12 fs from the tertiary carbon substrate to the nitrogen of the diaminium species. The trajectory continues for an additional 397 fs without any further bond formation or

breaking events. These results show that hydride transfer (via singlet spin state) leads to the formation of a persistent (i.e., without rebound) carbocationic complex.

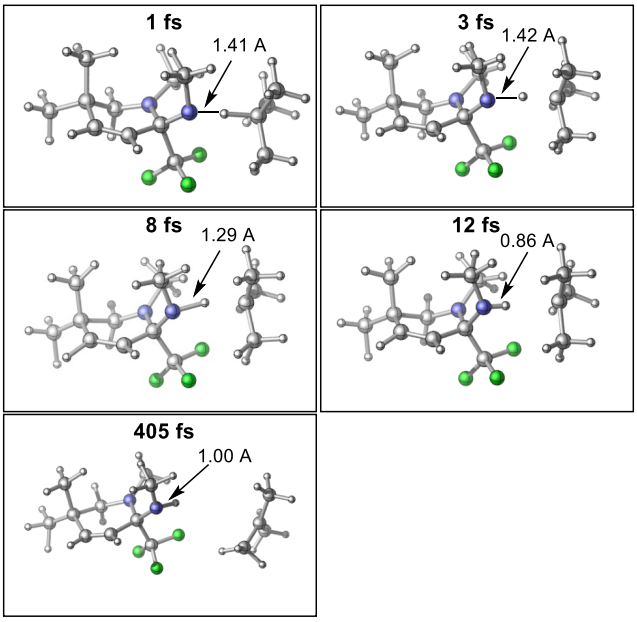


Figure 2.12 Snapshots of a typical reactive trajectory propagated in the gas phase leading to intermediate **F**. The hydrogen is transferred in the first 12 fs of the trajectory. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

Overall, 108 simulations were performed, and the results from analyzing these simulations show that most trajectories (84%) lead to the formation of the carbocationic complex **F** (**Figure 2.13**). The reverse reaction leading to the open, singlet biradical **D** is also observed in 10% of the trajectories, while only ~1% (after 1532 fs) of the trajectories lead to the much lower energy 3-membered diaziridinium **E**. These results suggest that a long-lived biradical species is responsible for C−H amination.

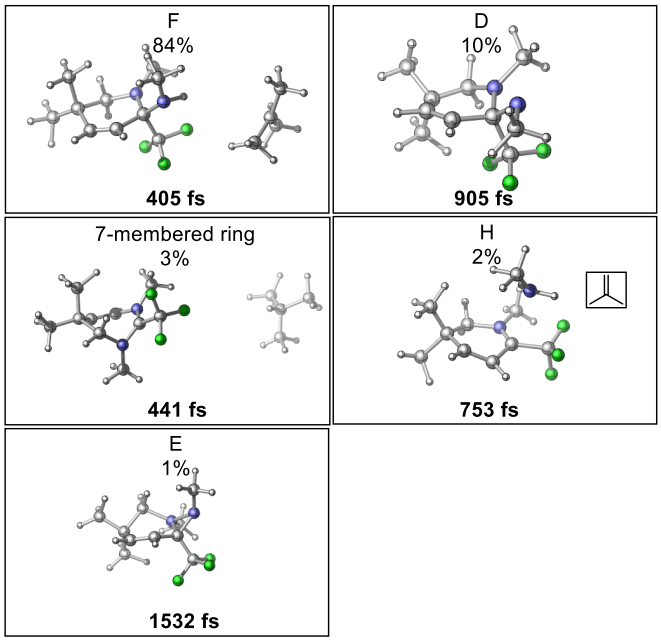


Figure 2.13 Summary of results from 108 MD simulations from the open-shell singlet transition state located. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

Consistent with this hypothesis, ring- expansion product (7-membered ring) was observed in ~3% of the trajectories (after ~441 fs), similar to the decomposition products of diaziridiniums that have previously been observed experimentally[54] and was explored computationally (see **Figure A2.16** in Appendix 2 for the potential energy surface including this side pathway). Notably, the Hilinski group previously published experimental results that support the notion that a tosyl or other sulfonyl groups lower the tendency of the organocatalyst to undergo ring expansion relative to hydrogen,[52] consistent with the calculations showing ring expansion as a minor pathway.

Finally, ~2% of the simulations led to intermediate **H** in which a second hydrogen from the tertiary carbocation is abstracted by the amine group, leading to 2-methyl propene, methyl amine, and regeneration of the iminium organocatalyst. Overall, these results support the mechanism shown in **Figure 2.14** and do not support a rapid rebound

mechanism. However, in the calculations, explicit solvent molecules and counterions were not considered, which are likely to play a key role in preventing the escape of discrete carbocations to undergo side bimolecular reactions.

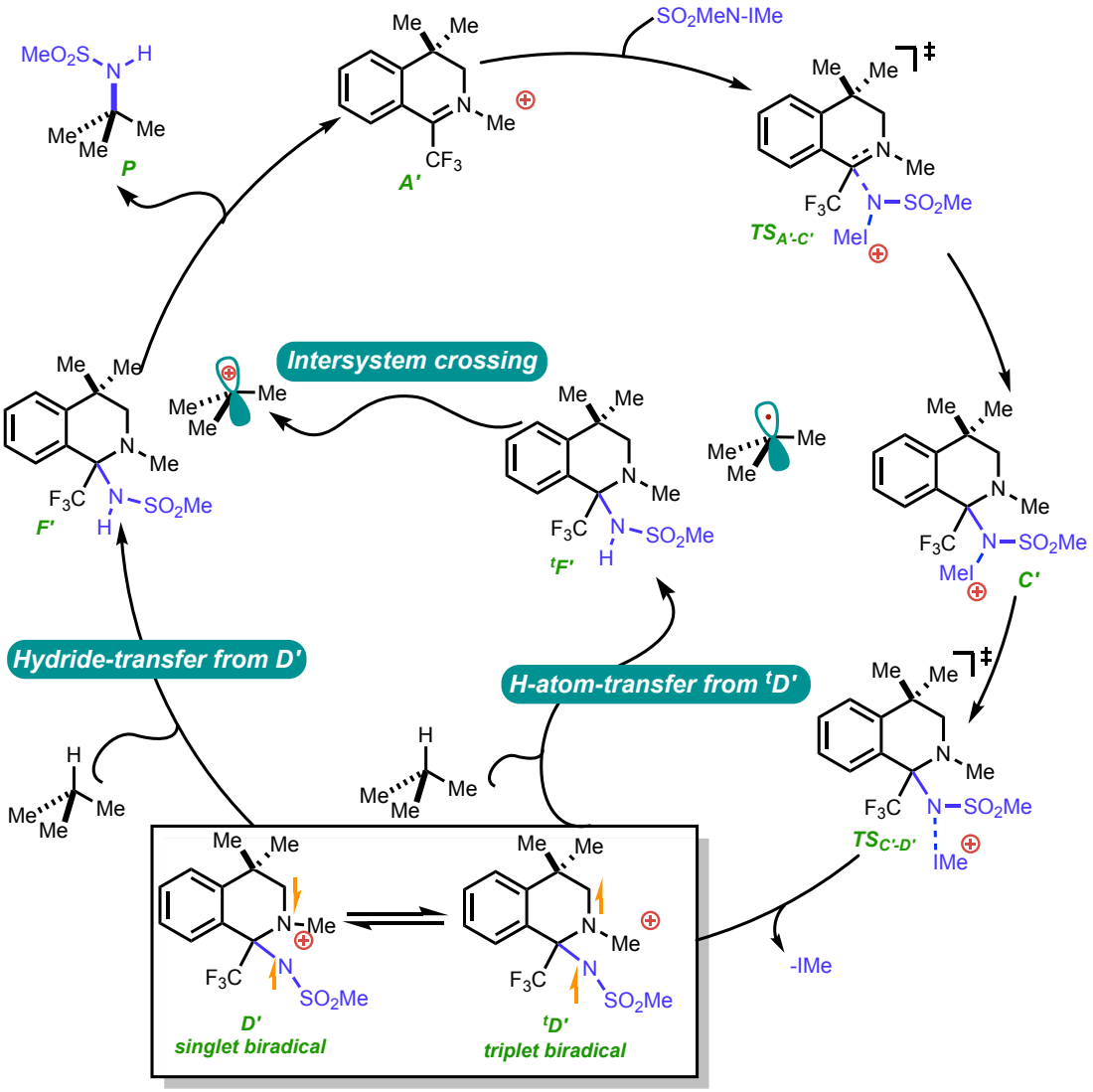


Figure 2.14 Mechanism of organocatalytic C-H amination as revealed by quantum mechanical and quasi-classical dynamic calculations. Reprinted with permission from ref 1. Copyright 2020 American Chemical Society.

2.3.6 Correlation of Results with Experiments

The initial hypothesis guiding the design of iminium-catalyzed C−H amination was centered on the idea that a diaziridinium might be accessed from the reaction of a nitrene precursor and the catalyst. Furthermore, that diaziridinium, like its cousins in the dioxirane and oxaziridine families, might be expected to transfer a heteroatom (in this case nitrogen) in a C−H functionalization process. Indeed, the calculations predict the formation of the expected diaziridinium as an intermediate along the reaction coordinate leading to C−H amination. However, unexpectedly and in contrast to the well-studied dioxirane case, the open biradical forms **D** and **D'** are also calculated to exist as intermediates and are found to be the relevant oxidants engaged in C−H bond cleavage. This result, along with the calculated nature of the subsequent C−H activation steps for each intermediate, is consistent with experimental results and provides important insight for future reaction design.

Experimentally and under conditions slightly modified from the computational model (i.e., use of PhINTs or PhINTces as the nitrene precursor), successful C−H amination is limited to benzylic C−H bonds or other C−H bonds that are substantially weakened by conjugative or hyperconjugative effects (see examples in **Figure 2.1**). Calculations suggest that, whereas hydride transfer and HAT transition states are isoenergetic for primary, secondary, and tertiary C−H bonds, benzylic hydride transfer begins to be favored (by 0.6 kcal/mol for toluene as shown in **Figure 2.8**). Previously, when studying the effect of substitution of the tetralin aromatic ring on relative reaction rates, we observed a strong correlation with the Hammett constant σ_p with a ρ value of

−2.5.[52] This suggests an increase in positive charge at the benzylic carbon. These data could be taken as evidence that, for the reported experimental results, a hydride transfer pathway via the singlet biradical is favored. Previous experimental investigations by the Hilinski group also found a primary kinetic isotope effect of 2.5 for amination of isochroman in an intermolecular competition experiment. The kinetic isotope effect (KIE) of the H transfer step for both the down and up conformers of the N−H bond formation transition state was computed. The computed values of k/k_{HD}[61] were 1.72 and 1.98 for the down and up conformers, respectively, in the truncated system. These computed KIE values are in accord with the experimental value ($k_H/k_D = 2.5$) for the isochroman molecule (see **Figure 2.15**). The magnitude of this effect is also consistent with predicted KIE values for reactions involving hydride transfer.[67] In addition, the observation of a primary KIE is consistent with the overall mechanism proposed, which shows that for benzylic amination, the rate-determining step is formation of **D** and **D'**, but an irreversible C−H bond cleavage occurs in a product-determining step following the rate- determining step.

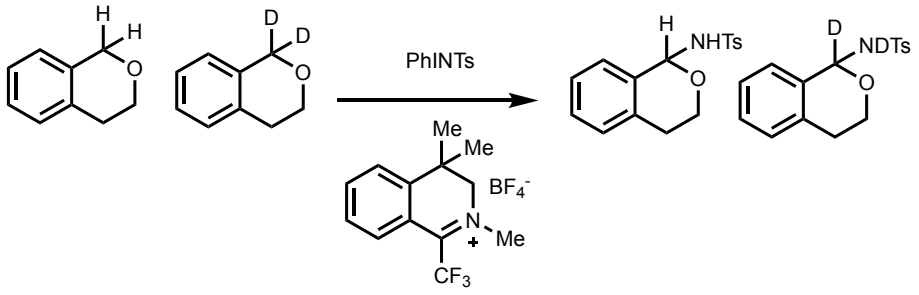


Figure 2.15 Experimental KIE of the isochroman system and the computed KIE of the system studied computationally.

The calculated mechanism and reaction barriers offer several potentially productive directions for reaction design. First, it is notable that both the overall barriers and calculated

transition state energies for the C−H functionalization step (<20 kcal/ mol in all cases) are lower than what might be predicted for a reaction exhibiting a scope at room temperature limited to benzylic or highly activated alkane substrates. One possible explanation for this is that the generation of an N-tosyl analog of **D** might, for steric reasons, occur with a higher barrier, and that this analog might subsequently exhibit lower reactivity than the calculated N-mesyl oxidant, given the proximity of the nitrogen protecting group to the substrate during the C−H functionalization step (**Figure 2.10**). In this regard, reducing the steric bulk of the terminal oxidant is potentially of interest. Moreover, the lack of reactivity with otherwise unactivated tertiary C−H bonds is puzzling given that formation of **D** is calculated to be the rate-determining step, as in the benzylic case. Sterics might play a role here. However, it was observed experimentally that PhINTs and PhINTces are poorly soluble in the reaction mixture and dissolve slowly (and not always entirely) over the time period of the reaction. Therefore, an alternative hypothesis is that the poor solubility of the terminal oxidant severely limits the concentration of **D** and **D'** in the reaction mixture, leading to rates of product formation that are below an observable level. This might be addressed by the use of more soluble nitrene precursors.

2.4 Conclusion

The mechanism of iminium-catalyzed C−H amination was explored through computational methods including quantum mechanical calculations and molecular dynamics simulations. Through the computational studies, a mechanism by which this C−H amination occurs is proposed. The iminoiodinane is added to the iminium catalyst followed by removal of the iodomethane. The resulting singlet biradical species can then

undergo N−H bond formation. The computational studies show that both hydride transfer and HAT mechanisms for activated C−H bonds are operative, competitive, and energetically accessible. However, for unactivated C−H bonds/sites (e.g., 1°), a HAT mechanism is operative but large energetic barriers are observed. Furthermore, in agreement with quantum mechanical calculations, molecular dynamics simulations do not support a rapid rebound mechanism. Modulating the organocatalyst to control the mechanism of C−H amination (hydride vs HAT mechanism) by tuning the substituents of the biradical intermediate can be studied in the future.

Chapter 3: The Role of the Trichloroacetimidate to Enable Iridium-Catalyzed Regio- and Enantioselective Allylic Fluorination

Excerpts from this chapter were published in: Sorlin, A. M.; Mixdorf, J. C.; **Rotella, M. E.**; Martin, R. T.; Gutierrez, O.; Nguyen, H. M. *J. Am. Chem. Soc.* **2019**, *141,* 14843 – 14852.

3.1 Abstract

Asymmetric allylic fluorination is a robust, efficient methodology with potential applications for the development of pharmaceuticals and practical synthesis for ^{18}F radiolabeling. A computational (dispersion-corrected DFT) approach was taken to interrogate the mechanism of the diene-ligated, iridium-catalyzed regio- and enantioselective allylic fluorination developed by the Nguyen group. In the presence of an iridium(I) catalyst and nucleophilic fluoride source (Et_3N•3HF), allylic trichloroacetimidates undergo rapid fluoride substitution to generate allylic fluoride products with excellent levels of branched-to-linear ratios. Experimental mechanistic studies by Nguyen et al. revealed the crucial role of the trichloroacetimidate as a potent leaving group and ligand to enable conversion of racemic allylic trichloroacetimidates to the corresponding enantioenriched allylic fluorides. The mechanism of this reaction was probed computationally using dispersion-corrected DFT, and it was found to occur via a dynamic kinetic asymmetric transformation (DYKAT) in the presence of the chiral bicyclo[3.3.0]octadiene-ligated iridium catalyst. This work in elucidating the mechanism of the iridium-catalyzed regio- and enantioselective allylic fluorination is crucial to future reaction development and catalyst design.

3.2 Introduction

The introduction of fluorine into organic molecules is a useful technique for the preparation of complex molecules with applications in pharmaceuticals, agrochemicals, and performance materials.[68] For example, fluorides are vital components of medicinal and imaging reagents, as shown through the use of ^{18}F labeled nuclei in positron emission tomography-computed tomography (PET-CT).[69] Fluorination often requires the aid of a transition metal catalyst to promote this reaction. Methods for allylic fluorination (**Figure 3.1**) have been developed by Doyle,[70] Governeur and Brown,[71] Wu,[72] and Liu[73] among others.[74]

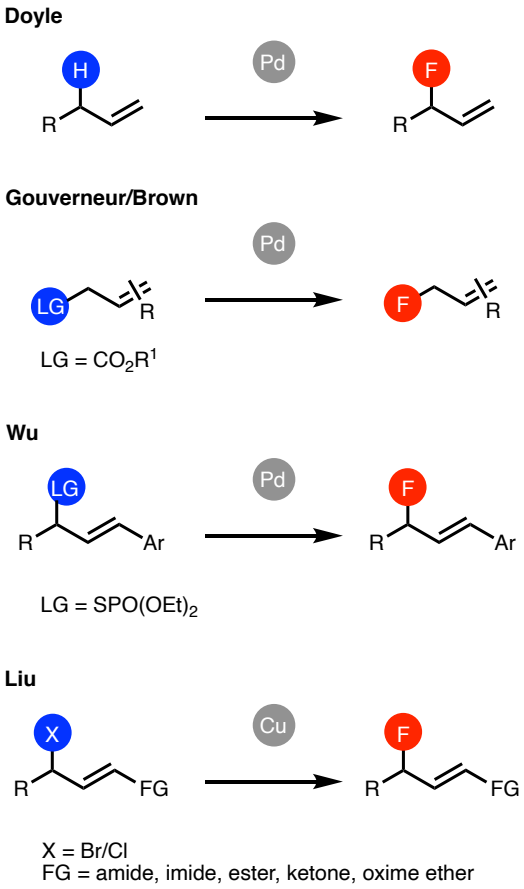


Figure 3.1 Transition metal-catalyzed methods for allylic fluorination by C-H activation or functional group exchange.

Although there have been several efficient methodologies reported for the regioselective formation of allylic fluorides,[75,76,77,78,79,80,81] there are few approaches available for the asymmetric synthesis of allyl fluorides.[8,82,83,84,85] In 2011, initial studies toward a regioselective fluorination reaction were undertaken in the Nguyen group. Accordingly, allylic trichloroacetimidates **1** were employed as electrophiles, $Et_3N{\cdot}3HF$ as a nucleophilic fluoride source, and cyclooctadiene iridium chloride dimer, $[Ir(COD)Cl]_2$, as a catalyst leading to the formation of branched allylic fluorides **2** in good yields and excellent regioselectivities (**Figure 3.2**). The trichloroacetimidate group employed in this work is widely used in synthetic organic chemistry, starting with Schmidt's use of the

leaving group in glycosylation reactions[86] as well as in Overman's development of a [3,3]-sigmatropic rearrangement[87] to generate an allylic trichloroacetimidate. In subsequent studies, racemic secondary allylic trichloroacetimidates **3** were transformed to enantioenriched allylic fluorides **4** using a chiral bicyclo[3.3.0]octadiene *(S,S)*-ligated iridium complex.[88,89]

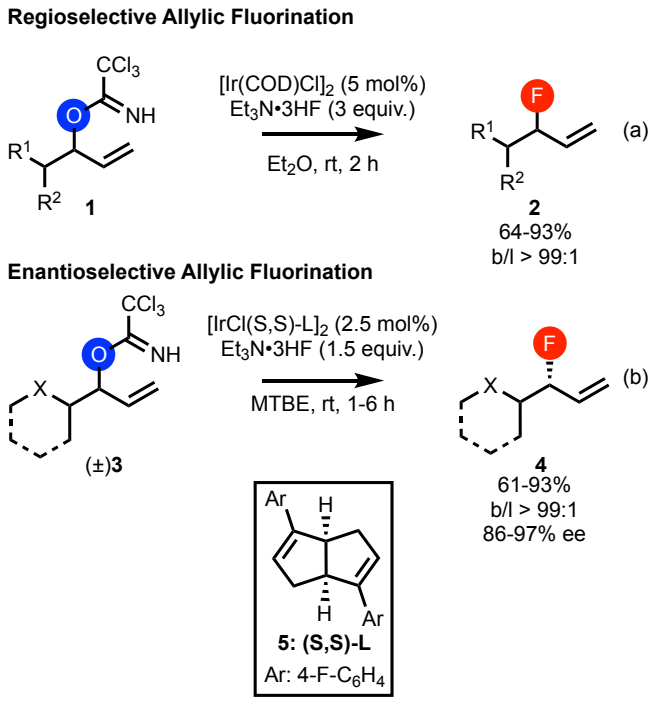


Figure 3.2 Regio- and enantioselective allylic C-F bond formation developed by Nguyen.

An understanding of the mechanism underlying this transformation can provide insight into the origin of the observed regio- and enantioselectivity as well as the vital role of the trichloroacetimidate leaving group. Thus, in collaboration the Nguyen group, computational studies of the mechanism of this iridium-catalyzed allylic fluorination were performed to gain insight into the factors controlling reactivity.[90] Overall, the results described provide support for a dynamic kinetic asymmetric transformation (DYKAT) of racemic allylic trichloroacetimidate leading to regio- and enantioselective allylic C−F bond

formation. This work also highlights the dualistic nature of the trichloroacetimidate as a leaving/directing group and as a ligand to facilitate equilibration of diastereomeric π-allyl iridium intermediates via a π−σ−π mechanism, leading to enantioenriched allylic fluorides.

3.3 Results and Discussion

3.3.1 Ionization of the Allylic Trichloroacetimidate

Based on previous work focused on transition-metal-catalyzed allylic substitutions,[91] a general mechanism for iridium-catalyzed allylic fluorination could be hypothesized (**Figure 3.3**). First, allylic trichloroacetimidate **A** coordinates with [Ir] catalyst and then undergoes ionization of the C−O bond leading to the formation of π-allyl iridium intermediate **B**. The π-allyl iridium complex **B** is proposed to react with nucleophilic fluoride, resulting in allylic fluoride product **C**.

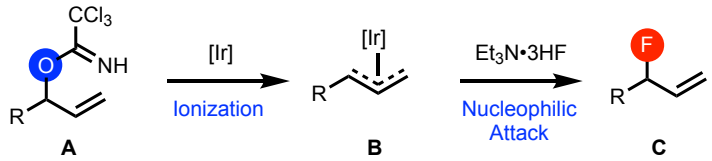


Figure 3.3 Proposed intermediate steps for the iridium-catalyzed allylic fluorination.

To gain insight into the vital role of the trichloroacetimidate group to facilitate the iridium-catalyzed allylic fluorination, dispersion-corrected DFT calculations were performed (M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether). To begin, the achiral (COD) system was studied extensively followed by the chiral system. In an effort to reduce computational cost without comprising the accuracy of the results, the truncated allylic trichloroacetimidate was used as a model substrate for all calculations (**Figure 3.4**). The validity of the use of this model substrate was verified experimentally. When exposed to the reaction conditions, allylic trichloroacetimidate **6** reacted to give allylic fluoride **7** with

the expected branched selectivity (>99:1 branched: linear). This experimental result validates the choice of model substrate for these computational studies.

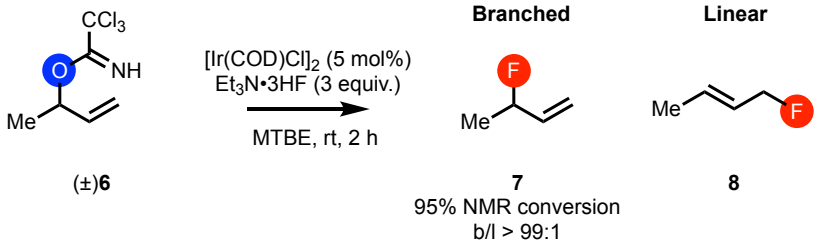


Figure 3.4. Fluorination of model substrate **6.**

Using this model system, the mechanism of iridium-catalyzed allylic fluorination was then investigated (for information on the choice of the computational method, see **Figure A3.1** in Appendix 3). First, the most energetically favored mode of complexation between allylic trichloroacetimidate **6** and $[Ir(COD)Cl]_2$, presumably resulting from fragmentation of dimeric $[Ir(COD)Cl]_2$ precatalyst, was explored.[92,93,94,95,96,97] After extensive conformational analysis (**Figure A3.2** in Appendix 3) and exploration of various modes of coordination, three distinct isomeric structures were identified. Overall, calculations revealed a strong energetic preference for bidentate coordination to the allylic trichloroacetimidate substrate via η^2-(π-coordination) of the olefin and η^1-(σ-coordination) to the nitrogen atom of the imine group, to form a pentacoordinated square pyramidal complex **6-Ir-A** (**Figure 3.5**).

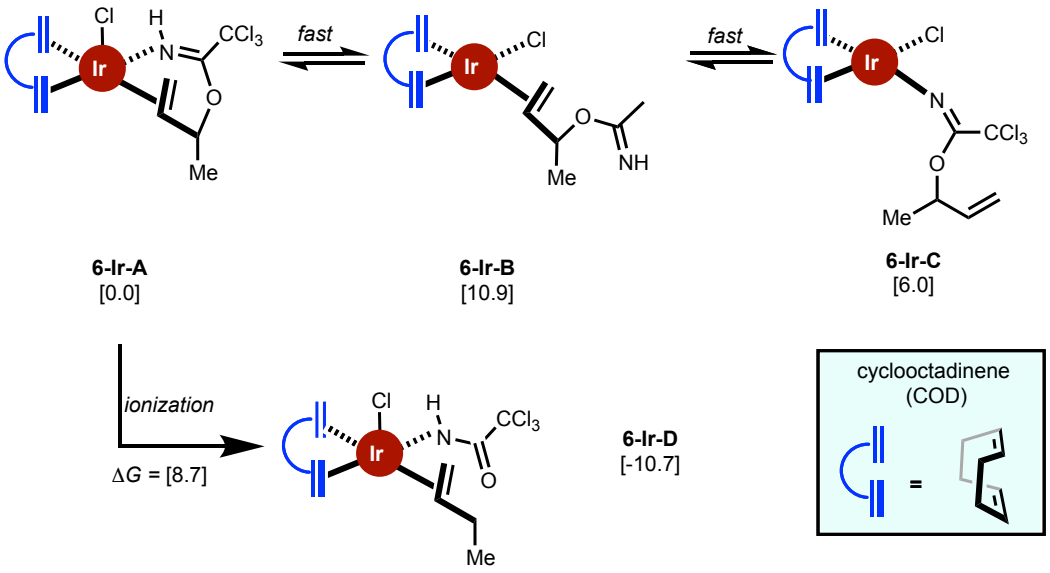


Figure 3.5 Identification of various modes of iridium coordination to allylic trichloroacetimidates. Free energies (kcal/mol) were computed using B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether) in brackets. Reprinted with permission from ref 23. Copyright 2019 American Chemical Society.

Monodentate coordination to either imine or olefin to form tetracoordinated square planar complexes **6-Ir-B** and **6-Ir-C** were also considered but are >6 kcal/mol higher in energy. Presumably, the strong ability of the imine and olefin to coordinate in a bidentate fashion overcomes the strain associated with the formation of the 7-member chelated complex **6-Ir-A**.[98] This mode of coordination (i.e., **6-Ir-A**) is crucial for reactivity as it preorganizes the catalyst−substrate complex for facile C−O bond breaking. Referring to **Figure 3.5**, the lowest energetic barrier for ionization is 8.7 kcal/mol, leading to π-allyl iridium intermediate **6-Ir-D** which is downhill in energy by 10.7 kcal/mol. Competing, higher energy pathways, are given in **Figure A3.3** in Appendix 3. To confirm that complex **6-Ir-D** is an active intermediate, the Nguyen lab reacted allylic trichloroacetimidate *(R)*-**9** with $[Ir(COD)Cl]_2$ catalyst **10** (**Figure 3.6**), isolating crystals of a pentacoordinated π-allyl Ir(III) species with η^1-(σ-coordination) of the trichloroacetamide nitrogen to the iridium. This coordination presumably arises from facile ionization of the bidentate Ir substrate

complex (e.g., **6-Ir-A**; **Figure 3.5**). Notably, examination of the orientation of the iridium from π-allyl iridium complex shows a retention in stereochemistry from trichloroacetimidate (*R*)-**9**. This evidence supports that the trichloroacetimidate is crucial to induce ionization and acts as both a leaving group and a ligand to the iridium.

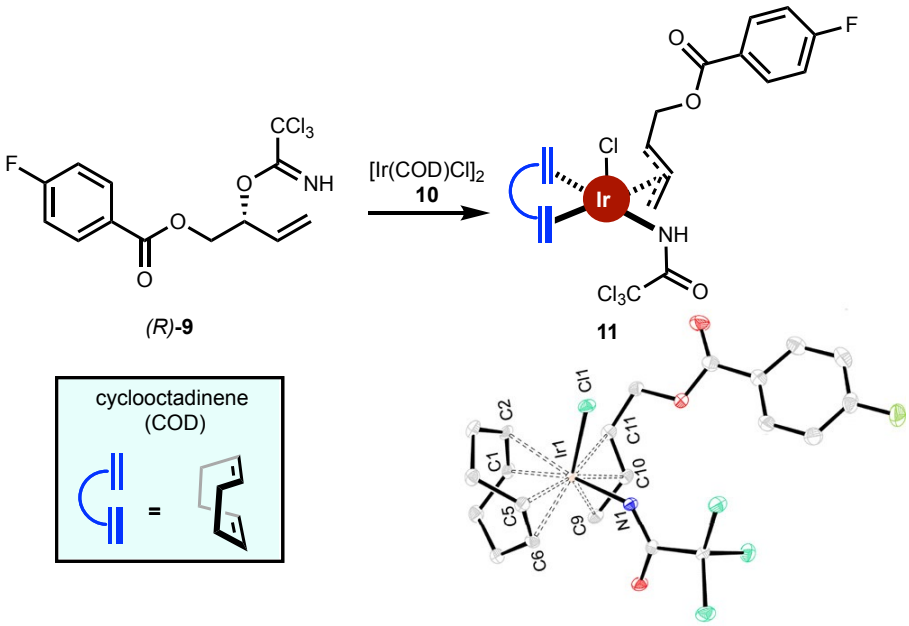
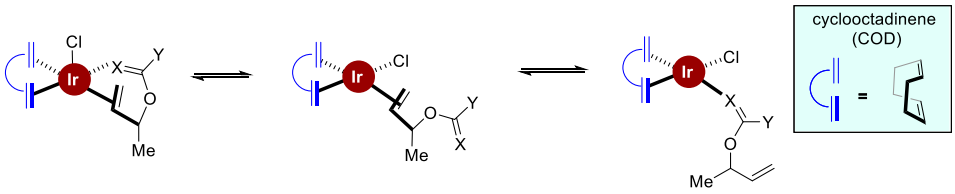


Figure 3.6 X-ray crystal structure of distorted square pyramidal π-allyl iridium intermediate **11** obtained by the Nguyen group. Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Gray, green, white, blue, red, and yellow ellipsoids represent C, Cl, Ir, N, O, and F atoms, respectively.

A distortion−interaction analysis (**Figure A3.4** in Appendix 3) was also performed to better understand the reactivity and, in particular, why the ionization via the 7-member chelated complex (**6-Ir-A**) is much lower in energy than the alternatives. The lowest energy transition state (**6-Ir-TS-N**) has a favorable interaction energy between the iridium metal center and the trichloroacetimidate group, making it a lower energy transition state. It is hypothesized that the iridium-nitrogen bond in **6-Ir-TS-N** may contribute to this favorable interaction through strong metal-to-ligand back bonding.

The role of the trichloroacetimidate group in the ionization step was further probed by comparing the ionization barriers of different electrophiles (trichloroacetimidate **1**, carbonate **2**, acetate **3** and imine **4** in **Figure 3.7**). The preference for the pentacoordinated intermediate **6-Ir-A** is observed only in the case of the trichloroacetimidate group. On the contrary, this same preference is not observed with the other leaving groups, as shown in **Figure 3.7**. Experimentally, the Nguyen group showed that the trichloroacetimidate group is vital for the allylic fluorination to proceed regioselectively and in high yield. With this observation, it is clear that the pentacoordinated intermediate, only favored in the case of the trichloroacetimidate group, is essential to the reaction by setting up a preorganized complex that allows the fluorination to occur.



Entry	X, Y	6-Ir-A	6-Ir-B	6-Ir-C
1	NH, CCl_3	0.0 [0.0] (0.0)	10.0[10.9] (17.2)	8.7 [6.0] (12.3)
2	O, OCH_3	0.0 [0.0] (0.0)	-4.1 [-6.6] (0.5)	-0.4 [-3.5] (1.7)
3	O, CH_3	0.0 [0.0] (0.0)	-2.9 [-3.8] (1.9)	-2.9 [-6.2] (-0.1)
4	NH, CH_3	0.0 [0.0] (0.0)	13.3 [13.5] (19.6)	3.6 [0.9] (6.9)

Figure 3.7 Energetic preference for bidentate coordination shown in **6-Ir-A** observed with trichloroacetimidate substrate (entry 1) using COD ligand**.** Free energies (kcal/mol) were computed using M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and, in brackets, B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and in parenthesis, DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)// M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether). Reprinted with permission from ref 23. Copyright 2019 American Chemical Society.

Having studied the ionization step leading to the formation of the key π-allyl intermediate in the achiral system, I moved on to explore the ionization pathway with the chiral (*S,S*)-diene bicyclo[3.3.0]octadiene ligand. As shown in **Figure 3.8** (red), the lowest

energy pathway from ***(S)*-II** (R = Me) proceeds via dissociation/re-association of the substrate to form the pentacoordinated complex ***(S)*-II′** (i.e., ionization directly from ***(S)*-II** complex is ~5 kcal/mol higher in energy; see **Figure A3.5** in Appendix 3). Notably, the ***(S)*-II′** complex is ca. 6 kcal/mol uphill in energy, presumably due to steric interactions between the substrate and the "Cl" group. Nonetheless, from ***(S)*-II′** complex, facile C−O bond breaking via 7-member bis-chelated transition state ***(S)*-II′-TS** (relative barrier is 11.3 kcal/mol from ***(S)*-II**) leads directly to the π-allyl iridium intermediate, **I-E3**, downhill in energy by 6 kcal/mol. I also located two distinct pathways for C−O bond breaking that included a [3,3]-sigmatropic rearrangement and 5-member π-O-chelation, but these pathways were much higher in energy than the 7-member π-N-chelation pathway (see **Figure A3.6** in Appendix 3 for information on these pathways); therefore, they were not considered further. Having established the lowest energy pathway for π-allyl iridium intermediate formation (**I-E3**) from the ***(S)*-II** complex, I next focused on the formation of π-allyl iridium intermediates from ***(R)*-II** (**Figure 3.8**, green).[99] Unlike the ***(S)*-II** complex, ***(R)*-II** favors ionization directly (via transition state **(R)-II-TS**) to form π-allyl iridium intermediate **I-E1** with an overall barrier of 11.2 kcal/mol (green solid).[100]

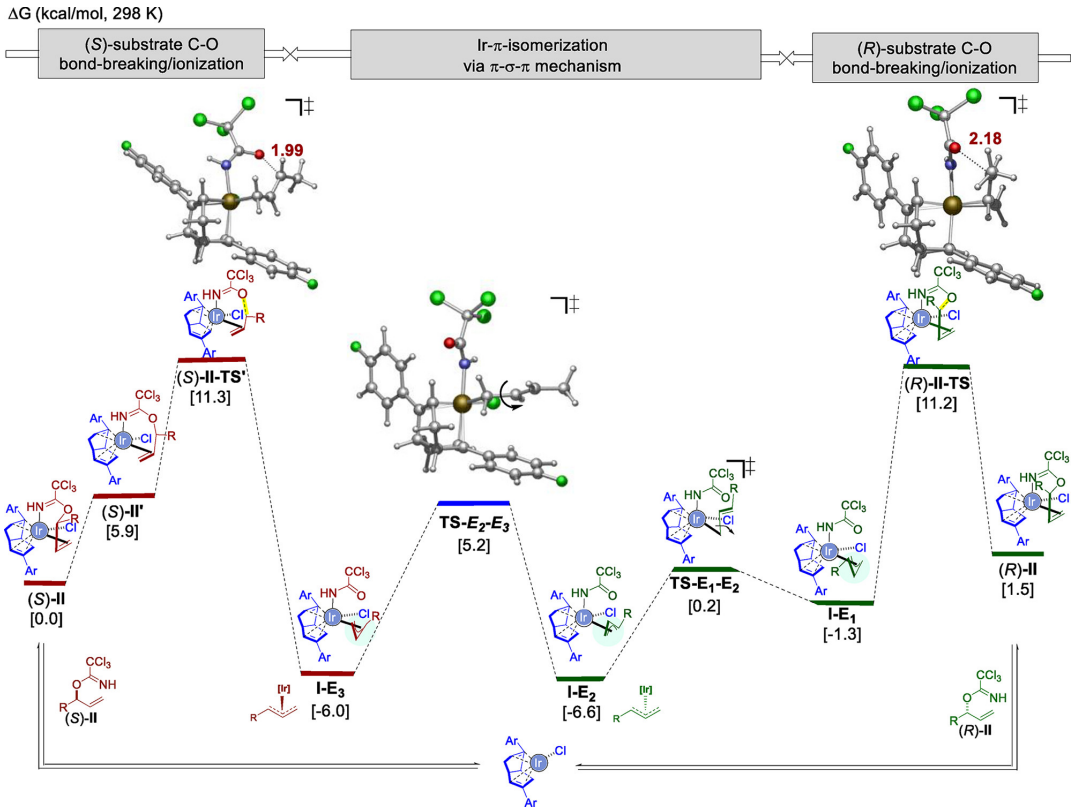


Figure 3.8 Relative energy (ΔG, kcal/mol) for the formation of the π-allyl iridium intermediates from both (*S*)- and (*R*)-allylic trichloroacetimidate (R = Me) using the chiral (*S*,*S*)-diene (L) ligated iridium catalyst (L = bicyclo[3.3.0]octadiene). Free energies (kcal/mol) were computed using B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethylether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) level of theory. Reprinted with permission from ref 23. Copyright 2019 American Chemical Society.

3.3.2 Isomerization of the π-Allyl Intermediates

From direct ionization of **(R)-II**, we obtain the intermediate **I-E1** while the ionization of **(S)-II'** leads to **I-E3**. Following ionization, the complexes **I-E1** and **I-E3** can interconvert through π-allyl isomerization (**Figure 3.8**). With regard to this isomerization, the complex **I-E1** can undergo facile sigma rotation (via **TS-E1-E2**) followed by σ- to- π slippage to form the lower energy π-allyl iridium intermediate **I-E2**. The intermediate **I-E2** can also undergo sigma rotation (via **TS-E2-E3**, barrier of 5.2 kcal/mol) followed by σ- to- π slippage to form **I-E3**, the same intermediate formed from direct ionization of **(S)-**

II'. Given a barrier of 5.2 kcal/mol for the interconversion of **I-E2 and I-E3**, the intermediates can rapidly interconvert and exist in equilibrium with one another. This interconversion through a π–σ–π mechanism is well-established for η^3-allyl metal complexes.[101,102]

3.3.3 Asymmetric Fluorination

Having located the lowest energy pathways for interconversion between (R)- and (S)-allylic trichloroacetimidate substrates and establishing rapid equilibration among the lowest energy π- allyl iridium intermediates (**Figure 3.8**), next the origin of regio- and enantioselectivity was explored.[103] For simplicity, only nucleophilic attack onto the lowest energy π-allyl iridium intermediates (**I-E3** and **I-E2**) is discussed, since all others were found to be much higher in energy (see **Figure A3.7** in Appendix 3 for details on nucleophilic fluorine attack on all π-allyl iridium intermediates **I-E1, I-E2, I-E3,** and **I-E4**).

Overall, the lowest energy pathway for iridium-catalyzed allylic fluorination proceeds via outer-sphere nucleophilic fluoride attack (see **Figure A3.8** for details on inner-sphere attack) onto the lowest energy π-allyl iridium intermediates (**Figure 3.9**).

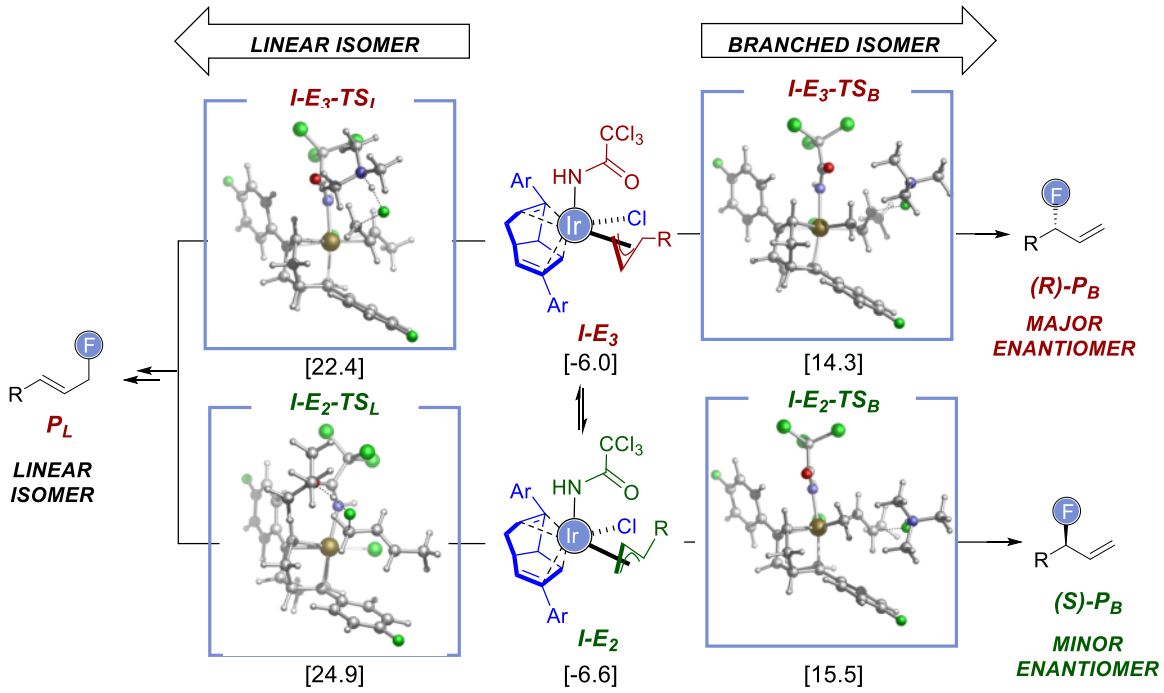


Figure 3.9 Relative energetics for allylic fluorination of π-allyl iridium intermediates and regioselectivity. Free energies (kcal/mol) were computed using B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) levels of theory. Reprinted with permission from ref 23. Copyright 2019 American Chemical Society.

The barriers for fluoride attack[104] onto the two lowest energy isomeric π-allyl iridium intermediates leading to linear and branched allylic fluorides are higher in energy (14.3−24.9 kcal/mol, **Figure 3.9**) than the barriers for isomerization (5.2 kcal/mol) of the π-allyl iridium intermediates (**Figure 3.8**). These results strongly support a Curtin−Hammett scenario in which both *(S)*- and *(R)*-allylic trichloroacetimidates can undergo facile racemization via formation of π-allyl iridium intermediates (i.e., **I-E2** to **I-E3**) followed by regio- and stereodetermining nucleophilic fluoride attack.

Moreover, concerning the regioselectivity, the computed barriers for nucleophilic attack at the least substituted carbon (leading to linear products) were significantly higher in energy (8−9 kcal/mol) than nucleophilic attack on the most substituted carbon (**Figure**

3.9, left versus right). Presumably, the branched transition states benefit from stronger interactions between the developing $\pi_{C=C}$ moiety and the iridium as evident by the shorter Ir-allyl distances in the transition state structures (see **Figure A3.7** in Appendix 3). Therefore, quantum mechanical calculations predict exclusive formation of branched allylic fluoride products. Collectively, these results are consistent with the experimental regioselectivity in which high branched-to-linear ratios (b:l > 99:1) were observed for a wide range of allylic trichloroacetimidates substrates.

Regarding the enantioselectivity of the branched allylic products, overall, transition state **I-E3-TS$_B$**, which will lead to the experimentally observed enantiomer, is 1.2 kcal/mol lower in energy than diastereomeric transition state **I-E2-TS$_B$**. This energy difference between the competing diastereomeric transition states is also in reasonable agreement with experiment (%ee$_{calc}$ = 76 vs %ee$_{exp}$ = 93; **Figure 3.8**) although other methods (UM06 and DLPNO) predict similar results, (M06) %ee$_{calc}$ = 96 and (DLPNO) %ee$_{calc}$ = 76, respectively (see **Figure A3.9** in Appendix 3).

Closer inspection at the two lowest energy **I-E2-TS$_B$** and **I-E3-TS$_B$** diastereomeric transition states (**Figure 3.10**) reveal nearly identical Ir−allyl distances (2.11 and 2.25−2.26 Å), suggesting similar electronic strength[105] of the transition metal fragment and the developing olefin interaction in both transition states. However, in **I-E2-TS$_B$** the allyl group has an unfavorable interaction with the −NHCOCl$_3$ moiety, while in **I-E3-TS$_B$** these two groups experience lesser steric interactions.

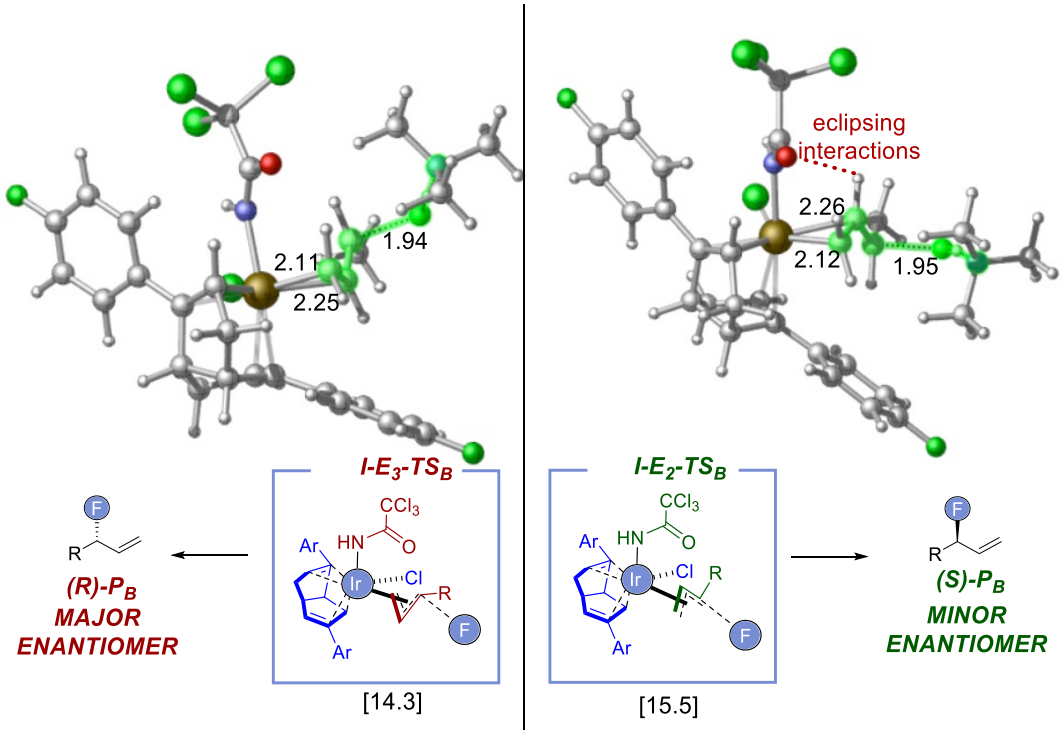


Figure 3.10 Lowest energy diastereomeric transition states leading to major and minor branched-selective allylic fluorides with relative energies of fluoride addition. Free energies (kcal/mol) were computed using B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) levels of theory. Reprinted with permission from ref 23. Copyright 2019 American Chemical Society.

With the establishment of the origin of regioselectivity and enantioselectivity, a deuterium labeling experiment was performed by the Nguyen group to probe the mechanisms of retention or inversion of stereochemistry.[106,107] The *cis*-alkene deuterium-labeled trichloroacetimidates **(*S*)-13** and ***(R)*-13** were submitted to the standard fluorination condition using [IrCl(*S,S*)-L]$_2$ catalyst (**Figure 3.11**). For the ***(S)*-13** substrate, the *(R)*-enantioenriched product **14** was obtained with retention of configuration of the olefin geometry *(cis)*. In contrast, for the ***(R)*-14** substrate, the *(R)*-enantioenriched product **15** was obtained with transposition of the deuterium on the terminal alkene (*trans*).

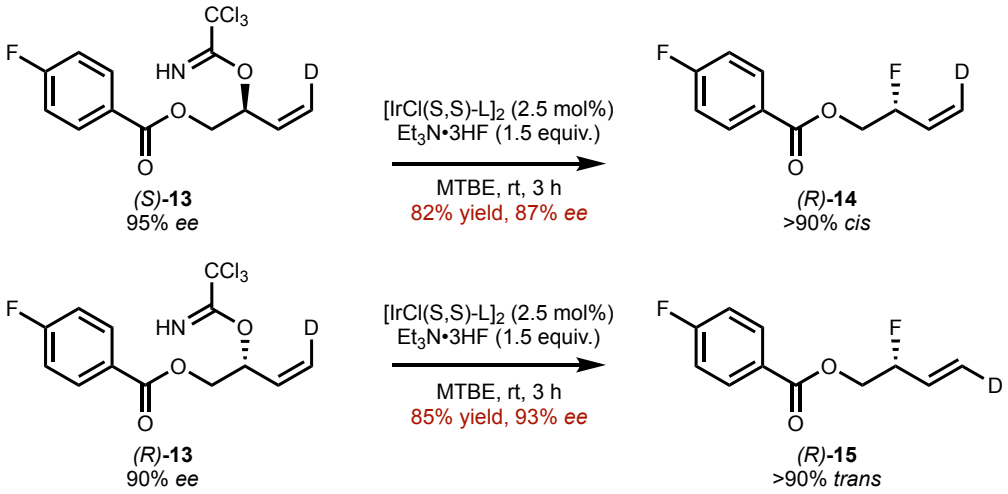


Figure 3.11 Fluorination of enantioenriched deuterium-labeled allylic trichloroacetimidates performed by the Nguyen group to support my computational mechanistic proposal.

Overall, these results, in agreement with my computational findings, are consistent with a retention−inversion pathway. Following this mechanism using [IrCl*(S,S)*-L]$_2$ catalyst (**Figure 3.12**), allylic trichloroacetimidate ***(S)*-13** would undergo ionization with retention of stereochemistry and outer sphere nucleophilic attack with inversion to afford *cis* product **14** without scrambling of deuterium on the terminal alkene. On the other hand, allylic trichloroacetimidate ***(R)*-13** would first proceed through ionization with retention of stereochemistry, and the π-allyl iridium intermediate would then undergo isomerization via a π−σ−π mechanism as predicted computationally in my work to eventually lead to fluoride nucleophilic attack with inversion to afford *trans* product **15**.

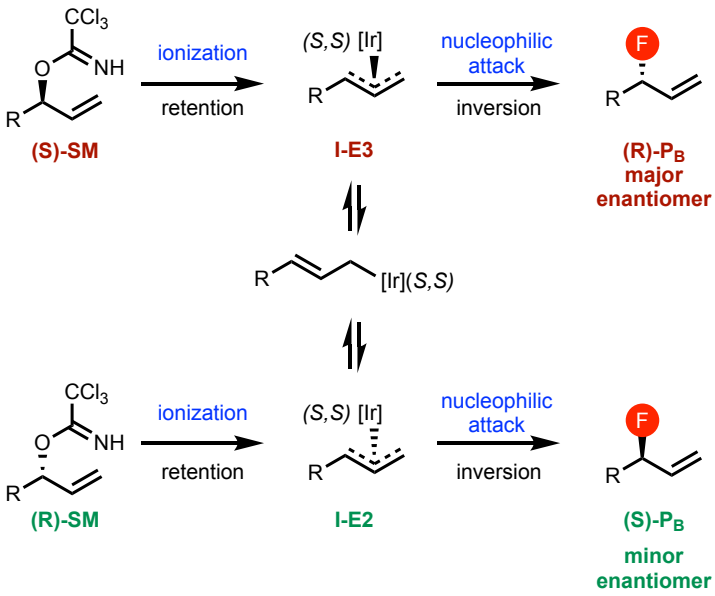


Figure 3.12 Possible mechanism of Ir-catalyzed DYKAT using $[IrCl(S,S)L]_2$ proposed computationally with experimental support.

3.4 Conclusion

The computational studies, in combination with experimental work by the Nguyen group, represent the systematic mechanistic investigation of the diene-ligated iridium catalysts that have been employed in the regio- and enantioselective fluorination of secondary allylic trichloroacetimidates. X-ray crystal structure analysis confirmed the presence of the π-allyl iridium intermediate in the reaction and, in combination with computational data, suggests that the ionization step would undergo retention of stereochemistry. Furthermore, DFT calculations in combination with deuterium-labeled trichloroacetimidate experiments by the Nguyen group suggest that the nucleophilic attack would lead to regio-determining C−F bond formation proceeding via outer-sphere fluoride attack at the more substituted allyl moiety of the η^3-bound π-allyl iridium complex. Taken together with the experimental studies, the computational studies support that the fluorination reaction of racemic allylic trichloroacetimidate substrates is likely to occur via a DYKAT process. The importance of the trichloroacetimidate is highlighted through its

multiple-purpose role as both a leaving/directing group and a ligand promoting the π−σ−π isomerization leading to a DYKAT process. In future work, the mechanistic findings obtained from these computational and experimental studies can be used to develop more effective catalysts with use of the trichloroacetimidate as the leaving group in other allylic substitutions.

Chapter 4: Mechanistic Studies of Photoredox/Nickel Dual-Catalyzed Carbon-Carbon Bond Formations

Excerpts from this chapter were published in: a) Matsui, J.; Gutierrez-Bonet, A.; **Rotella, M.;** Alam, R.; Gutierrez, O.; Molander, G. A. *Angew. Chem. Int. Ed.* **2018**, *57*, 15847-15851. and b) Youran, L.; Gutiérrez-Bonet, A.; Matsui, J.; **Rotella, M. E.;** Dykstra, R.; Gutierrez, O.; Molander, G. A. *ACS Catal.* **2019**, *9,* 8835 – 8842.

4.1 Abstract

A wide range of organic transformations can be performed under photocatalysis using visible light. When paired with a metal or organocatalyst in a dual catalytic method, photocatalysts can be used to perform stereoselective reactions under relatively mild conditions. Specifically, nickel can be used in conjunction with a photocatalyst (and light) to perform a wide range of cross-coupling reactions such as the allylation of vinyl epoxides and the alkylation of oxa- and azabenzonorbornadienes. These regioselective (and in the case of the latter, diastereoselective) transformations developed by the Molander group have a broad substrate scope with specific applications in the functionalization of carbohydrate compounds. However, an understanding of the mechanisms of these nickel/photoredox dual-catalyzed reactions is lacking despite its potential utility for the development of new metallaphotoredox-catalyzed reactions. Herein, I used quantum mechanical calculations to study the underlying mechanism of these transformations. Specifically, both density functional theory (DFT) and DLPNO-CCSD(T) calculations were used to probe the mechanism of the regioselective nickel-catalyzed/photoredox allylation of vinyl epoxides, providing support for a Ni^0 to Ni^{II} oxidative addition pathway followed by radical addition and inner sphere allylation. Also, DFT calculations were used to study the nickel/photoredox dual-catalyzed regio- and diastereoselective alkylation of

oxabenzonorbornadienes, providing support for an oxidative addition/reductive elimination mechanism, followed by a Curtin-Hammett scenario that controls the regioselectivity of the reaction.

4.2 Introduction to Photoredox/Nickel Dual-Catalyzed Single-Electron Tsuji-Trost Reaction

The combination of a photocatalyst, light, and a transition metal catalyst is a particularly attractive method for the development of selective organic transformations under mild reaction conditions.[108] For example, the Tsuji-Trost reaction which creates $C(sp^3)$-$C(sp^2)$ bonds[109] is limited in the choice of nucleophile coupling partner by pKa constraints required for the interaction of the nucleophile with the π-allyl transition metal intermediate.[110] Often, Zn-,[111] Sn-,[112] B-,[113] Mg-,[114] Si-,[115] and Li-based[116] enolates are used successfully as nucleophilic coupling partners in the Tsuji-Trost reaction. However, these enolate-based methods require highly basic conditions. To address these challenges, the Tunge group developed a palladium/photoredox dual-catalyzed radical-based intramolecular allylation. However, the intermolecular allylation was limited to the coupling of unsubstituted allyl groups with alkyl carboxylic acids.[117] In order to expand upon Tunge's precedent in radical-based Tsuji-Trost reactions, the Molander group sought to use cost effective nickel-based catalysts, which have comparatively slower rates of β-hydride elimination of the allylnickel species than palladium.[118] In this vein, the group first developed a regioselective nickel/photoredox dual-catalyzed allylation of vinyl epoxides with alkyltrifluoroborates as the radical precursor.[119] The scope of radical precursor was then expanded from alkyltrifluoroborates to include 1,4-dihydropyridines (DHPs), affording primarily the *trans* isomer (**Figure 4.1**). An understanding of the factors that

control the reaction's selectivity will allow for the development of methods with complementary reactivity and selectivity.

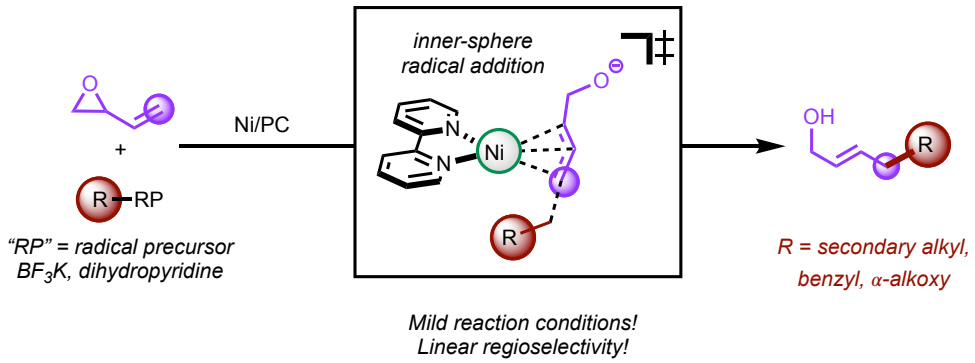


Figure 4.1 Exploring radical-based Tsuji–Trost reactivity under photoredox conditions.[12]

4.3 Results and Discussion: Mechanistic Insights into the Photoredox/Nickel Dual-Catalyzed Single-Electron Tsuji-Trost Reaction

Seeking to expand the scope of the Tsuji-Trost reaction, the Molander group developed a regioselective, nickel-catalyzed/photoredox allylation of secondary, benzyl, and α-alkoxy radical precursors and vinyl epoxides to produce linear allylic alcohols primarily in the *trans* isomer (**Figure 4.1**). Using an iridium photocatalyst ($Ir[dFCF_3ppy]_2(bpy)PF_6$), light, and a nickel catalyst ($[Ni(dtbbpy)(H_2O)_4]Cl_2$), alkyltrifluoroborates can be cross coupled with vinyl epoxides to give linear allylic alcohols (**Figure 4.2**) in high yield and *E/Z* ratios (**3a, 3b**). However, *E/Z* selectivity was greatly diminished when *tert*-butyl ether moieties were explored (**3c**).

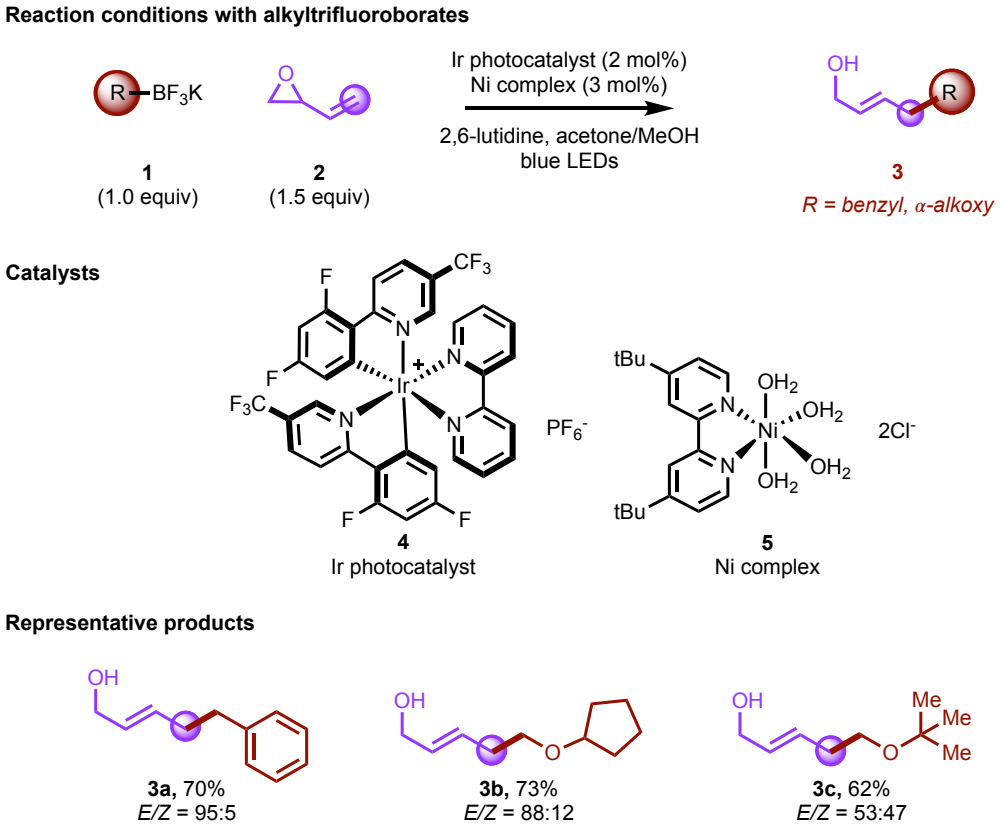


Figure 4.2 Reaction conditions developed by the Molander group for the regioselective nickel/photoredox Tsuji-Trost cross-coupling. Catalysts **4** and **5** are shown as well as representative products **3a, 3b,** and **3c**.

By modifying the photocatalyst from the iridium complex to an organic photocatalyst (4CzIPN) and the radical precursors to dihydropyridines, heterocyclic and alkenyl moieties could be incorporated within the coupling partners as well **(Figure 4.3**). These conditions also allowed for the production of allylated monosaccharides in high *E/Z* ratios (**Figure 4.3, 8c**). Notably, the stereochemical outcome of the photoredox/nickel dual-catalyzed alkylation is complementary to that of the palladium-catalyzed transformations. The latter provided net retention by double inversion,[120] whereas in the present case, 1,2-epoxy-3,4-cyclohexene afforded primarily the *trans* isomer (**8d**), suggesting the nickel coordinates the alkene and adds to the opposite face of the epoxide, but then the resulting nickel complex engages the radical and undergoes reductive elimination by a

stereoretentive, inner-sphere mechanism. To explore this mechanistic hypothesis, I undertook DFT and DLPNO-CCSD(T) quantum mechanical calculations.

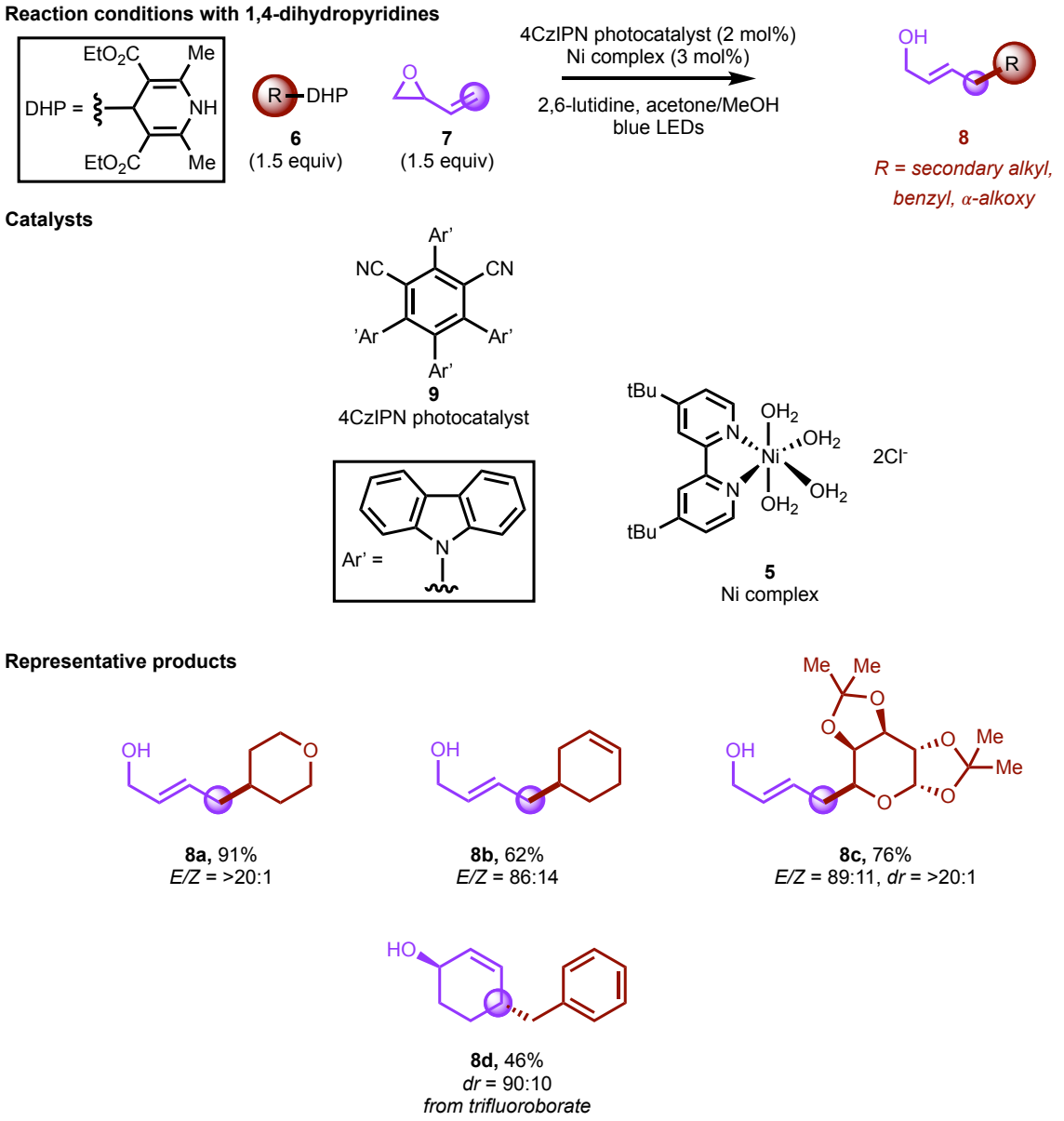


Figure 4.3 Reaction conditions developed by the Molander group using 1,4-dihydropyridines (DHP) as the radical precursors in the regioselective nickel/photoredox Tsuji-Trost cross-coupling. Catalysts **9** and **5** are shown as well as representative products **8a, 8b, 8c** and **8d**.

I used quantum mechanical calculations (DFT and DLPNO-CCSD(T) methods) to gain insight into the underlying mechanism of the photoredox/nickel dual-catalyzed Tsuji-Trost transformation, with particular focus on the goal of probing the factors controlling selectivity in the reaction.[121] The energetics of the mechanistic proposal are given in **Figure 4.4**.

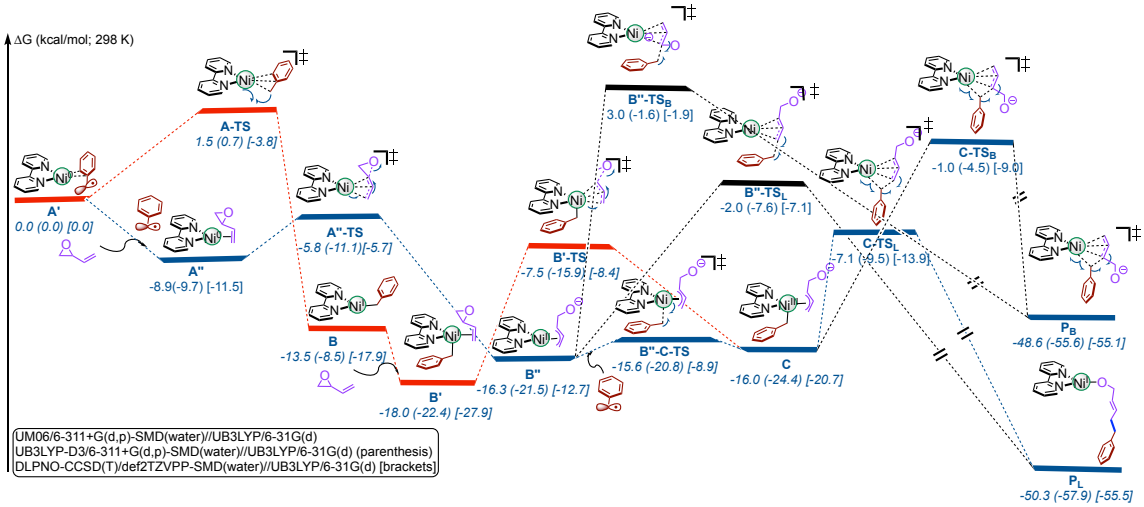


Figure 4.4 Competing $Ni^0/Ni^I/Ni^{III}$ (red), $Ni^0/Ni^{II}/Ni^{III}$ (blue), Ni^0/Ni^{II} (blue and black) pathways leading to $C(sp^3)$-$C(sp^3)$ bond formation.

I began the study with the benzyl radical (**A'**) which forms from the photocatalytic cycle (see **Figure A4.1** in Appendix 4 for energetics of radical formation). From here, complexation of Ni^0 to vinyl epoxide (**A''**) is energetically favored over that of complexation to benzyl radical **A'** by 8.9 kcal mol^{-1}, as shown in **Figure 4.4** (blue). Subsequently, this vinyl epoxide/Ni^0 (**A''**) complex can quickly undergo an S_N2-like ring-opening (via **A''-TS**; barrier is only 3.1 kcal mol^{-1} from **A''**) to form the π-allyl nickel(II) intermediate **B''**. As anticipated by previous calculations,[122] **B''** can quickly engage the benzyl radical, generated by single-electron transfer (SET) oxidation of $BnBF_3K$ by the photocatalyst to form the Ni^{III} intermediate **C** (via **B''-C-TS**). Overall, radical addition is

facile (the barrier is ca. 1–3 kcalmol^{-1}, dependent on the method). Finally, inner-sphere C(sp^2)-C(sp^3) bond formation via **C-TS$_L$** (the barrier is 8.9 kcal mol^{-1} from **C**) leads to formation of the linear product (**P$_L$**), 50.3 kcal mol^{-1} downhill in energy.

A series of reductive elimination transition states leading to formation of branched products (e.g., **C-TS$_B$**) were also located, but these were much higher in energy (>5 kcal mol^{-1}) than **C-TS$_L$**, presumably because of unfavorable electronic repulsion and steric interactions between the charged oxygen and the benzyl group (**Figure 4.4**). Moreover, C(sp^2)-C(sp^3) bond formation by an outer-sphere pathway (black) was also found higher in energy. Formation of **C** from a Ni^0-Ni^I-Ni^{III} pathway (**Figure 4.4**, red) is also overall higher in energy than the Ni^0-Ni^{II}-Ni^{III} pathway (blue). Albeit low, the barrier for radical addition (**A-TS**) from Ni^0 is still 7.3 kcal mol^{-1} higher in energy than oxidative addition to vinyl epoxide (via **A''-TS**). However, it is likely that formation of **C** is highly dependent on the local concentration of the benzyl radical and vinyl epoxide. Overall, DFT and DLPNO-CCSD(T) calculations support a Ni^0-Ni^{II}-Ni^{III} reaction pathway and an inner-sphere reductive elimination as the product-determining step, leading to formation of the linear product as the major product (see **Figure A4.2** in Appendix 4 for the overall catalytic cycle).[123] This model is in accord with the stereochemical results observed with cyclohexadiene monoxide. Further, although computational studies favored the linear product, the branched pathway is only 5 kcal mol^{-1} higher in energy, suggesting branched products may be observed in some cases (likely dependent on the nature of the substrate, ligand, etc.). To test this hypothesis, the Molander group subjected sterically hindered aryl-substituted vinyl epoxides to the standard reaction conditions and indeed found a mixture of linear and branched products, albeit in low yields.

In summary, a dual catalytic allylation reaction which demonstrates complementarity to traditional Tsuji–Trost reactions was developed by the Molander group. In juxtaposition with classical reactivity in the palladium-catalyzed transformations (stabilized anionic carbon nucleophiles), carbon-centered radicals were employed, enabling the allylation of secondary, benzyl, and α-alkoxy radical precursors. Additionally, net inversion of stereochemistry was observed in the photoredox/nickel dual-catalyzed systems, as opposed to the net retention by double inversion observed in the traditional palladium-catalyzed processes. To gain insight into the mechanistic pathway, I conducted quantum mechanical calculations (using dispersion-corrected (U)DFT and DLPNO-CCSD(T) methods) to determine the energetic favorability of the oxidative addition step. Here, a Ni^0 to Ni^{II} oxidative addition step was found to occur before radical addition to the nickel center. This proposal is a deviation from previous mechanistic studies of photoredox/nickel dual cross-coupling pathways where Ni^0 to Ni^I has been involved in the putative pathway.[124]

4.4 Introduction into the Use of Oxabenzonorbornadiene as Electrophilic Coupling Partners under Photoredox/Nickel Dual Catalysis

Following the development of the regioselective nickel/photoredox dual-catalyzed Tsuji-Trost reaction by the Molander group, the use of oxa- and azabenzonorbornadienes as electrophilic coupling partners under nickel/photocatalytic conditions was explored.[125] Oxa- and azabenzonorbornadienes were targets for this reaction owing to their literature precedent as compounds capable of forming new $C(sp^3)$-$C(sp^3)$ bonds.[126] With the overall goal in mind of building molecular complexity rapidly, it is logical to target compounds which can readily introduce $C(sp^3)$-hybridized centers in a molecule as these centers

increase a compound's complexity by way of increasing its 3D character.[127] Along these lines, oxabenzonorbornadienes have been employed in transition metal-catalyzed cross-coupling reactions, most notably in reaction with organozinc reagents.[128] While palladium is widely used to generate diastereoselective and enantioenriched products[129] in this coupling, other transition metals such as nickel, copper, and cobalt have been employed in asymmetric versions of this reaction.[130] Although excellent enantiocontrol is possible through these methods, most of the examples are limited to dialkylzinc compounds as the coupling partner, where only one alkyl motif is coupled with the substrate. In simple systems, the loss of the other alkyl residue is inconsequential but in the case of complex alkyl side chains, this limitation can become a handicap. Additionally, the alkyl residue is limited in scope to benzylic, allylic and simple alkyl chains. To address these challenges, the Molander group replaced the organometallic species with an aryl halide radical precursor in the cross-coupling following work done by the Cheng group in 2015.[131] Although Cheng reported the successful nickel-catalyzed reductive cross-coupling of oxabenzonorbornadienes with alkyl halides, the yields were low, limiting the utility of the method. Building on this work, Molander reported a nickel/photoredox dual-catalyzed cross-coupling of oxa- and azabenzonorbornadienes with alkyl motifs leading to exclusive formation of the 1,2-*syn* addition product (**Figure 4.5**).

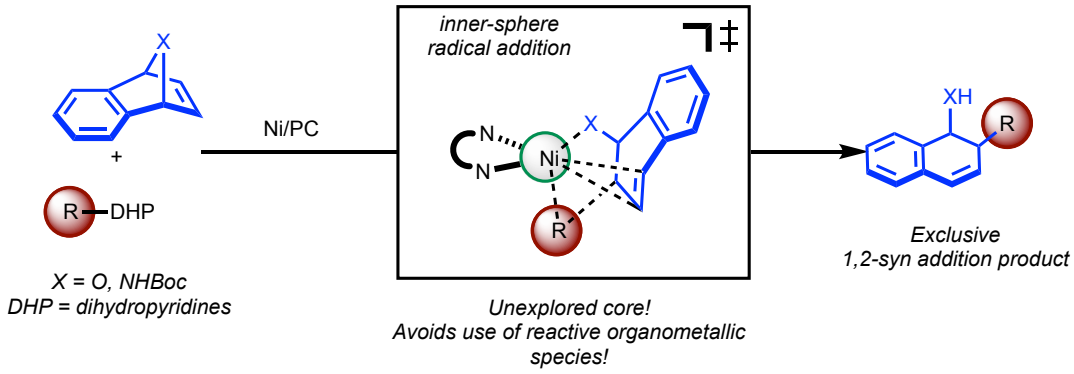


Figure 4.5 Ni/photoredox dual catalysis as a strategy to overcome previous limitations of the alkylation of oxa- and azabenzonorbornadienes.[132]

This reaction serves as a complement to existing methodology based on copper catalysis which results in anti-selective product formation.[133] In general, mechanistic knowledge of this nickel/photoredox dual-catalyzed 1,2-*syn* addition is limited, despite the potential for new reaction development that such knowledge would allow. Thus, density functional theory (DFT) calculations were undertaken to probe the underlying mechanism of this transformation, with particular emphasis on understanding the observed regio- and diastereoselectivity.

4.5 Density Functional Theory Study of the Mechanism of Photoredox/Nickel Dual-Catalyzed Alkylation of Oxabenzonorbornadienes

Having identified alkyl-substituted 1,4-dihydropyridines as excellent radical precursors in the nickel/photoredox dual-catalyzed Tsuji-Trost reaction, the Molander group moved on to explore the radical precursor's capabilities in the combination of saccharyl-DHPs with epoxynaphthalene electrophiles. If successful, this method would allow for the straightforward preparation of Group II *C*-aryl glycoside antibiotics which, previously had limited synthetic routes available, all of them involving the use of organometallic reagents.[134,135] Conceptually, alkylation of the oxa- and

azabenzonorbornadienes poses several challenges, including the various regio- and stereochemical scenarios available (1,2- and 1,4-addition products,[136] as well as *syn/anti*-stereoisomers). However, the Molander group anticipated that the judicious choice of the ancillary ligand for the nickel catalyst would lead to a satisfactory and useful product distribution. With this hypothesis in mind, the group optimized reaction conditions for the cross-coupling of epoxynaphthalene with 4-alkyl-1,4-dihydropyridines. Specifically, the reaction used $NiCl_2 \cdot$dme as the precatalyst, acetone as the solvent, and 2,4,5,6-tetra-9H-carbazol-9-yl-1,3-benzenedicarbonitrile (4-CzIPN) as the photocatalyst with **L1** (**Figure 4.6**) to deliver products in quantitative yields with excellent regio- and diastereocontrol. To expand the scope, Molander et. al focused on different 4-alkyl-DHPs, finding that secondary and stabilized primary radicals were successfully coupled with oxo- and azabenzonorbornadienes while tertiary radicals failed to deliver the desired product. Secondary radicals, including heterocycles (**Figure 4.6, 12a**), bicyclic structures (**12b**), and masked diols (**12c**), could be introduced in good to high yields. Notably, the reaction was not limited to epoxynaphthalenes, as azabenzonorbornadienes were suitable substrates as well, affording only the *syn*-1,2-addition product (**12d**). Intrigued by the excellent regio- and diastereocontrol observed, the Molander group examined diverse epoxynaphthalene cores to determine whether substrate control could be tuned based on steric or electronic factors and found that regardless of the substituents on the aromatic ring, exclusive *syn*-1,2-addition was observed. Thus, to understand this regioselectivity, I employed quantum mechanical calculations.

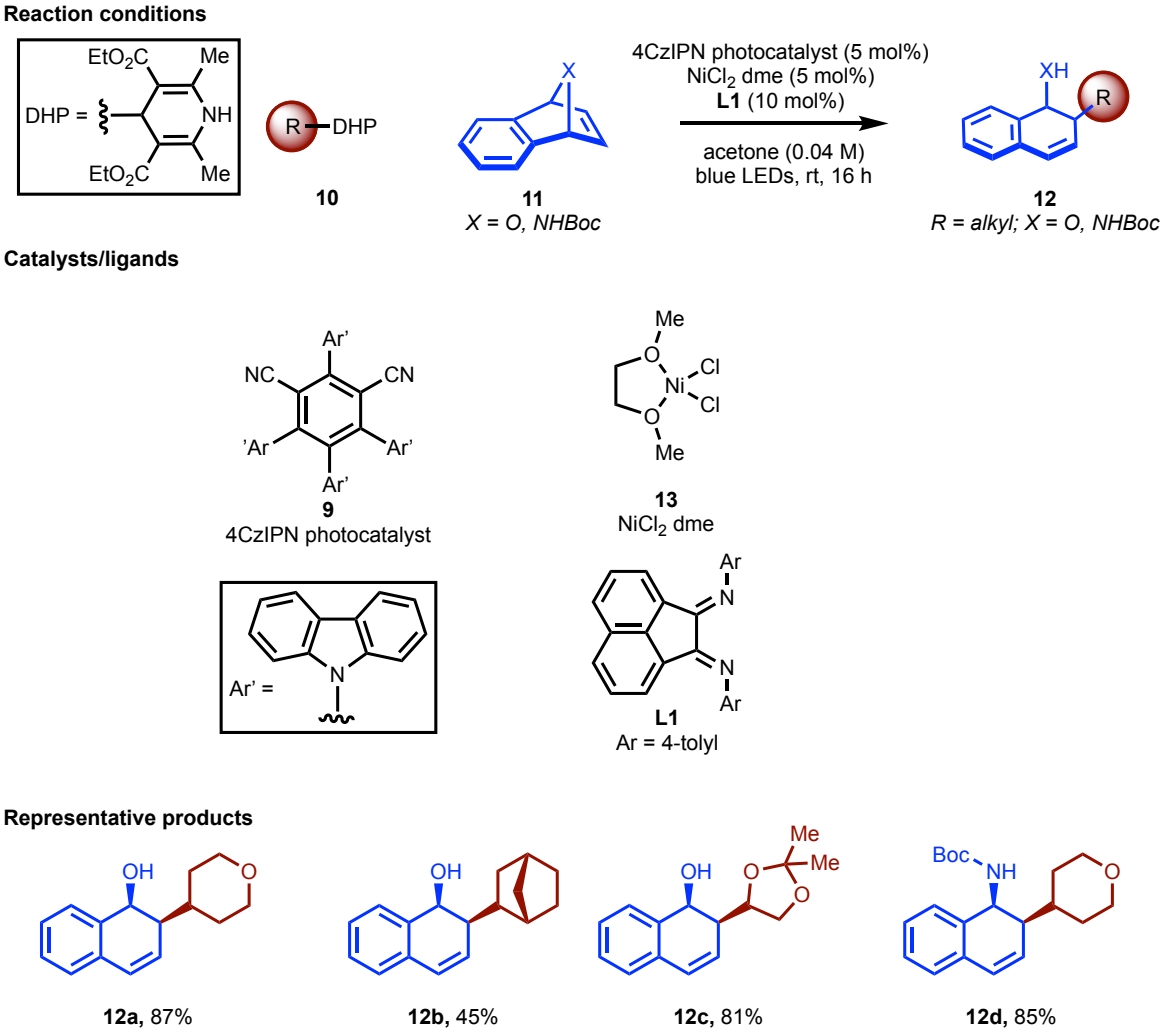


Figure 4.6 Reaction conditions developed by the Molander group in the nickel/photoredox-catalyzed cross-coupling of oxa- and azabenzonorbornadienes with 4-alkyl DHPs. Catalyst **9**, $NiCl_2$-dme **13** and **L1** are shown as well as representative products **12a, 12b, 12c,** and **12d.**

I used density functional theory [UM06/6-311+G(d,p)-CPCM-(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)] to gain insights into the mechanism and factors controlling regioselectivity of the nickel/photoredox dual-catalyzed cross-coupling of oxabenzonorbornadienes with alkyl motifs. Epoxynaphthalene was used as the representative oxabenzonorbornadiene. For simplicity, only the lowest energy pathway is discussed (see **Figure A4.3** in Appendix 4 for full details on higher energy pathways).

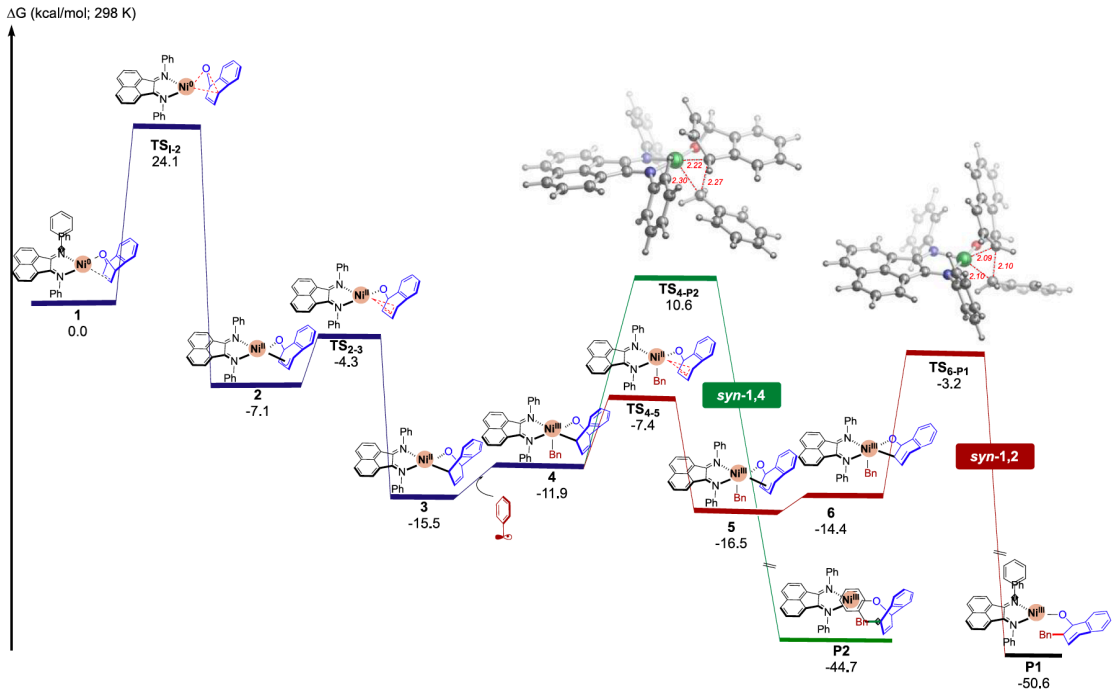


Figure 4.7 Energetics of the lowest energy pathway. Free energies (kcal/mol) are computed at the UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone) level of theory. Reprinted with permission from ref 18. Copyright 2019 American Chemical Society.

As shown in **Figure 4.7**, syn complexation of the epoxynaphthalene to the Ni (0) complex **1** allows direct oxidative addition to the C−O bond via **TS-1-2** (overall barrier is 24.1 kcal/mol) to form a Ni-O-π-allyl complex **2** (exergonic by 7.1 kcal/mol). In turn, this intermediate favors a low barrier π−σ rearrangement (via **TS-2-3**), leading to the 1,4-Ni (II)-O-alkyl complex **3**. At this stage, the benzyl radical, presumably generated from the photocatalytic cycle (not calculated), will add to the Ni (II) intermediate **3**, leading to formation of Ni (III) complex **4**. Despite various attempts, the transition state could not be located for radical addition at this level of theory. Analysis of relaxed scans of the forming Ni−C bond[137,138,139] (see **Figure A4.4** in Appendix 4) revealed a barrierless interconversion

between **3** and **4**, while calculations optimized in the gas phase revealed a small energetic barrier (ca. 3 kcal/ mol) between these two species.

Importantly, from this Ni (III) complex **4** intermediate, two pathways were found that could lead to the formation of the 1,4- and 1,2 products. As shown in the green pathway, Ni (III) intermediate 4 could undergo direct reductive elimination (via **TS-4-P2**) to form the 1,4-product (after protonation; not calculated) with an overall barrier of ~26 kcal/mol from 3. Although the barrier is reasonable, the formation of the 1,2-product (red) is significantly lower in energy. Specifically, 4 will preferentially undergo a facile σ–π–σ isomerization (barrier is only ~5 kcal/mol via **TS-4-5**), leading to the more energetically favored π-allyl Ni (III) 5 intermediate. In turn, this π-allyl intermediate will then form the 1,2-Ni (III) intermediate **6**, which is poised to undergo facile (barrier is ~11 kcal/mol) reductive elimination via **TS-6-P1**, leading to the experimentally observed 1,2-syn product **P1** (after protonation; not calculated).

The distortion-interaction model[140] was used to explore the regioselectivity of the reaction. Specifically, **TS-6-P1** and **TS-4-P2** (**Figure 4.8**) were analyzed. $\Delta E_{dist}^{\ddagger}$ is the energy required to distort intermediate **3** and the benzyl radical into the transition state geometry. $\Delta E_{int}^{\ddagger}$ is the energy of the interaction between the distorted fragments. The distortion energy of **TS-4-P2** is higher than that of **TS-6-P1** (~7 kcal/mol), indicating that it takes more energy for intermediate **3** and the benzyl radical to distort into the transition state geometry required by **TS-4-P2** than by **TS-6-P1**, contributing to the overall higher energy of this transition state. Furthermore, the interaction energy between the distorted intermediate **3** and benzyl radical fragments in **TS-6-P1** is 8 kcal/mol lower than that in

TS-4-P2. This result indicates that **TS-6-P1** has a more favorable interaction energy, leading to the observed 1,2-regioselectivity. It is worth noting that the C−C bond length between the benzyl radical and the epoxynaphthalene substrate in **TS-6-P1** is shorter (2.1 Å) than the same bond length in **TS-4-P2** (2.27 Å), indicating that **TS-6-P1** is a more dissociative transition state, which contributes to the more favorable interaction energy in **TS-6-P1**. Overall, the distortion-interaction model offers insight into the preference for the 1,2-product, as observed experimentally.

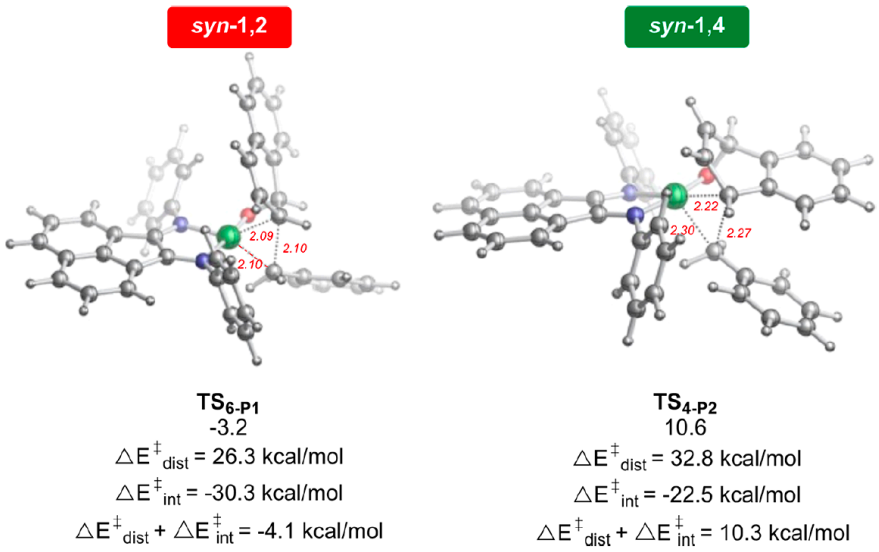


Figure 4.8 Distortion-interaction analysis of $\mathbf{TS_{6\text{-}P1}}$ and $\mathbf{TS_{4\text{-}P2}}$. Energies (kcal/mol) are computed at the UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone) level of theory. The favorable interaction energy in $\mathbf{TS_{6\text{-}P1}}$ leads to the observed regioselectivity. Reprinted with permission from ref 18. Copyright 2019 American Chemical Society.

Overall, favorable exo-coordination [via Ni(0) **1**] dictates the syn-selectivity, whereas the exclusive 1,2-regioselectivity observed arises from a Curtin−Hammett scenario,[141] owing to a rapid σ−π−σ isomerization that interconverts benzyl radical/ Ni(II), σ-Ni(III), and π-allyl Ni(III) intermediates (**3, 4, 5, 6**) prior to undergoing regio-

determining reductive elimination. The previously reported mechanism under palladium catalysis[142] (i.e., carbometalation followed by a β-oxygen elimination) would be unlikely for this system because there is no precedent in the literature for a β-oxygen elimination with nickel. Indeed, computations predict this pathway to be unfavorable because of the high energy of the syn carbometalation transition state.

In summary, taking advantage of the inherent mild reaction conditions of nickel/photoredox dual catalysis, the Molander group developed the first general and efficient regio- and diastereoselective alkylation of oxa- and azabenzonorbornadienes which tolerates an array of functional groups and complex alkyl motifs, including saccharyl units, thus allowing for the synthesis of arylated C-glycosyl antibiotic precursors. Through computational mechanistic studies, I unraveled a new mechanistic paradigm, invoking a Ni(0) oxidative addition to form an π-allylnickel complex, followed by radical addition to generate a Ni(III) species, which under Curtin−Hammett conditions undergoes preferential reductive elimination from the 1,2-nickel adduct, resulting in complete regiocontrol.

4.6 Conclusion

In summary, quantum mechanical calculations were used to study the underlying mechanism of two nickel/photoredox dual-catalyzed reactions developed by the Molander group, including the allylation of vinyl epoxides and the alkylation of oxa- and azabenzonorbornadienes. In the regioselective Tsuji-Trost reaction, computations provide support for a Ni^0 to Ni^{II} oxidative addition pathway followed by radical addition and inner sphere allylation. Further, linear product formation was favored over branched computationally, in agreement with experimental observations. Additionally, DFT

calculations were used to study the nickel/photoredox dual-catalyzed regio- and diastereoselective alkylation of oxa- and azabenzonorbornadienes. It was found that the reaction proceeds by an oxidative addition/reductive elimination mechanism, followed by a Curtin-Hammett scenario that controls the observed regioselectivity of the reaction.

Chapter 5: Mechanistic Insights into the Nickel-Catalyzed Diarylation of Unactivated Alkenes in Ketimines

5.1 Abstract

Olefins are a prevalent motif in natural products and feedstock chemicals and widely used in organic synthesis.[143] For example, rapid diversification of alkenes can be accomplished through transition metal-catalyzed dicarbofunctionalization reactions. Recently, the Giri group developed a method for 1,3-, and 1,2-diarylation of alkenes. In this work, I used quantum mechanical calculations to explore the mechanism of these nickel-catalyzed diarylation reactions. Key findings from these studies were the role of the phosphine ligand in promoting reductive elimination and the role of silver and copper salts in suppressing β-hydride elimination and enabling reductive elimination.

5.2 Introduction

Selective dicarbofunctionalization of alkenes is a powerful strategy to rapidly build molecular complexity using readily available starting materials.[144] Extensive efforts have been placed towards the development of selective reductive cross-coupling methods to difunctionalize alkenes.[145,146] Generally, these methods are successful with activated alkenes[147] while examples of the dicarbofunctionalization of unactivated alkenes are rare.[148] Notably, an appealing strategy for the dicarbofunctionalization of unactivated alkenes is via the interception of *in situ* generated Heck intermediates with organometallic reagents (**Figure 5.1**).[149]

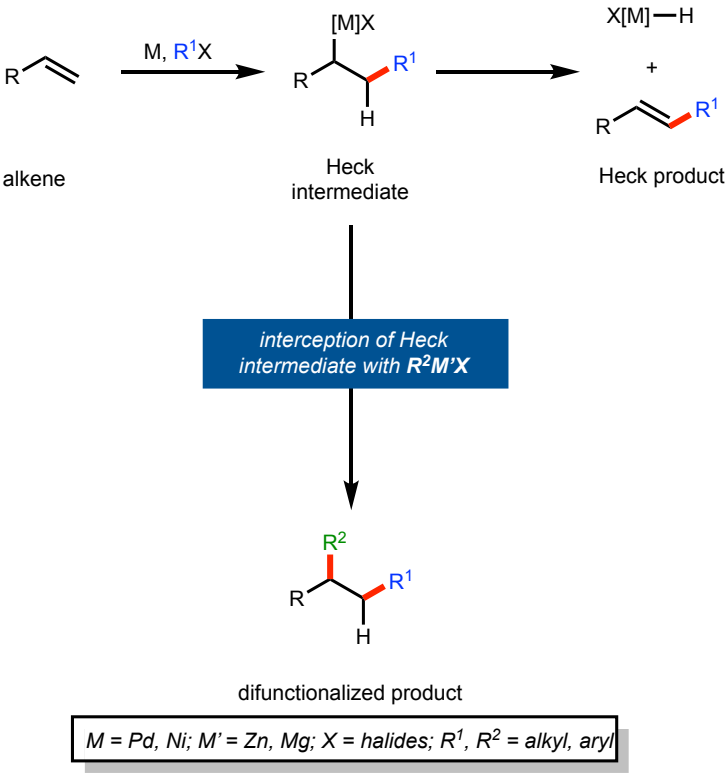


Figure 5.1 Strategies for alkene difunctionalization via the interception of the Heck intermediate.

Recently, Giri and co-workers[150] and Engel, Zhao, and Zhang[151] have utilized a directing group strategy to promote selective dicarbofunctionalization of unactivated alkenes, which they hypothesize occurs by control of the migratory insertion stage via stabilization of the 6-membered metallacycle intermediate. Notably, by implementing either *neutral* or *cationic* reaction conditions, the Giri group was able to selectively generate the 1,3- or 1,2-diarylated products from this metallacycle intermediate (**Figure 5.2**).

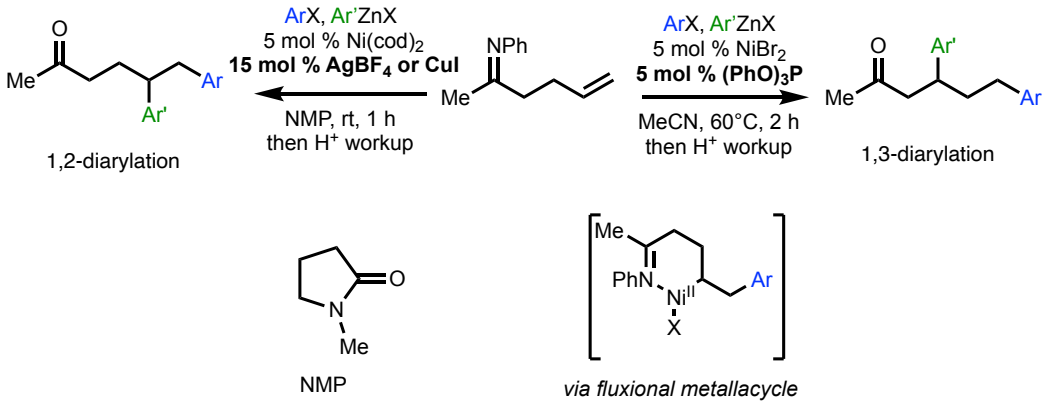


Figure 5.2 Nickel-catalyzed dicarbofunctionalization of unactivated olefins in ketimines. The 1,3-diarylated product (right) can be accessed through *neutral* conditions while the 1,2-diarylated product (left) can be accessed using *cationic* conditions by way of a silver or copper salt.

In particular, the phosphine ligand **P(OPh)$_3$** in conjunction with $NiBr_2$ can be used to obtain a wide range of 1,3-diarylated ketones from the corresponding alkenes, aryl halides, and aryl zinc reagents.[152] On the other hand, by incorporating 15 mol % of silver or copper salt, 1,2-diarylated ketones can be synthesized.[153] To elucidate the mechanism and shed light into the origin of the divergent reactivity, I used dispersion-corrected density functional theory calculations to map out the potential energy surface with both the neutral nickel/phosphine system (yielding the 1,3-diarylated product) and the cationic nickel/silver or nickel/copper system (yielding the 1,2-diarylated product).

5.3 Results and Discussion

5.3.1 Mechanistic Insights into the 1,3-Diarylation of Unactivated Alkenes in Ketimines

First, I focused on using quantum mechanical calculations to elucidate the mechanism of nickel-catalyzed 1,3-diarylation of unactivated alkenes (**Figure 5.3**).[10]

Overall, I expect that these calculations will lead to a greater understanding of the underlying mechanism of the transformation and aid in future rational reaction design.

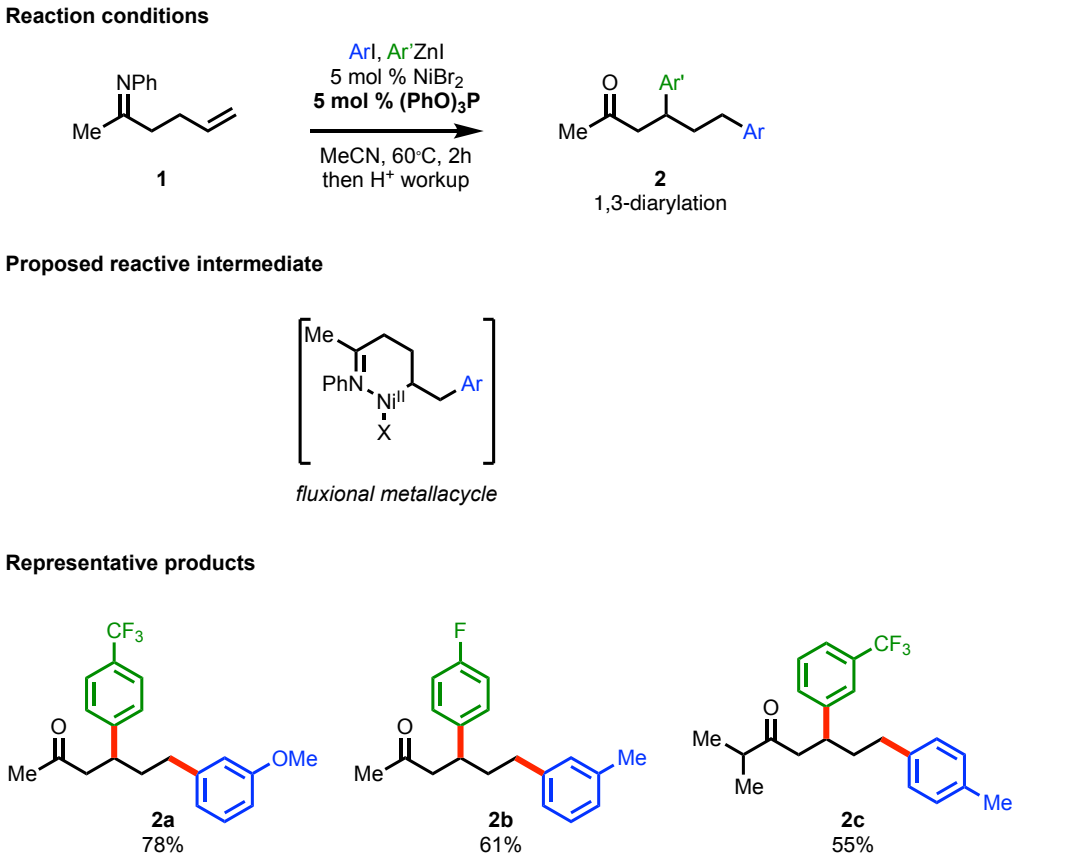


Figure 5.3 Conditions developed by the Giri group for 1,3-diarylation of unactivated olefins in ketimines via a fluxional metallacycle intermediate.

To investigate the mechanism of this transformation I used dispersion-corrected density functional theory with the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) method (see **Figures A5.1 – A5.4** in Appendix 5 for full details on the energetics of the pathway). The energies of both the singlet and triplet states of all species were computed in addition to the energies of different conformers from an exhaustive conformational search of each intermediate and transition state (see **Figures A5.5 – A5.31** in Appendix 5 for details on the conformational search). As shown in **Figure 5.4**, **A** can complex to the aryl iodide to give **A'** via ligand dissociation followed by oxidative addition

via **A'-TS-B** (barrier of 19.2 kcal/mol) to form **B (Figure 5.4)**. Notably, calculations shown that migratory insertion from **B** is facile via **B-TS-C** (barrier of 6.3 kcal/mol) to form **C.** In turn **C** but undergo an isomerization to move aryl ring away from the metal center. (not calculated) to form species **C-conf** (downhill by 8.9 kcal/mol).

Singlet **C-conf** can then undergo direct β-hydride elimination via ^{1}**C-TS-D** to form ^{1}**D** (**Figure 5.4**, barrier of 28.1 kcal/mol). Alternatively, ^{1}**C-conf** could undergo intersystem crossing to the triplet-spin species ^{3}**C-conf**, which is uphill by 4.0 kcal/mol. From here, the triplet ^{3}**C-conf** can then undergo β-hydride elimination via the lower energy ^{3}**C-TS-D** (barrier of 18.3 kcal/mol) to lead to triplet ^{3}**D** (downhill in energy by 15.9 kcal/mol respective to **A**). The triplet intermediate ^{3}**D** can undergo intersystem crossing again to form the lower energy singlet ^{1}**D**. The pathway for β-hydride elimination with the involvement of the phosphine ligand was computed as well (see **Figure A5.2** in Appendix 5, gray pathway) but found to be higher in energy, leaving the role of the phosphine ligand unknown.

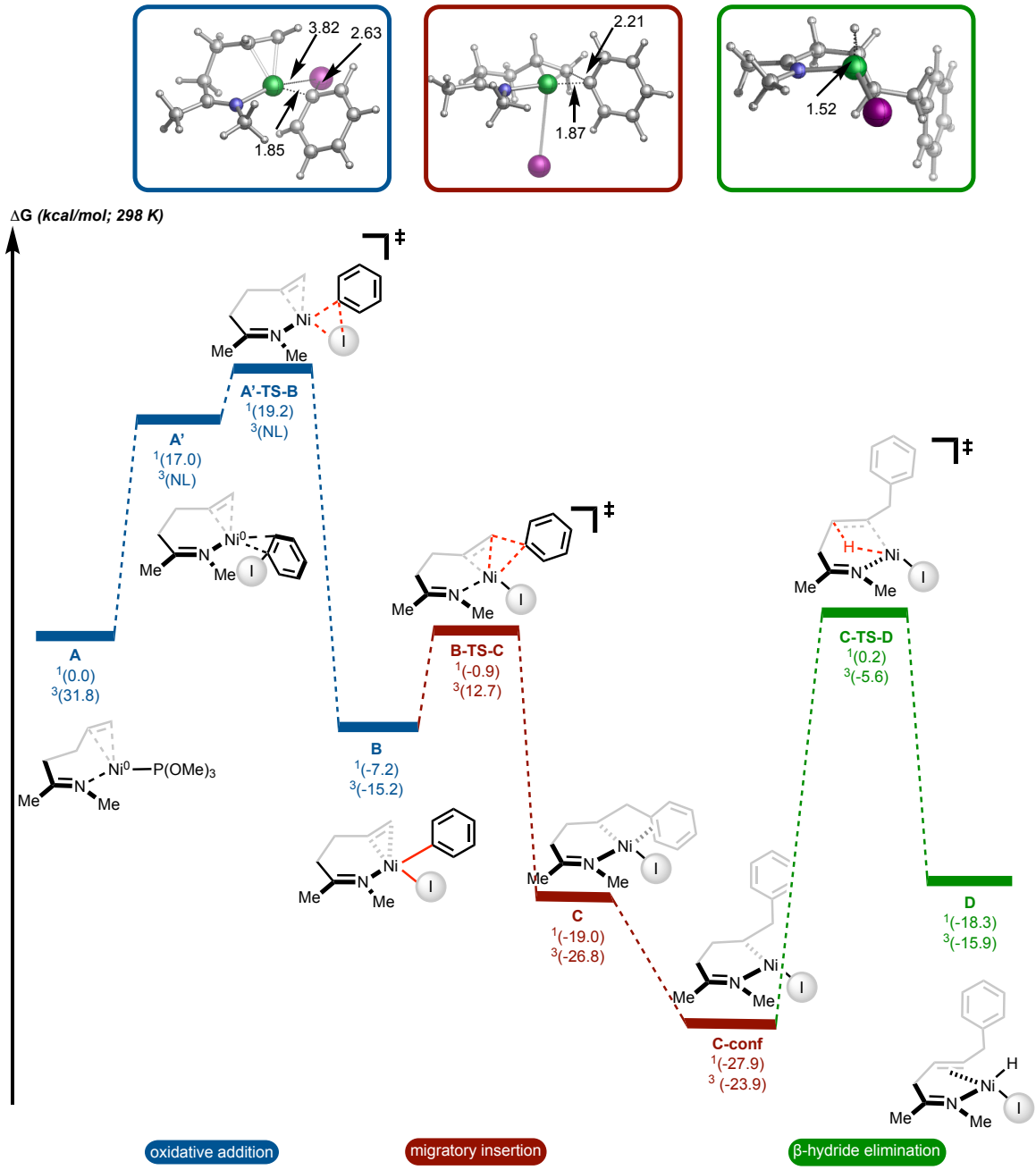


Figure 5.4 Reaction coordinate diagram showing oxidative addition, migratory insertion, and β-hydride elimination leading to intermediate **D** calculated at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory. NL indicates that these intermediates could not be located at the spin indicated in the superscript.

Next, intermediate **^{1}D** can quickly undergo a ring contraction through nickel-hydride reinsertion via **D-TS-E** (**Figure 5.5,** barrier of 4.4 kcal/mol) to form intermediate **E**. From **E**, the phosphine ligand can bind to the nickel center leading to the lower energy intermediate **E'** (downhill in energy by 7.0 kcal/mol). Finally, the phenyl group from the phenyl zinc iodide can then undergo transmetalation to form the lower energy intermediate **G** (-34.4 kcal/mol). Notably, calculations show that the rate-determining step is the reductive elimination step and it occurs with the aid of the phosphine ligand to give product **H** with a barrier of 27.8 kcal/mol.

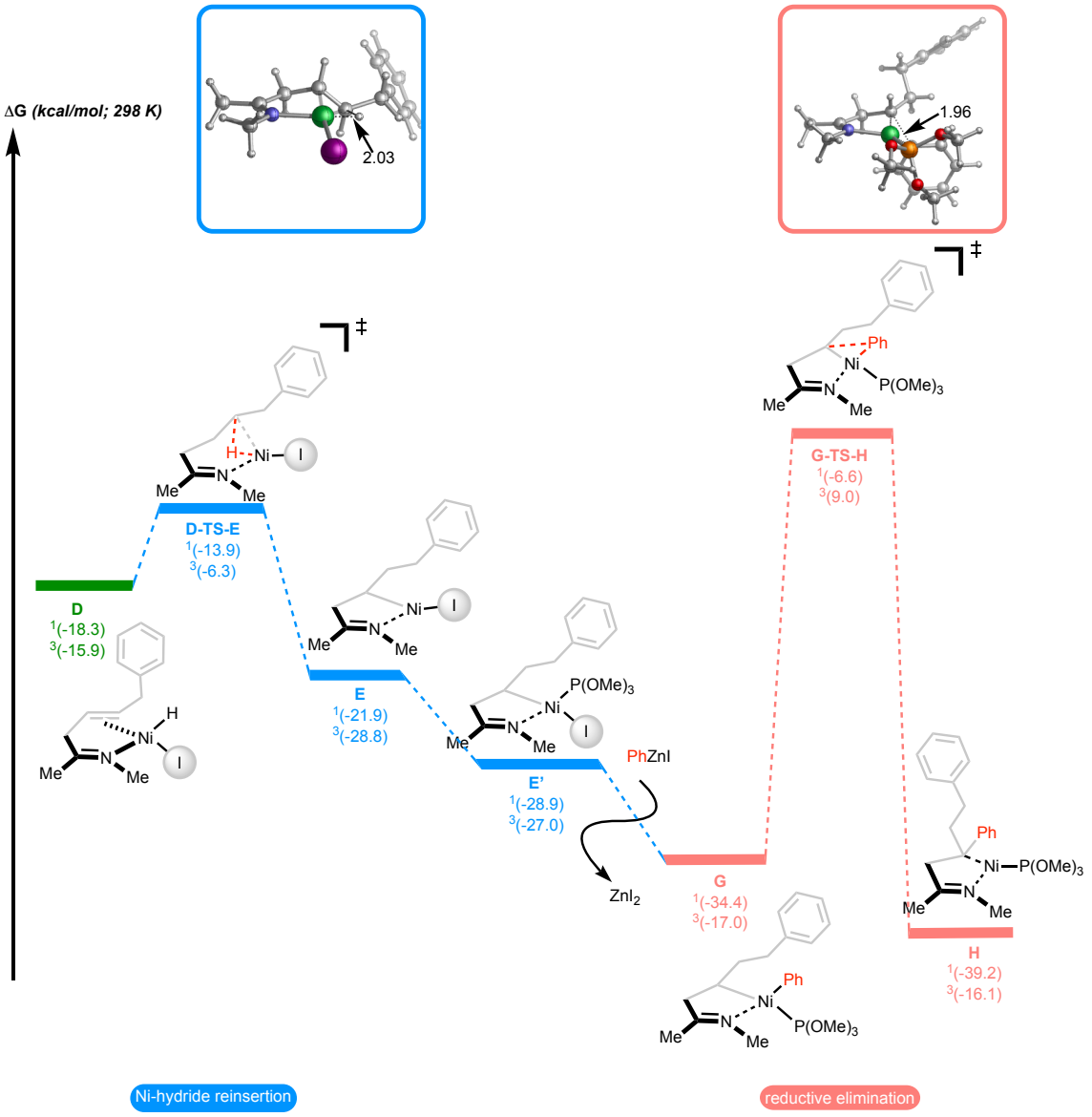


Figure 5.5 Reaction coordinate diagram showing nickel-hydride reinsertion and reductive elimination leading to 1,3-diarylated product calculated at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

Reductive elimination was also computed without phosphine ligand but was found to be prohibitively high in energy (overall barrier of 49.2 kcal/mol; see **Figure A5.4** in Appendix 5 for details). Thus, these calculations provide evidence for the role of the *phosphine ligand for reactivity*. Overall, calculations are consistent with the catalytic cycle shown in **Figure 5.6**. From these calculations, we can attribute observed 1,3-regioselectivity as a result of the β-hydride elimination/Ni-hydride reinsertion leading to a ring contraction from the 6-membered (^{1}**C**) to a 5-membered metallacycle (^{1}**E**).

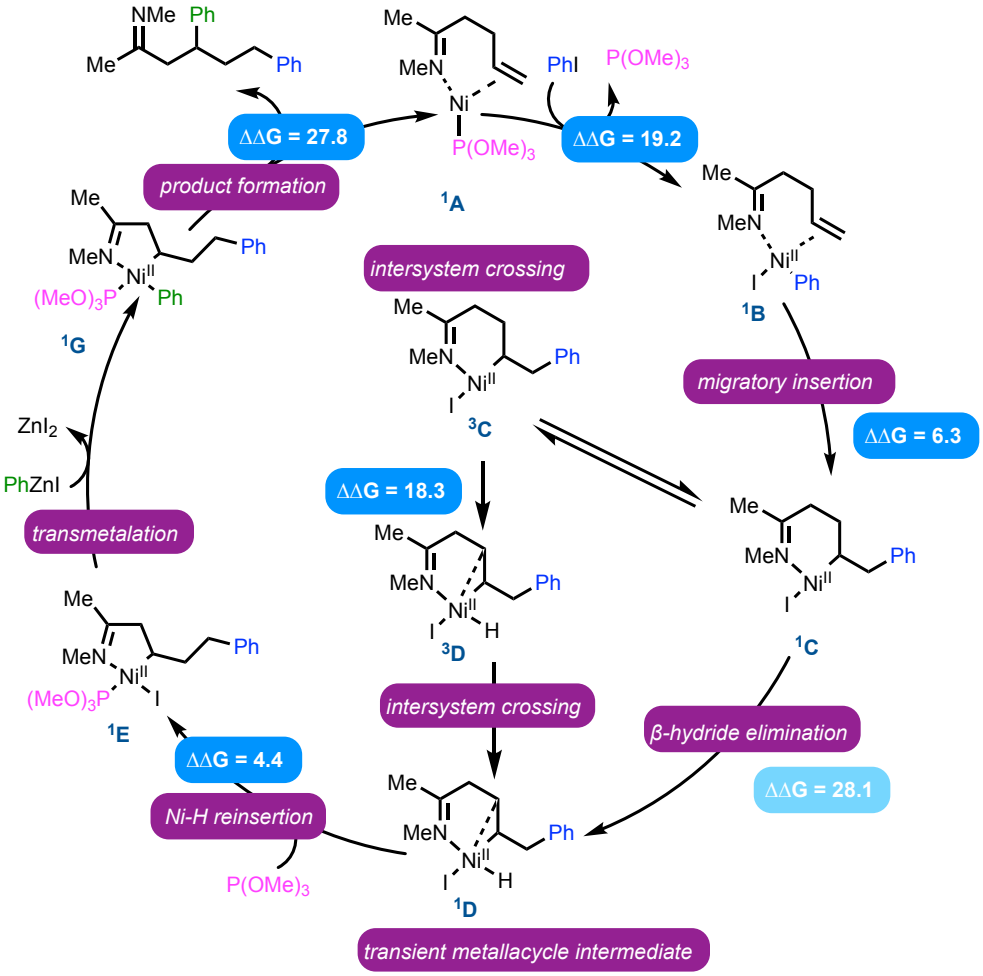


Figure 5.6 Overall neutral catalytic cycle of Ni-catalyzed 1,3-diarylation. Free energy values (kcal/mol) were calculated at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

5.3.2 Mechanistic Insights into the 1,2-Diarylation of Unactivated Alkenes in Ketimines

Next I explored the mechanism of the cationic nickel-catalyzed 1,2-diarylation of unactivated alkenes in ketimines (**Figure 5.7**) with focus on elucidating the role of the silver and copper salt as well as understanding the origin of the observed 1,2-regioselectivity.

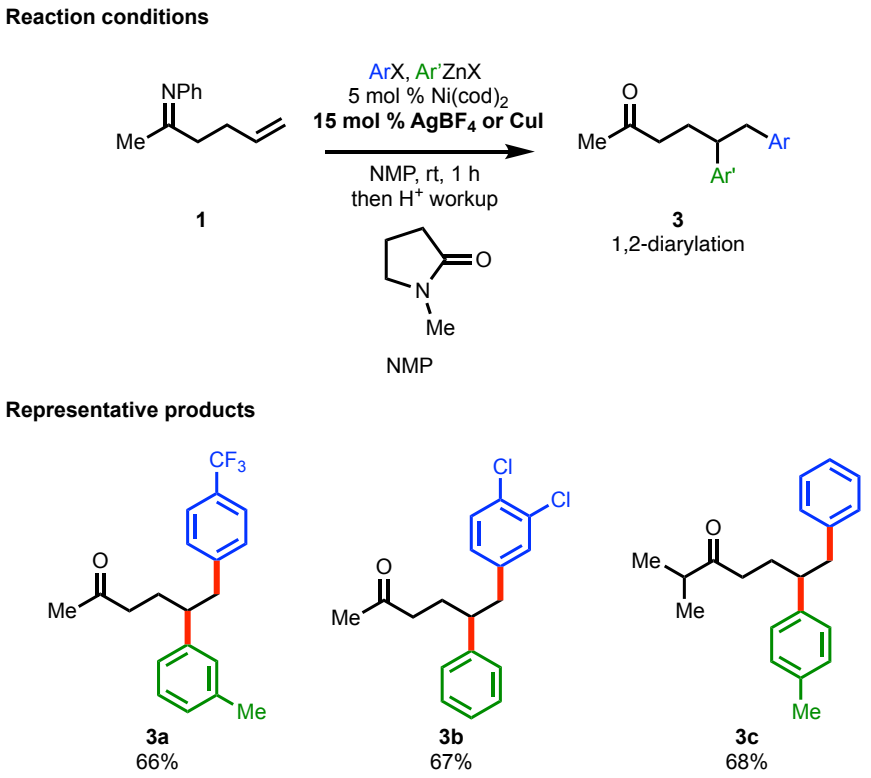


Figure 5.7 1,2-diarylation of unactivated olefins in ketimines enabled by silver or copper salts.

To investigate this system, dispersion-corrected DFT calculations (UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)) were used. Both the singlet and triplet states were computed as in the case of the neutral system, but the singlet state was found to be lower in energy for all intermediates and transition states in this case and therefore only the singlet energy values are given for simplicity. The full reaction coordinate diagram for the Ni/$AgBF_4$-catalyzed system is given in **Figure 5.8**.

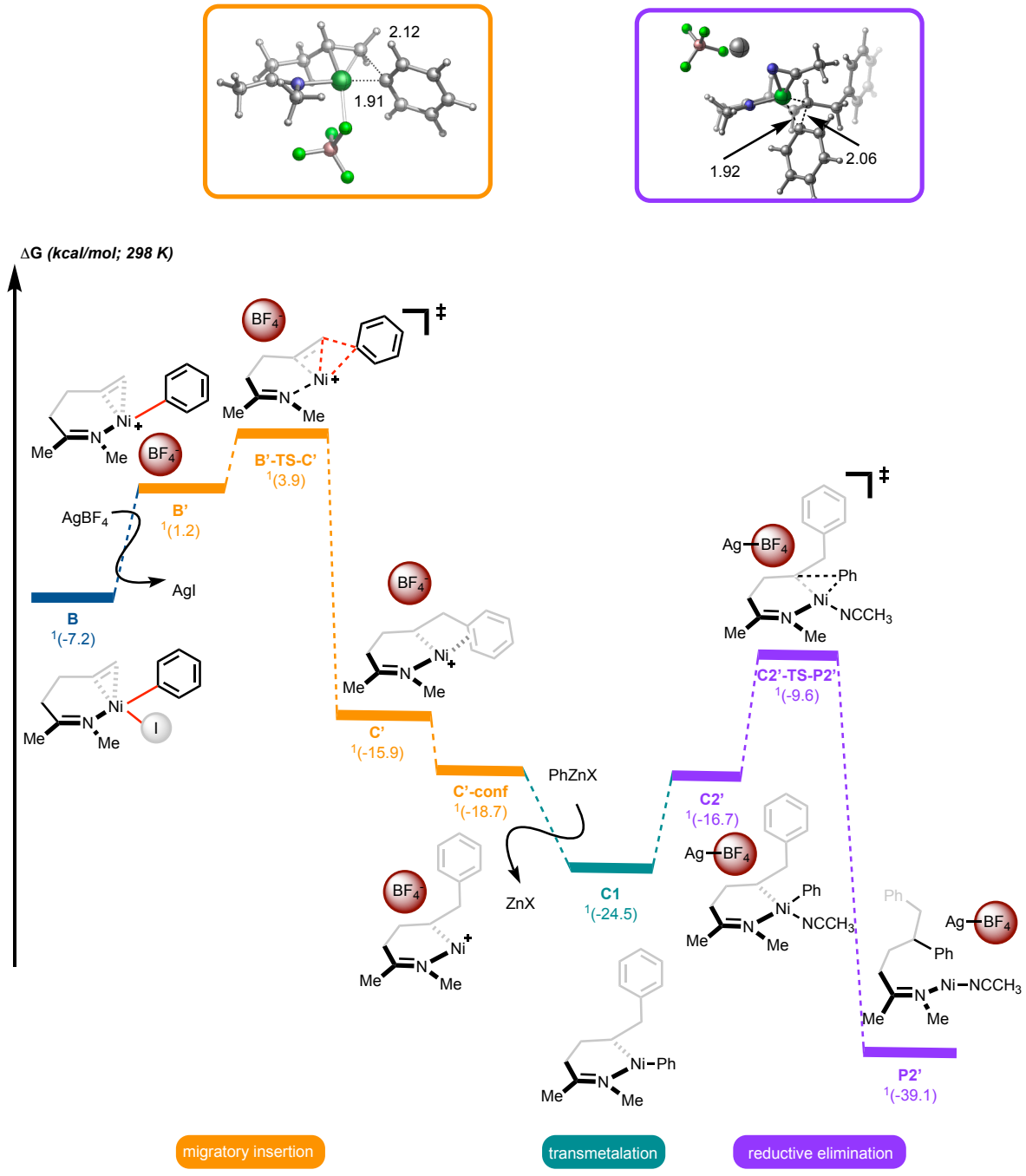


Figure 5.8 Reaction coordinate diagram of the lowest energy pathway with $AgBF_4$ showing migratory insertion, transmetalation and reductive elimination leading to 1,2-diarylation calculated at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

Notably, the iodine atom of **B** (from oxidative addition of nickel complex A', see **Figure 5.4**) can dissociate from nickel to form the higher energy cationic nickel species **B'** (uphill in energy by 8.4 kcal/mol). Next migratory insertion occurs via **B'-TS-C'** (barrier of 11.1 kcal/mol from **B**) to form **C'**. Similar to the neutral system, intermediate **C'** can isomerize to the lower energy intermediate **C'-conf**. However, unlike the neutral nickel system, the cationic intermediate **C'-conf** is less likely to undergo β-hydride elimination (see **Figure A5.32** in Appendix 5 for details on this higher energy pathway) as the barrier to this process is prohibitively high in energy (38.9 kcal/mol, **Figure 5.9**). These results suggest that a role of the silver salt is to suppresses the β-hydride elimination. Further, since β-hydride elimination is unlikely, ring contraction via nickel-hydride reinsertion is suppressed, thereby leading to the observed 1,2-regioselectivity.

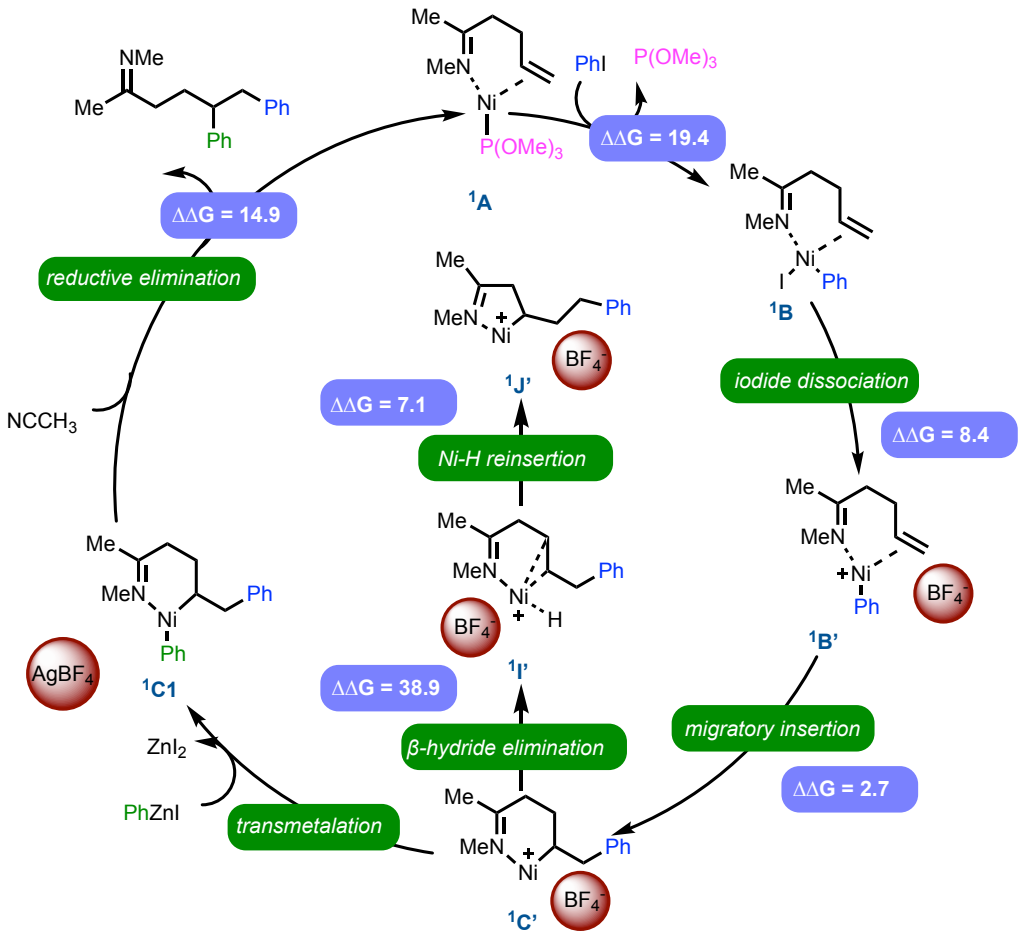


Figure 5.9 Overall cationic catalytic cycle of Ni/Ag-catalyzed 1,2-diarylation. Free energy values (kcal/mol) were calculated at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

In place of β-hydride elimination, the cationic intermediate **C'-conf** can undergo transmetalation with the organozinc reagent to form the lower energy intermediate **C1** (-24.5 kcal/mol). Intermediate **C1** is expected to then undergo reductive elimination to form the desired product. Various conformers of transition states were explored for this stage and the lowest energy conformers of each was given in the pathway in **Figure A5.33** in Appendix 5. This reaction coordinate diagram shows that unassisted reductive elimination is the highest in energy (orange pathway which occurs without the aid of a solvent molecule or $AgBF_4$ salt to lower the energy).

With the incorporation of an acetonitrile molecule, the metal-π coordination lowers the energy of the reductive elimination by ~3 kcal/mol (**Figure 5.10, C2-TS-P'**). However, this structure does not explain the kinetic data collected by the Giri group in which the silver or copper salt increases the rate of reaction. To explore the enhanced rates with the Ag or Cu additives, I located the reductive elimination transition state **C1'-TS-P1'** in which a molecule of $AgBF_4$ was coordinated to the nickel center. Interestingly, it was found that this salt lowers the barrier of reductive elimination by 16 kcal/mol (**Figure 5.10**), hinting at a potential role of the silver salt in the reaction.[154,155]

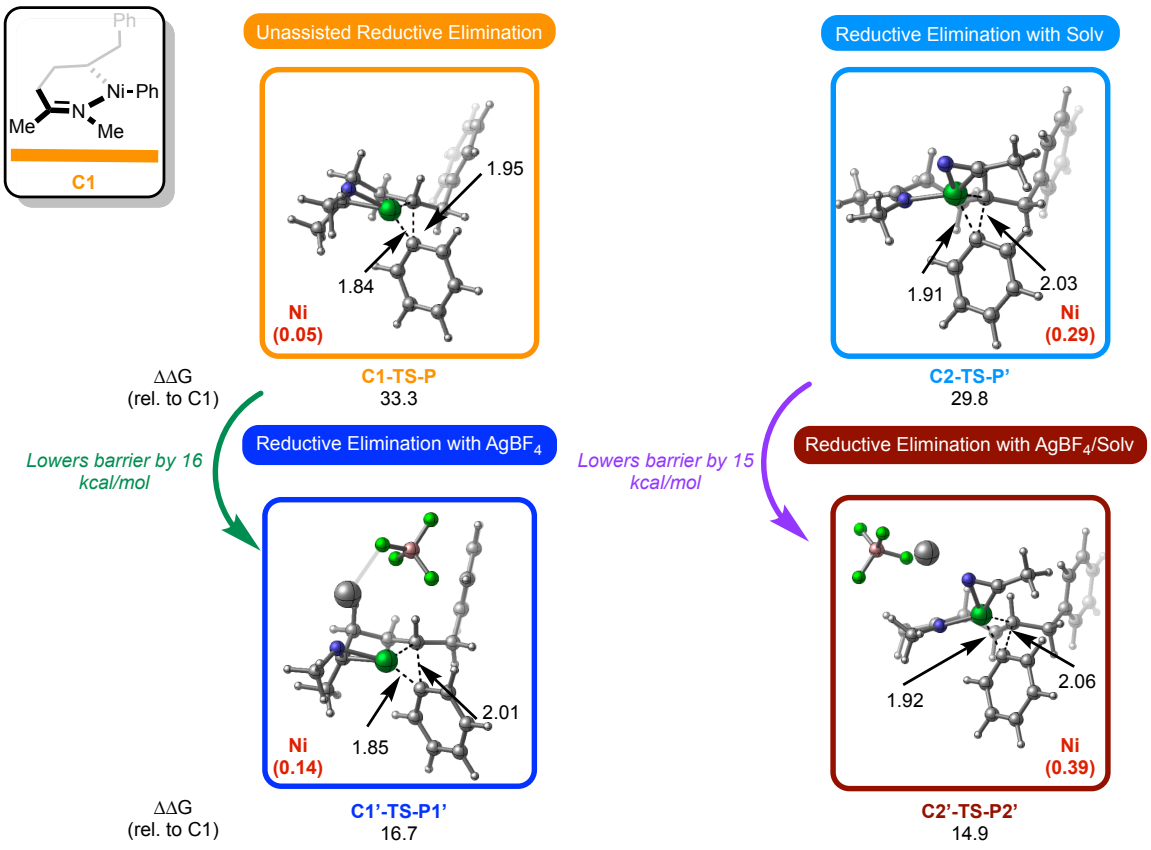


Figure 5.10 Role of $AgBF_4$ in enabling reductive elimination. Free energy values (kcal/mol) were calculated at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory. Mulliken charges for nickel, calculated at the same level, are given in red (parenthesis).

For comparison, the copper/nickel-catalyzed 1,2-diarylation was also explored computationally leading to similar conclusions (see **Figure A5.34** in Appendix 5 for the reaction coordinate diagram of this system). Like the silver/nickel bimetallic pathway and the neutral nickel 1,3-diarylation, the mechanism begins with oxidative addition (barrier of 19.2 kcal/mol), leading to intermediate **B (Figure 5.11)**. From here, iodide abstraction occurs to form the cationic nickel species **B1'** which is downhill in energy (-9.2 kcal/mol) unlike the silver/nickel pathway in which halogen abstraction was an uphill process. Following the formation of the cationic nickel species, migratory insertion occurs via **B1'-TS-C1'** (barrier of 5.7 kcal/mol) to form intermediate **C1'**. The role of copper was revealed in suppressing β-hydride elimination (see **Figure A5.35** in Appendix 5 for details) and thereby controlling the regioselectivity of the reaction from the computed barrier of 28.5 kcal/mol (**Figure 5.11**) for this process.

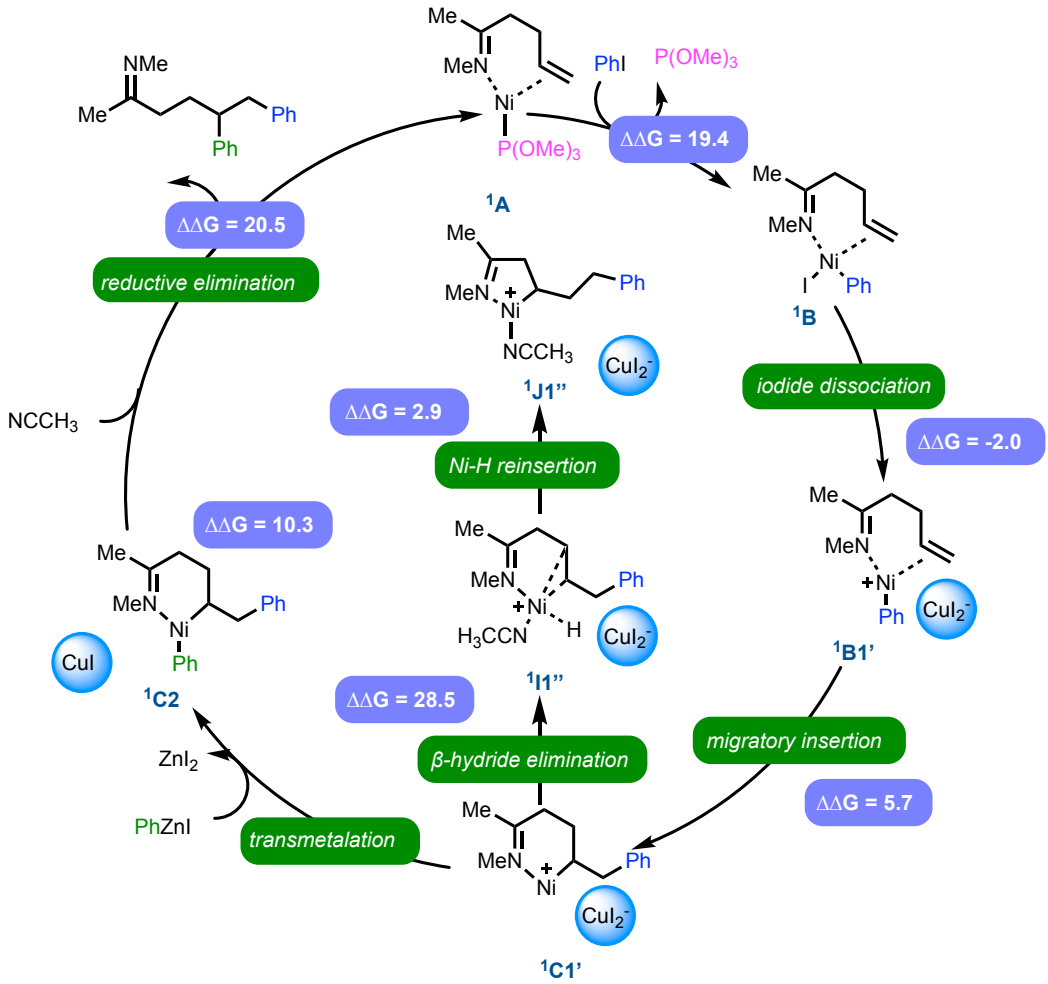


Figure 5.11 Overall cationic catalytic cycle of Ni/Cu-catalyzed 1,2-diarylation. Free energy values (kcal/mol) were calculated at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

Instead of undergoing β-hydride elimination, intermediate **C1'-conf**, formed by isomerization of **C1'**, reacts with the arylzinc reagent to form **C1**. Reductive elimination relies on the presence of the copper iodide salt at the nickel center to lower the barrier by 9.0 kcal/mol (**Figure 5.12, C2''-TS-P1'**) which agrees with experimental kinetic data suggesting that the reaction rate is increased in the presence of copper iodide.

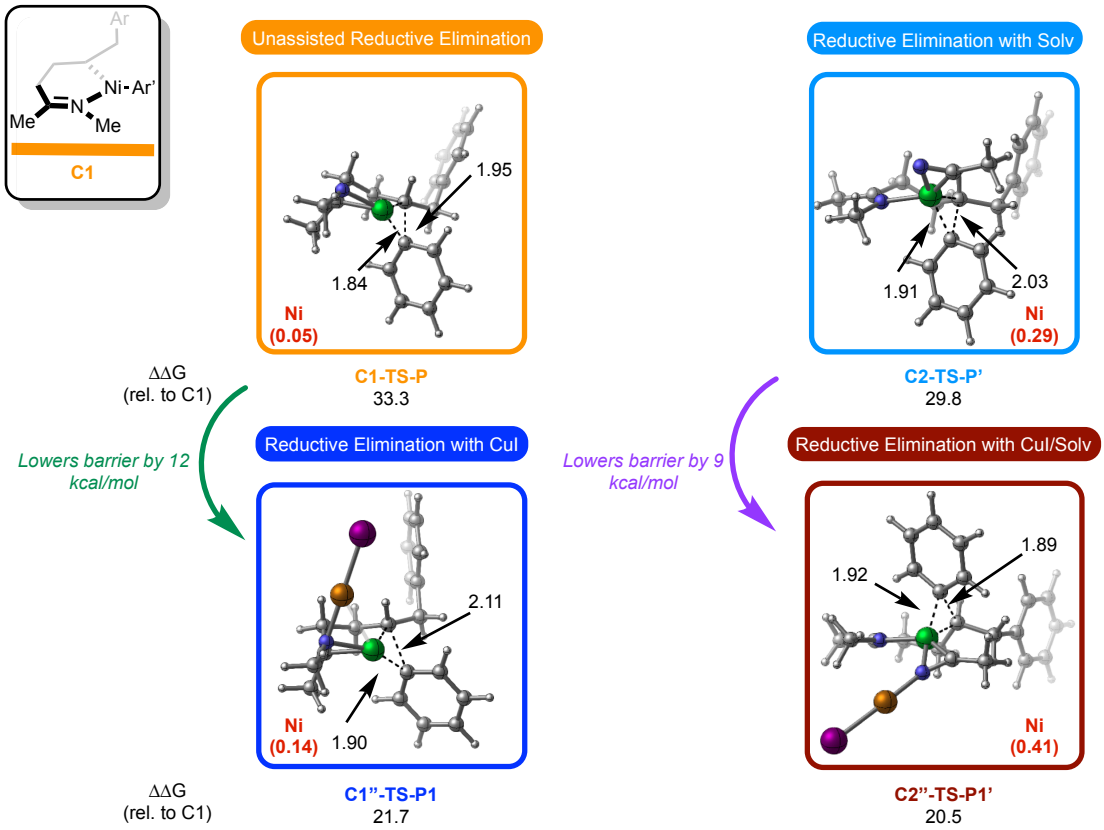


Figure 5.12 Role of CuI in enabling reductive elimination. Free energy values (kcal/mol) were calculated at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory. Mulliken charges for nickel, calculated at the same level, are given in red (parenthesis).

5.4 Conclusion

In conclusion, the mechanisms of the nickel-catalyzed 1,3-diarylation and nickel/silver (copper) bimetallic catalyzed 1,2-diarylation of unactivated olefins using a ketimine as directing group were explored using quantum mechanical calculations. In the 1,3-diarylation, it was found that the regioselectivity is controlled by β-hydride elimination through the triplet state followed by a rapid nickel-hydride reinsertion which results in a ring contraction of the nickel metallacycle from a 6-membered ring to a 5-membered species. Further, the role of the phosphine ligand was explored, with computations

revealing its critical role in promoting reductive elimination. Next the mechanism of the cationic nickel-catalyzed 1,2-diarylation of alkenes using silver or copper salts was explored. The silver/copper salts were found to serve a dual role in the reaction. On the one hand, they control the 1,2-regioselectivity of the product formation by raising the barrier of β-hydride elimination to a prohibitively high energy such that ring contraction to give the 1,3-product will not occur. Additionally, the silver and copper salts were found to be crucial to enabling reductive elimination in agreement with kinetic data. These mechanistic insights provided computationally are vital to the development of future nickel-catalyzed dicarbofunctionalization reactions and are currently being used in the reaction design of an analogue with an anionic ligand in place of the silver/copper salt in the cationic system.

Chapter 6: Impact of Ligands and Metals on the Formation of Metallacyclic Intermediates and a Nontraditional Mechanism for Group VI Alkyne Metathesis Catalysts

Excerpts from this chapter were published in a) Thompson, R. R.; **Rotella, M. E.**; Du, P.; Zhou, X.; Fronczek, F. R.; Kumar, R.; Gutierrez, O.; Lee, S. *Organometallics* **2019**, *38,* 4054 – 4059. And b) Thompson, R. R.; **Rotella, M. E.**; Zhou, X.; Fronczek, F. R.; Gutierrez, O.; Lee, S. *J. Am. Chem. Soc.* **2021**,*143*, 9026 – 9039.

6.1 Abstract

Triphenylsiloxide is an effective ancillary ligand for Mo(VI)-catalyzed alkyne metathesis owing to its flexibility which allows for the modulation of the Mo≡C electrophilicity, thereby promoting the metathesis. To probe the effect of ligand flexibility on Mo≡C electrophilicity, the Lee group synthesized a tethered variant of triphenylsiloxide. The basal arene limits the Mo-O-Si bond angles that the complex can adopt, thereby controlling the possible electrophilicity of the metal center. Quantum mechanical calculations were used to predict ^{13}C NMR shifts of the alkylidyne carbon as an evaluation of its electrophilicity, with more downfield carbyne shifts occurring on more electrophilic molybdenum centers. A metallatetrahedrane (MTd) Mo(VI) intermediate was isolated by Lee et. al in the experimental studies in place of the expected metallacyclobutadiene (MCBD) intermediate, raising the question of this intermediate's role, if any, in catalysis. For comparison, the analogous tungsten catalyst was synthesized but only the MCBD intermediate was isolated. Thus, I employed quantum mechanical (dispersion-corrected DFT) calculations to probe the mechanism of Mo(VI)- and W(VI)-catalyzed alkyne metathesis, revealing the intermediacy of both MTd and MCBD intermediates. Further, I used computations to study the role of the metal in determining the nature of the most stable intermediate.

6.2 Introduction

Alkyne metathesis, the metal-catalyzed C≡C triple bond exchange variant of olefin metathesis, has recently gained interest[156] after laying relatively dormant[157] following its discovery in 1968 by Pennella, Banks, and Bailey.[158] The surge in interest for the method[159] is owed to a realization of its potential applications in a wide range of fields including polymer synthesis,[160] supramolecular chemistry,[161] and natural product synthesis.[162]

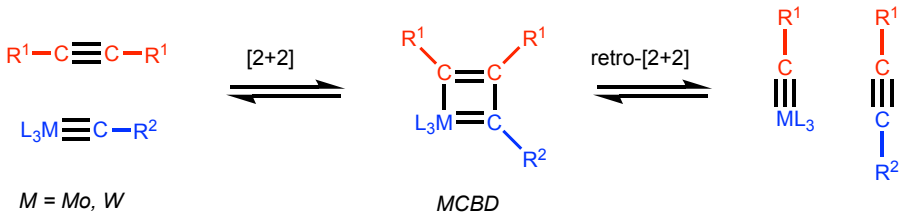


Figure 6.1 Commonly accepted mechanism for alkyne metathesis of [2+2] cycloaddition/retro-[2+2] by way of a MCBD intermediate.

Until recently, the generally accepted mechanism for this process[163] (shown in **Figure 6.1**) involved [2+2]-cycloaddition to form the key metallacyclobutadiene (MCBD) intermediate which dissociates by retro-[2+2]-cycloaddition to expel product and regenerate the active metal alkylidyne complex. Inspired by the development of a fluorinated alkoxide ligand by Johnson,[164] Fürstner designed an extremely effective triphenylsiloxide ligand[165] which tolerated a range of functional groups and achieved high turnover frequencies at low catalyst loadings.[166] This ancillary ligand **L_3** (**Figure 6.2**) is hypothesized to be so successful in promoting Mo(VI)-catalyzed alkyne metathesis owing to its flexibility.[167]

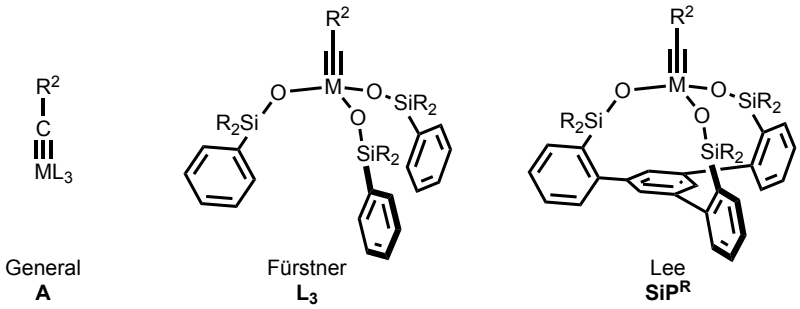


Figure 6.2 General structure **A** for an alkyne metathesis catalyst (left), Fürstner's triphenylsiloxide scaffold $\mathbf{L_3}$ (middle), and Lee's siloxide podand scaffold $\mathbf{SiP^R}$ (right; R = Ph, Et).

In particular, the Mo-O-Si bond angles are thought to modulate the electrophilicity of the Mo≡C center. Specifically, acute Mo-O-Si bond angles limit the extent of π-donation from the oxygen lone pairs into the metal center, thereby increasing its electrophilicity and encouraging MCBD formation. As the Mo-O-Si bond angle becomes more linear, π-donation once again becomes possible, increasing the electron density at the molybdenum center and encouraging product formation. To probe the hypothesis that the efficacy of the triphenylsiloxide ligand $\mathbf{L_3}$ in promoting alkyne metathesis is due to its flexibility, this property can be limited by tethering the three phenylsiloxide fragments together using a basal arene linker. The Lee group synthesized this preorganized siloxide podand ligand $\mathbf{SiP^R}$ (**Figure 6.2**) to probe the relationship between ligand flexibility and Mo≡C electrophilicity by a comparison of the catalytic activity of $\mathbf{L_3}$ and $\mathbf{SiP^R}$.[12] In particular, the Mo≡C electrophilicity in both metal complexes can be probed through ^{13}C NMR, with more downfield carbyne shifts serving as an indicator of a more electrophilic Mo≡C center. However, experimental NMR studies are limited to the Mo-O-Si bond angles accessible by the catalyst. To systematically probe the effect of Mo-O-Si bond angle on the Mo≡C electrophilicity, I computed carbyne ^{13}C chemical shifts for complexes with varying bond angles and compared these shifts with computed Mulliken charges of the

molybdenum center. This computational study comparing molybdenum complexes **L_3** and **SiP^R** is detailed herein.

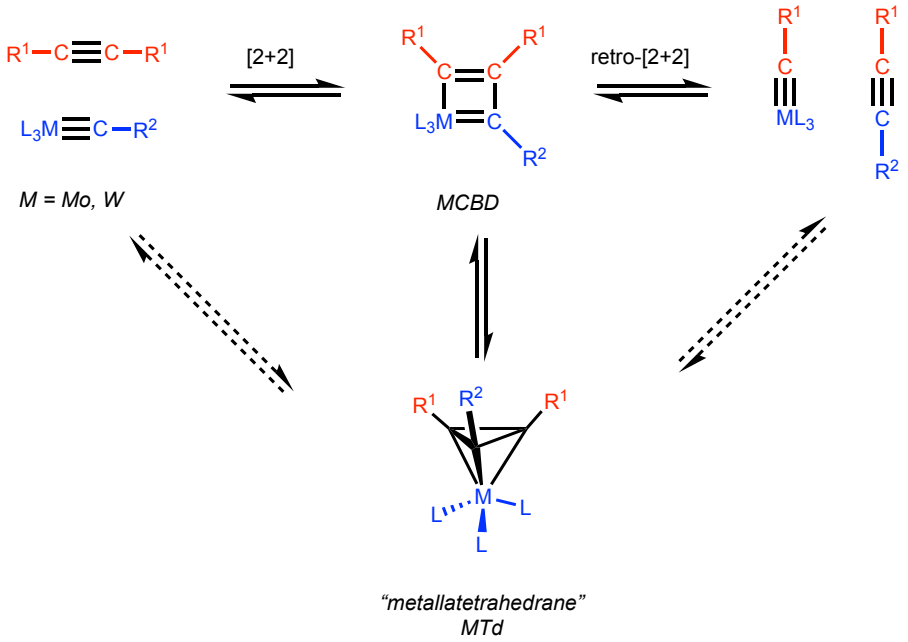


Figure 6.3 Commonly accepted mechanism for alkyne metathesis by way of a MCBD intermediate. MT_d formation is considered as an off-cycle intermediate.

Further during the experimental study of the siloxide podand ligand **SiP^R**, a metallatetrahedrane (MT_d) of Mo(VI) was isolated and characterized for its solid state structure by x-ray crystallography. This intermediate was found to be dynamic in solution, reverting to the active metal alkylidyne complex under vacuum and even promoting alkyne metathesis of 3-hexyne. Until this point, MT_d intermediates were generally viewed as off-cycle thermodynamic sinks[168] that serve to deactivate alkyne metathesis (**Figure 6.3**). This finding that the MT_d can promote alkyne metathesis led the Lee group to attempt the synthesis and isolation of a W(VI) MT_d variant.[169] Surprisingly, with both the phenyl siloxide podand ligand and the less sterically encumbered but analogous ethyl siloxide podand ligand **SiPh^R** (**Figure 6.4, R = Et**), a metallatetrahedrane of tungsten could not be obtained. Instead, the MCBD of tungsten was isolated. In order to study the role of metal

choice on the identity and stability of reactive intermediates, I turned to computations. This work also served to probe the mechanism of Mo(VI)- and W(VI)-catalyzed alkyne metathesis and the role of ligand sterics in the pathway.

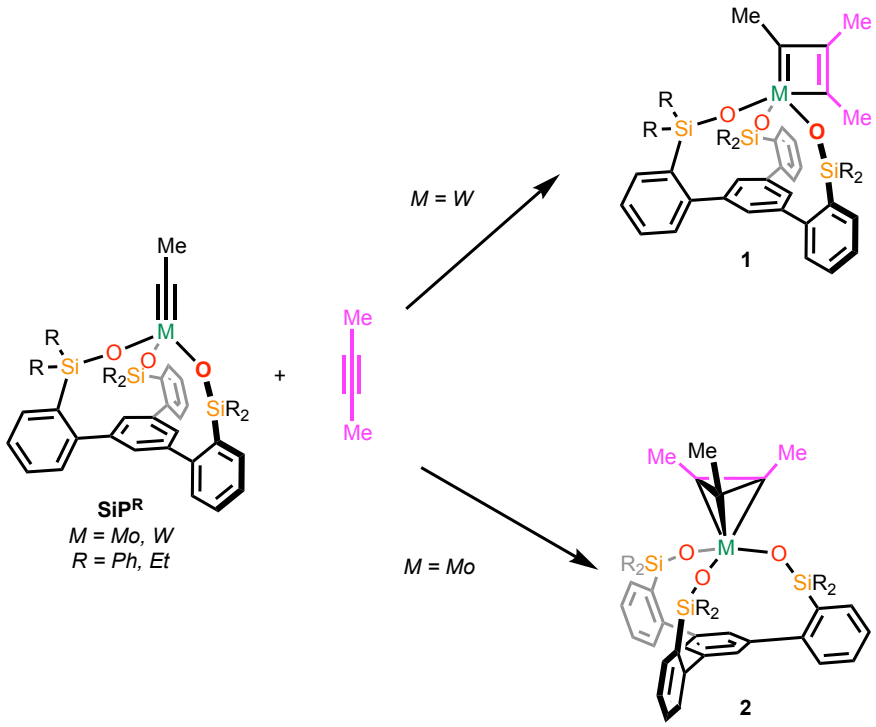


Figure 6.4 In the case of either siloxide podand ligand **SiP^{R}** (R = Ph, Et), only the MCBD could be isolated with tungsten (**1**) and only the MT_d could be isolated with molybdenum (**2**).

6.3 Results and Discussion

6.3.1 Computational Investigation of the Siloxide and Siloxide Podand Ligand Scaffold

At the outset of the work, the Lee group sought to synthesize the siloxide podand scaffold **SiP^{R}** (**Figure 6.2**), a variant of Fürstner's highly active triphenylsiloxide scaffold **L$_3$**, to test the role of the Mo-siloxide bond's flexibility in promoting alkyne metathesis. Fürstner suggested that acute Mo−O−Si angles render the metal center more electrophilic and encourage the formation of the metallacyclobutadiene (MCBD) intermediate. Subsequent straightening of the Mo−O−Si angle then drives product release to regenerate

the alkylidyne functionality. Principal to this design element, therefore, is the flexibility of the Mo−siloxide bond to sample a wide range of angles. A conceptually simple means for probing its importance would be to limit flexibility by tethering the three Ph_3SiO groups together as a single, tridentate chelate.

Further, Tamm and Coperet have shown that the ^{13}C chemical shift of the Mo-C can be used as a probe for the electrophilicity of the metal and alkyne metathesis activity of structurally related catalysts[170] with electrophilicity of the Mo≡C center increasing as the chemical shift increases. Experimentally, it is not possible to vary the Mo-O-Si bond angle systematically from 135° to 180°. However, computationally it can be done, with the chemical shift of the Mo-C carbyne calculated for increasing bond angles to study the effect that ligand geometry has on ^{13}C carbyne chemical shift and more importantly, the molybdenum-carbyne bonding.

Thus, I employed dispersion-corrected density functional theory calculations [B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)] to study the relationship between Mo-siloxide bond flexibility and electrophilicity of the molybdenum center. First, Lee et. al synthesized and characterized Mo-alkylidyne complexes with both siloxide podand ligand (**Figure 6.5**, complexes **3, 4**) and triphenylsiloxide (complexes **5, 6**). From the crystal structures of compounds **3** and **5**, I obtained the computed structures $\mathbf{3_{calc}}$ and $\mathbf{5_{calc}}$. The core experimental geometries are in reasonable agreement with computations (Mo-O-Si average = 164.5 vs. 160.0° for **3** and 149.1 vs. 146.2° for **5**), although the Mo-O-Si angles in each were found to be more acute (see **Figures A6.1-A6.2** in Appendix 6), possibly suggesting that crystal-packing forces may cause these angles to distort from ideal geometry.

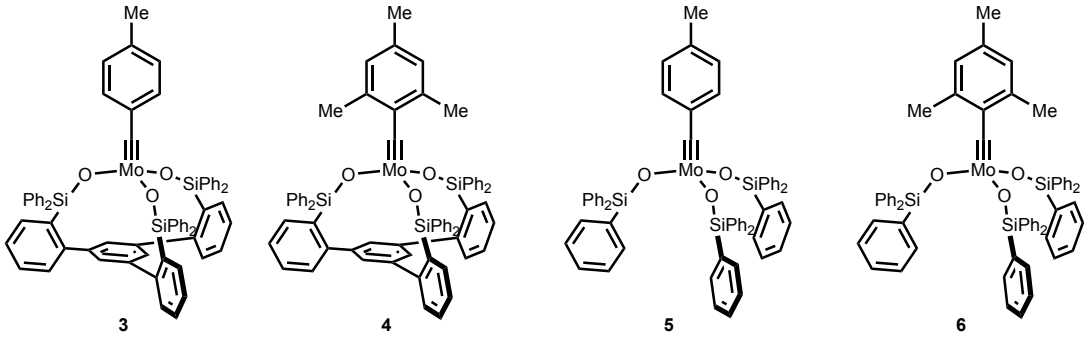
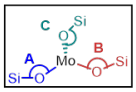


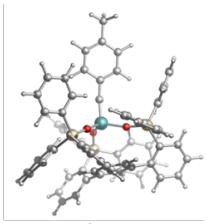
Figure 6.5 Molybdenum-alkylidyne complexes of the siloxide podand ligand (**3,4**) and the untethered triphenylsiloxide ligand (**5,6**). All four complexes were synthesized and characterized by x-ray crystallography by the Lee group.[12]

Next, I systematically changed one of the Mo-O-Si bond angles of both catalysts $\mathbf{3}_{\mathbf{calc}}$ and $\mathbf{5}_{\mathbf{calc}}$ to probe the effect of Mo-O-Si bond angle on the electronic properties of the catalysts. While linearization of one the Mo-O-Si bond angle did not show a significant change on the ^{13}C chemical shift (**Figure A6.3** in Appendix 6), as the Mo-O-Si angle becomes more linearized, the electron density on both oxygen and carbon decreases while electron density on Mo increases as observed via Mulliken charges of the oxygen carbon and Mo for $\mathbf{5}_{\mathbf{135°}}$ going from -0.99 and +1.92, respectively to -0.87 and +1.89 for $\mathbf{5}_{\mathbf{175°}}$ (see **Figure A6.4** in Appendix 6). Similarly, the alkyne carbon and Mo charges for $\mathbf{3}_{\mathbf{135°}}$ were -0.68 and +1.87, respectively, while increasing the Mo-O-Si bond angle to 175º led to C and Mo charges of -0.52 and +1.77, respectively (**Figure A6.5** in Appendix 6).

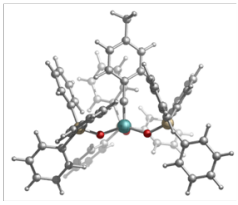
To explore the effect of linearization of the Mo-O-Si angle on the chemical shift, the three siloxide angles of **5** were locked into linearized geometry (**Figure 6.6**). Interestingly, the constrained linearized geometry of **5** resulted in an intermediate chemical shift (^{13}C = 320.99 ppm) and Mulliken charge (C = -0.69, Mo = +1.87). On the other hand,

constraining the Mo-O-Si bond angles of the triphenylsiloxide in **5** to match that of **3** (i.e., $\mathbf{5_{constrained}}$; **Figure 6.6**) resulted in nearly identical chemical shifts (i.e., ^{13}C = 328.73 versus 330.02) and Mulliken charges on the Mo atom (1.84 vs. 1.86) as **3**. These results suggests that while linearization of the Mo-O-Si bond angle has an important contribution to the electronic environment of the carbyne *the overall geometry imparted by the tripodal* ***SiP*** *scaffold is the greater determinant of electrophilicity as evaluated by the calculated* ^{13}C *NMR shifts.*

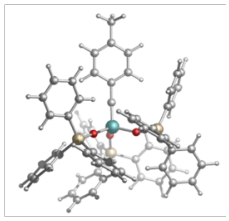




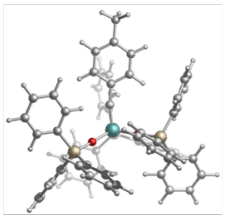
$\mathbf{3_{Calc}}$



$\mathbf{5_{Calc}}$



$\mathbf{5_{Constrained}}$



$\mathbf{5_{178°}}$

	$\mathbf{3_{Calc}}$	$\mathbf{5_{Calc}}$	$\mathbf{5_{Constrained}}$	$\mathbf{5_{178°}}$
^{13}C Alkyne Shift	330.02 ppm	314.92 ppm	328.73 ppm	320.99 ppm
Mo-Carbyne Distance	1.75 Å	1.75 Å	1.75 Å	1.75 Å
Si-O-Mo (A)	160.0°	153.6°	160.0°	178.0°
Si-O-Mo (B)	145.6°	145.8°	145.6°	178.0°
Si-O-Mo (C)	173.5°	139.3°	173.5°	178.0°
Mulliken Charge (Mo)	1.86	1.94	1.84	1.87
Mulliken Charge (Alkyne C)	-0.61	-0.95	-0.70	-0.69

Figure 6.6 Optimized structures of $\mathbf{3_{Calc}}$, $\mathbf{5_{Calc}}$, **5** constrained to the geometry of $\mathbf{3_{Calc}}$ ($\mathbf{5_{Constrained}}$) and 5 constrained to all Si-O-Mo bond angles of 178° ($\mathbf{5_{178}}$). A bond angle of 180º is not allowed in the Gaussian09 program due to convergence issues so instead a nearly linear angle of 178º was used. All structures given are optimized at the B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene) level of theory while ^{13}C shifts are computed relative to TMS standard at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene) level of theory.

To further compare the activity of the two ligand sets, I modeled an initial reaction coordinate of both $\mathbf{[Mo]L_3}$ and **[Mo]SiP** with acetylene (**Figure A6.6** in Appendix 6) and 2-butyne (**Figure 6.7**) as simplified systems for a preliminary mechanistic study. Using

acetylene as the substrate, calculations predict nearly identical barriers for the [2+2] cycloaddition between acetylene and **[Mo]L$_3$** and **[Mo]SiP**, 12.8 and 12.0 kcal/mol, respectively (**Figure A6.6** in Appendix 6).

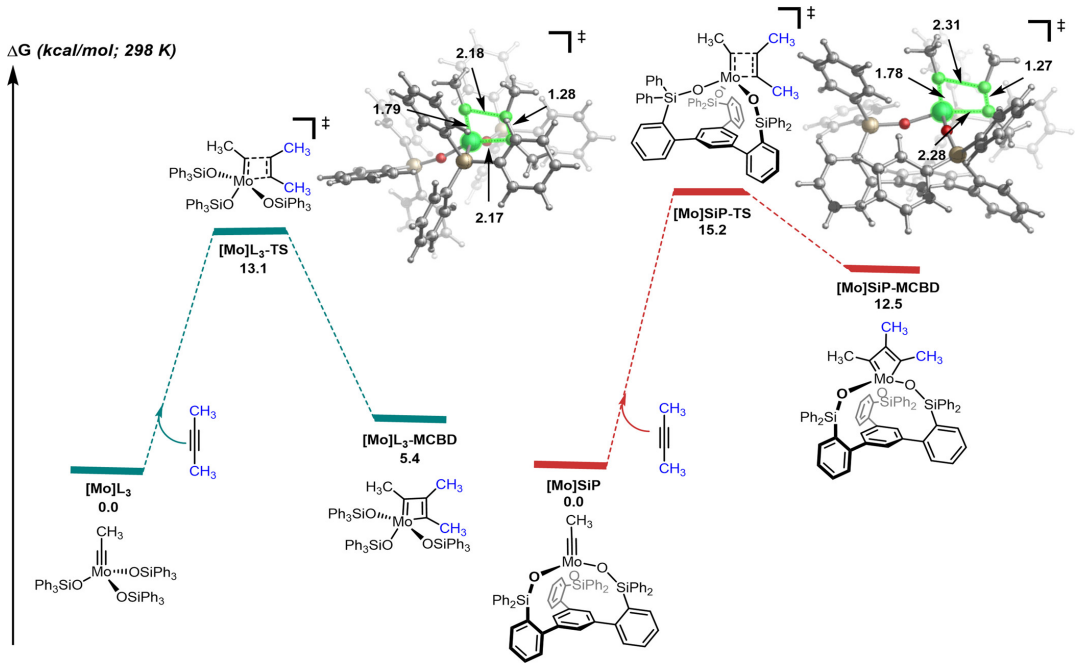


Figure 6.7 Energetics of MCBD formation via [2+2] cycloaddition for **[Mo]L$_3$** (left, green) and **[Mo]SiP** (right, red). Free energies (kcal/mol) are computed at the B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ level of theory. Reprinted with permission from ref 12. Copyright 2019 American Chemical Society.

Notably, the barrier associated with **[Mo]L$_3$** is slightly higher, suggesting that the ligand geometry of **SiP** may be beneficial in the cross-metathesis of case of sterically unhindered, unsubstituted alkynes. However, upon increasing the steric bulk of the model substrate to ethylidynes reacting with 2-butyne, the [2+2] cycloaddition transition state from the **[Mo]SiP** system was found to be 2.1 kcal/mol higher in energy than that for the **[Mo]L$_3$** system (**Figure 6.7**), supporting experimental results that the **[Mo]L$_3$** system reaches equilibrium faster. Furthermore, there is a significant destabilization of the MCBD of **[Mo]SiP** relative to **[Mo]L$_3$**, likely as a result of steric clashing between the methyl groups of the MCBD and the phenyl groups of the ligand (see **Figure 6.8**).

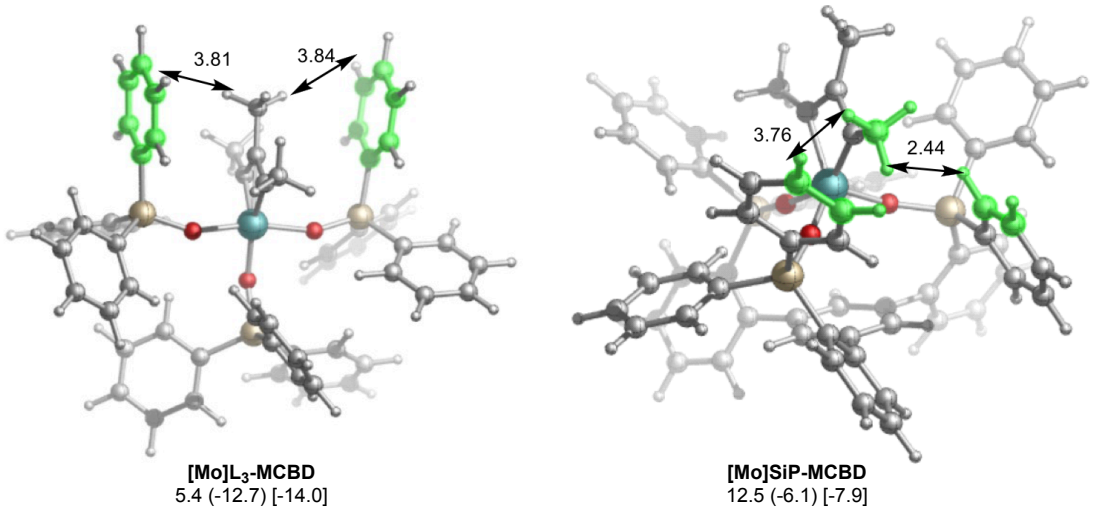


Figure 6.8 Comparison of MCBD intermediates **[Mo]L$_3$-MCBD** (left) and **[Mo]SiP-MCBD** (right). Free energies are given as well as enthalpies (parenthesis) and the Hartree-Fock (HF) energy (brackets) computed at the B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ level of theory. **[Mo]SiP-MCBD** is higher in energy by 7.1 kcal/mol than **[Mo]L$_3$-MCBD**, presumably due to the steric clashing between the methyl groups and neighboring phenyl groups (highlighted in green), which are closer than those in **[Mo]L$_3$-MCBD**. Key distances between neighboring atoms are given.

These preliminary results suggest that as steric bulk of the substrate increases, the energy of the initial [2+2] transition state and corresponding MCBD adduct increases as consequence of steric interactions between the substrate and the more rigid ligand in **[Mo]SiP**. Finally, in agreement with experiment, it was found that with this model system that the metallatetrahedrane (MTd) motif was more stable than the MCBD analog by 11.2 kcal/mol (**Figure 6.9**) and nearly isonergetic to the **[Mo]SiP** catalyst. Intrigued by these results, a more extensive computational investigation into the mechanism of alkyne metathesis was undertaken.

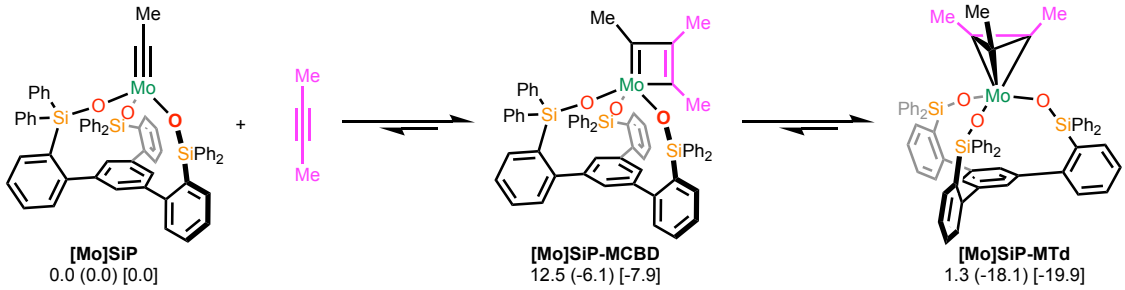


Figure 6.9 Energetic comparison of **[Mo]SiP-MCBD** and metallatetrahedrane computed at the B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ level of theory. Free energies are given as well as enthalpies (parenthesis) and the Hartree-Fock (HF) energy (brackets). The metallatetrahedrane **[Mo]SiP-MTd** is lower in free energy than the **[Mo]SiP-MCBD** intermediate by 11.2 kcal/mol.

6.3.2 Mechanistic Proposal for Group VI Alkyne Metathesis Catalysts

The Mo(VI) metallatetrahedrane (MT_d) that was isolated and characterized by x-ray crystallography in the experimental study (**Figure 6.9**) was shown to promote alkyne metathesis of 3-hexyne. This finding led to interest in the intermediate's part in the reaction. To probe its role, the Lee group attempted the synthesis and isolation of a W(VI) MT_d variant.[14] However, a metallatetrahedrane of tungsten could not be obtained. Instead, the MCBD was isolated. These experimental studies led to several questions on the role of these intermediates in alkyne metathesis. Namely, it was unclear how the metal choice (Mo or W) affected the identity and stability of reactive intermediates as well as what the exact role of the MT_d was in alkyne metathesis. To begin to answer these questions, I undertook a computational study of the mechanism of Mo(VI)- and W(VI)-catalyzed alkyne metathesis and the role of metal choice and ligand sterics in the pathway.

Specifically, I employed dispersion-corrected density functional theory calculations [B3LYP-D3/def2TZVP-SDD(M)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(M)-CPCM(benzene)] (where M is W or Mo depending on the system being studied)[171,172,173,174,175] to construct the potential energy surface of the reaction. Initially, to

reduce computational cost,[176] the conformationally flexible ethyl groups on the podand ligand (**SiP^{Et}**) were modeled as methyl groups (**SiP^{Me}**) and the tolyl substrate was modeled as a methyl. Overall, this method was able to capture the structural parameters of the isolated species, confirming the suitability of the computational method (see **Figure A6.7** in Appendix 6).

To explore the ligand effect, the mechanism for alkyne metathesis and formation of MCBD and MT_d species of tungsten paired with the **SiP^{Me}** and **SiP^{Ph}** ligands was studied (**Figure 6.10**). In the case of the **SiP^{Me}** ligand (black values), the barrier for concerted [2+2] cycloaddition to form the symmetrical MCBD **[W]-B** intermediate is only 11.3 kcal/mol (via an early transtion state **[W]-A-TS**). In turn, this MCBD could undergo a rapid isomerization (via a pseudoroation of the MCBD moiety with a barrier of 9.1 kcal/mol) to form **[W]-*ent*-B** followed by a retro-[2+2] to furnish the desired product (red pathway). These barriers are reasonable with experimental results for which the observed rate of reaction for alkyne metathesis was approximately 1 hour. Alternatively, as shown in green, the symmetrical MCBD **[W]-B** could instead isomerize to the most energetically favored (and experimentally observed and characterized) unsymmetrical MCBD **[W]-B'** (downhill by 9.1 kcal/mol with respect to **[W]-B)** via [**W]-B-TS-B'** (barrier of 10.7 kcal/mol) prior to undergoing alkyne metathesis. The traditional mechanistic pathway proposed for alkyne metathesis in which the MCBD forms by [2+2] cycloaddition and the product is expelled by a retro-[2+2] transition state directly from **[W]-B'** to product (**Figure 6.10**, green) was also explored.

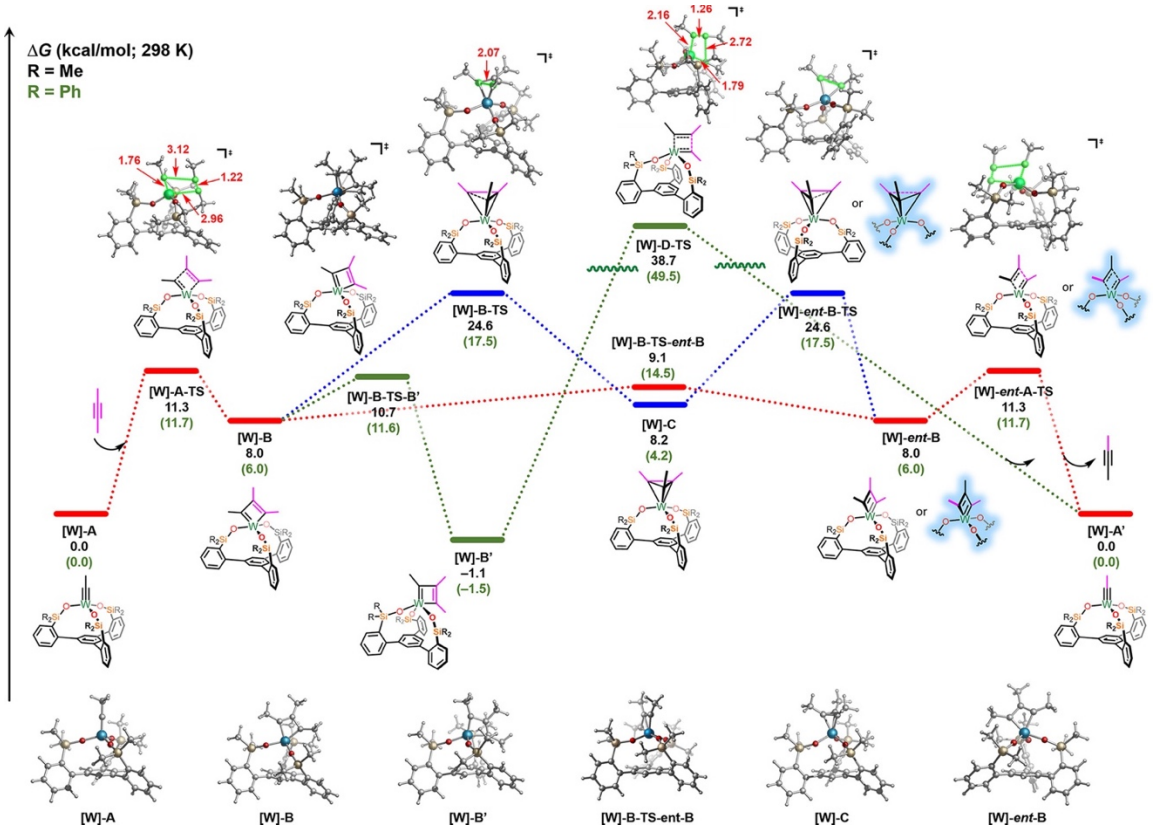


Figure 6.10 Energetics of MCBD and MT_d formation via [2+2] cycloaddition for tungsten with **SiP^{Me}** (outside parenthesis) and **SiP^{Ph}** (inside parenthesis) ligands. Free energies (kcal/mol) are computed at the B3LYP-D3/def2TZVP-SDD(W)-CPCM(benzene)// B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)level of theory. The red pathway shows the [2+2] cycloaddition followed by pseudorotation and finally retro-[2+2] to yield product. Alternatively, the red pathway from the [2+2] cycloaddition can lead to the blue pathway in which the metallatetrahedrane is involved in the product formation. The structures highlighted in blue are accessible via the metallatatetrahedrane pathway (blue lines). Notably, the green pathway in which the [2+2]/retro-[2+2] occurs with no pseudorotation is energetically inaccessible. Reprinted with permission from ref 14. Copyright 2021 American Chemical Society.

However, the barrier for this process is found to be prohibitively high in energy (38.7 kcal/mol via [**W]-D-TS**) and therefore energetically inaccessible at the experimental conditions. Consequently, this system does not follow the traditional [2+2]/retro-[2+2] mechanism that has previously been proposed and instead the C_3-symmetric ligand changes the mechanism to [2+2]/*isomerization(pseudorotation)*/retro-[2+2] as observed

independently by Fürstner/Neese in parallel to this study.[177] A comparison of the energetics of this study and that of Fürstner/Neese is given in **Figure A6.8** in Appendix 6. A related "turnstile" rotation was previously invoked by Schrock as taking part in olefin metathesis.[178]

Finally, another possible pathway was explored in which the metallatetrahedrane **[W]-C** was an on-cycle intermediate involved in product formation. As shown in **Figure 6.10** (blue), the MCBD **[W]-B** forms the nearly isoenergetic metallatetrahedrane **[W]-C** directly via a ring-closing transition state (**[W]-B-TS**) with a relative barrier of 16.6 kcal/mol (with respect to **[W]-B**). In this pathway, this symmetrical metallatetrahedrane **[W]-C** can then undergo ring opening followed by retro-[2+2] to form the alkyne metathesis product. Overall, while the blue pathway is energetically feasible, the pathway shown in red in **Figure 6.10** is much lower in energy and therefore the most likely mechanism the reaction follows. These computational results are in accord with experiment where only the thermodynamically more stable MCBD intermediate (akin to **[W]-B'**) was observed and not the (much higher in energy) transient MT_d intermediate (akin to **[W]-C**). Further, to probe the effect of the ligand on this process, the reaction coordinate was then explored for the tungsten **SiP^{Ph}** system (**Figure 6.10**; green values). Overall, similar energetics were observed for the alkyne metathesis pathway but there are pronouced effects of the ligand scaffold on the pathway for formation of the MT_d intermediate. Specifically, both the overall (17.5 kcal/mol vs. 24.6 kcal/mol) and relative (11.5 kcal/mol vs. 16.6 kcal/mol) barriers for the MT_d-formation (via **[W]-B-TS**) are significantly lower and more exergonic (4.2 kcal/mol vs. 8.2 kcal/mol) with the more sterically hindered ligand (green

values). As such, qualitatively, these results suggest faster and more favorable MT_d-formation via more sterically hindered **SiP^{Ph}** podand ligands.

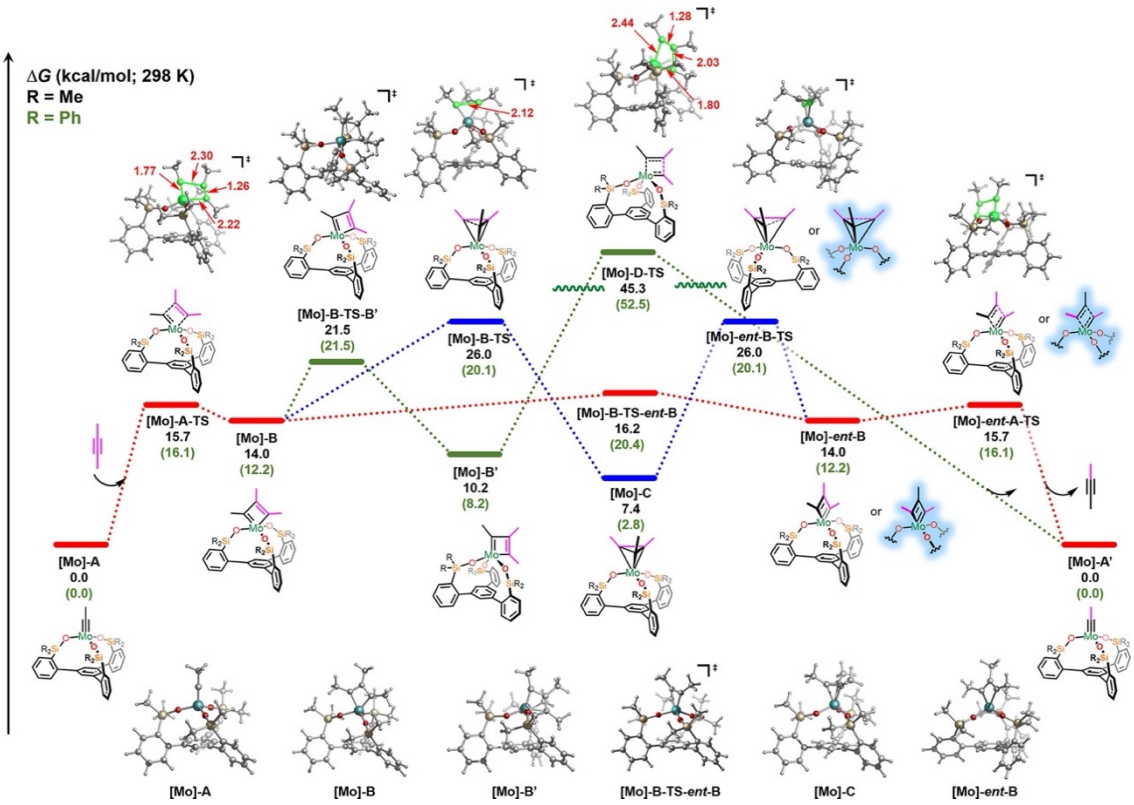


Figure 6.11 Energetics of MCBD and MT_d formation via [2+2] cycloaddition for molybdenum with **SiP^{Me}** (outside parenthesis) and **SiP^{Ph}** (inside parenthesis) ligands. Free energies (kcal/mol) are computed at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)// B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)level of theory. The red pathway shows the [2+2] cycloaddition followed by pseudorotation and finally retro-[2+2] to yield product. Alternatively, the red pathway from the [2+2] cycloaddition can lead to the blue pathway in which the metallatetrahedrane is involved in the product formation. The structures highlighted in blue are accessible via the metallatatetrahedrane pathway (blue lines). Notably, the green pathway in which the [2+2]/retro-[2+2] occurs with no pseudorotation is energetically inaccessible. Reprinted with permission from ref 14. Copyright 2021 American Chemical Society.

Next the reaction coordinates for the **SiP^{Me}** and **SiP^{Ph}** ligands for the molybdenum system (**Figure 6.11**) were explored. The operative mechanism of alkyne metathesis in the case of either ligand for the molybdenum catalyst is relatively the same as that observed

for tungsten but proceeds via a flatter surface. Starting with the **SiP^{Me}** ligand, **[Mo]-A** undergoes [2+2]-cycloaddition via **[Mo]-A-TS** (barrier of 15.7 kcal/mol) to form the very shallow symmetrical MCBD **[Mo]-B** (14.0 kcal/mol) intermediate. The MCBD can then undergo a rapid isomerization (via pseudorotation) with a barrier of 16.2 kcal/mol to form [**Mo]-ent-B**, which then undergoes retro-[2+2] via to form the desired product. On the other hand, the symmetrical MCBD [**Mo]-B** can also isomerize to the unsymmetrical and more thermodynamically favored MCBD [**Mo]-B'** via [Mo]-B-TS-B' (barrier of 21.5 kcal/mol) prior to product formation. However, this unsymmetric intermediate, in contrast to the tungsten systems, is overall uphill in energy by 10.2 kcal/mol compared to the catalyst **[Mo]-A**! These results are in agreement with experimental evidence in which the unsymmetrical (and significantly thermodynamically unstable) MCBD **[Mo]-B'** was not observed. On the other hand, the metallatetrahedrane **[Mo]-C** (7.4 kcal/mol) which forms by ring-closing of **[Mo]-B** via **[Mo]-B-TS** (barrier of 26.0 kcal/mol), is more thermodynamically favored than the MCBD intermediates and is in qualitative accord with experiment in which this intermediate is observed experimentally.

Notably, the computationally predicted metallatetrahedrane **[Mo]-C** has similar structural features to the X-ray structure (**Figure A6.9** in Appendix 6). It is worth noting that while the metallatetrahedrane **[Mo]-C** with both the truncated ligand and substrate is uphill in energy from **[Mo]-A**, the system studied experimentally (3-hexyne) yields a thermodynamically favorable metallatetrahedrane (see **Figure A6.10** in Appendix 6). From the metallatetrahedrane intermediate **[Mo]-C**, ring opening via [**Mo]-ent-B-TS** followed by retro-[2+2] can lead to product formation. However, this pathway (highlighted in blue, **Figure 6.11**) is higher in energy than the red pathway ([2+2]/isomerization/retro-[2+2])

and therefore is likely a secondary route toward product formation. Finally, similar to the tungsten system, the traditional [2+2]/retro-[2+2] mechanism in which the MCBD **[Mo]-B** forms product prior to isomerization to **[Mo]-ent-B** was also explored but, akin to W-system, the barrier for this pathway to be insurmountable and therefore is likely not operative for this system.

These computational results are consistent with experimental observations for the **SiP^{Ph}** ligand, in which the barrier to MCBD formation through the [2+2] transition state is higher than that of the tungsten system (16.1 kcal/mol vs. 11.7 kcal/mol) given that slower reaction rates were observed for alkyne metathesis with the molybdenum system. Akin to the tungsten system, the symmetrical MCBD **[Mo]-B** with the **SiP^{Me}** ligand (14.0 kcal/mol) is also energetically favored to isomerize to the unsymmetrical MCBD [Mo]-B' (10.2 kcal/mol) albeit this intermediate **[Mo]-B'** being significantly higher in energy (and uphill) than the analogous structure for the tungsten system (**[W]-B'**). Overall, these results are also consistent with experiment in which the MCBD is not observed for molybdenum.

To investigate the steric effects of the ligand, the barriers to metallatetrahedrane formation were computed for the **SiP^{Me}** system with the **SiP^{Ph}**. The destabilization of the **SiP^{Me}** molybdenum MT$_d$ can partially be attributed to greater steric hindrance as the methyl fragments of the ligand and the substrate are much closer in the case of the **SiP^{Me}** ligand. Furthermore, the noncovalent interactions in the **SiP^{Ph}** system between the CH of the substrate and the π system of the phenyl ring, which can be observed in the NCI plots (**Figure 6.12**) and in calculated ^{1}H NMR shifts of diastereotopic hydrogens, are responsible for the stabilization of the MT$_d$ and the transition state to its formation. However, the other

stages of the alkyne metathesis pathway are unaffected by the CH•••π interactions, which are not present in the NCI plots of the MCBD (**Figure A6.11**).

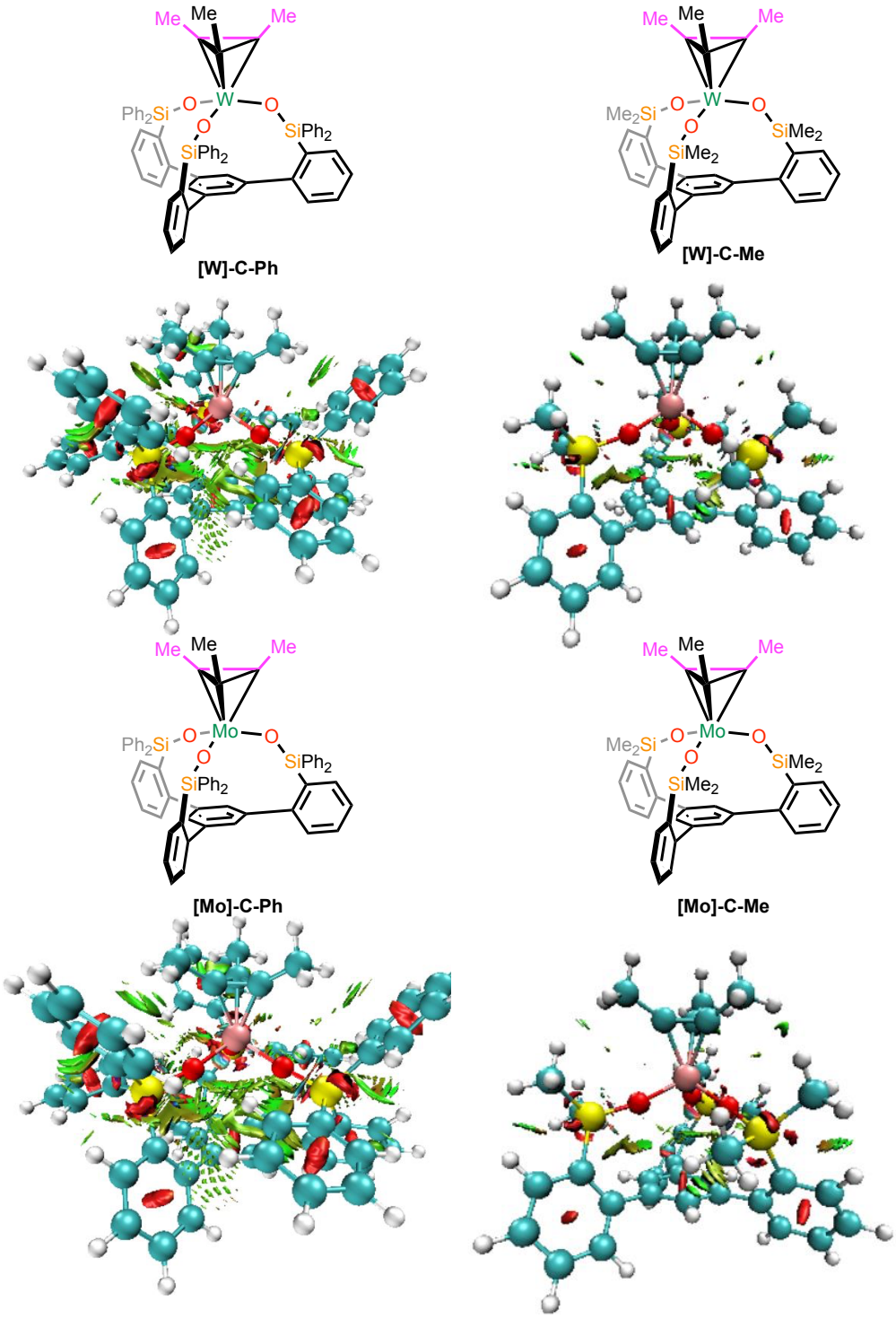


Figure 6.12 NCI plots showing the comparison between metallatetrahedranes in the tungsten (top) and molybdenum (bottom) systems with both the **SiP^{Ph}** and **SiP^{Me}** ligands. Key C-H···π noncovalent stabilizing interactions are visible in the NCI plots of the **SiP^{Ph}** metallatetrahedranes, as indicated by the green colors between substrate C-H and ligand aryl groups. Reprinted with permission from ref 14. Copyright 2021 American Chemical Society.

Energy decomposition analysis (EDA) based on the absolutely localized molecular orbitals[179] (ALMO-EDA) method implemented in Q-Chem 5.0[180] and described by Liu[181] was utilized to investigate the specific energetic contributions that control MCBD or MT_d formation. Specifically, the energy of the MCBD and MTd intermediates for both metals was decomposed into its energetic components including the Pauli repulsion (ΔE_{Pauli}), the electrostatic (ΔE_{elstat}), the polarization (ΔE_{pol}), and the charge transfer (ΔE_{ct}) energies using the HF method with the 6-311G(d,p) basis set as employed by Liu.[182] It was found that ΔE_{elstat}, or electrostatic energy between the ligand and the alkyne substrate, appeared to contribute to controlling the intermediate formation. Overall, the ΔE_{elstat} was lowest in the case of the favored intermediate (MCBD for W and MT_d for Mo; see **Figure 6.13** below and **Figures A6.12 and A6.13** in Appendix 6 for full details).

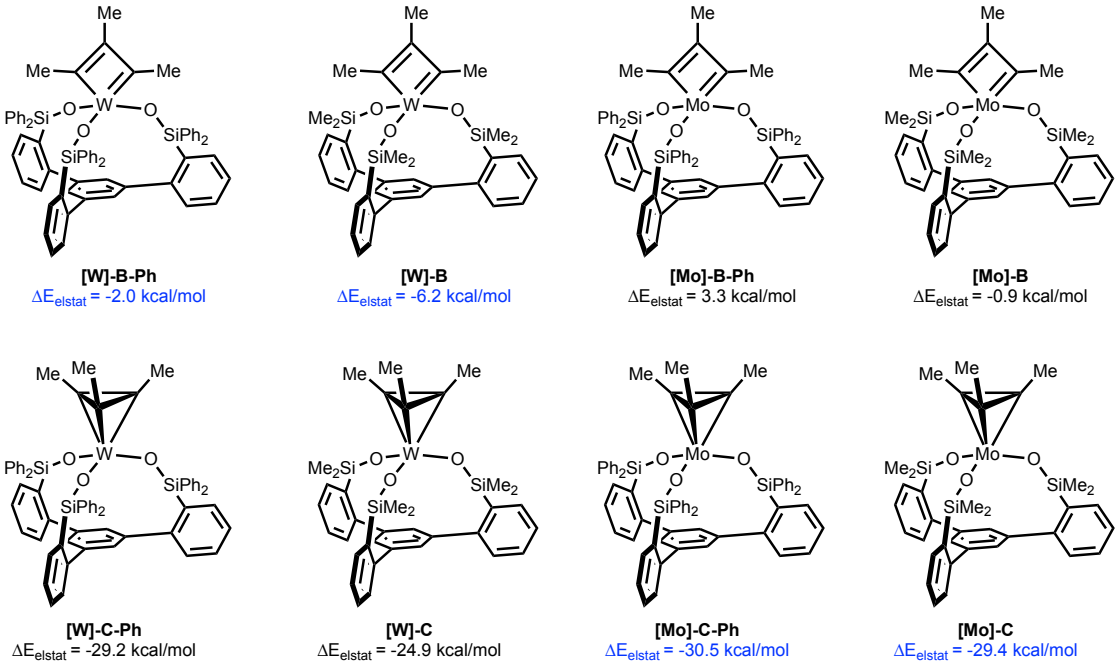


Figure 6.13 Electrostatic energies for the MCBD intermediates, **[W]-B** and **[Mo]-B** and MTd intermediates**, [W]-C** and **[Mo]-C**, computed by the second-generation ALMO-EDA method using HF/6-311G(d,p). The electrostatic energies are lower for **[W]-B** than **[Mo]-B** and for **[Mo]-C** than **[W]-C** showing that the electrostatic energy likely contributes to metal's preference to form the observed intermediate.

Furthermore, the distortion energy[183] required to convert the geometry of the intermediate into the transition state geometry was also calculated for the MCBD and MT_d formation transition states. It was found that the low distortion energy required to form the MCBD in the case of tungsten drives the formation of this intermediate and explains this observed preference while the distortion energy does not appear to play a role in the preference for the MT_d in the molybdenum case (see **Figures A6.14 and A6.15** in Appendix 6). Instead, for molybdenum it appears to be the favorable CH•••π interactions in the MT_d intermediate that drive its formation. Overall, the formation of the metallocyclobutadiene or metallatetrahedrane intermediates using these podand ligands appears instead to be dependent on the nature of the metal with the favorable electrostatic

energy between the ligand and substrate leading to its preference for the MCBD intermediate in the case of tungsten and the MT_d intermediate in the case of molybdenum.

6.4 Conclusion

In conclusion, to explore the role that siloxide ligand geometry has on catalyst activity and electrophilicity, the Lee group synthesized a tethered variant in which the three siloxide motifs were connected by a single arene linker. Through a computational investigation of the effect of Mo-O-Si bond angle on ^{13}C carbyne shift and Mulliken charge of the molybdenum, the relationship between ligand flexibility and electrophilicity was explored. It was found that rather than the bond angle controlling the electrophilicity of the molybdenum center, it was the geometry of the complex imparted by the ligand that had the strongest effect. Further, the Lee group discovered that treatment of the SiP-supported alkylidyne with a slight excess of 3-hexyne resulted not in the expected MCBD intermediate but rather a rare instance of a molybdenum metallatetrahedrane. This species was found to be dynamic, both by being able to revert to the original alkylidyne under vacuum and being able to participate in alkyne metathesis. A preliminary investigation into the energetics of the MCBD and MT_d formation was performed, revealing that MCBD formation has a lower barrier in the case of the siloxide ligand while MT_d formation is favorable for the siloxide podand ligand.

These studies prompted a more detailed investigation into the metallatetrahedrane, a previously scantly investigated organometallic species despite its potential role in alkyne metathesis as well as its similarity to analogous heteroatom-based E_3 species which are abundant in the chemical literature. Through computations in conjunction with

experimental studies by the Lee group, it was shown that the isolation of such species requires a confluence of myriad and subtle factors including metal choice, supporting ligand rigidity and the presence of non-covalent interactions. The greater electrophilicity of W (relative to Mo) stabilizes MCBD over MT_d, regardless of all other factors. The ability of ancillary ligand(s) to more readily distort to accommodate catalyst geometries also leads to a MCBD preference. Additionally, CH•••π interactions appear to be indispensable in stabilizing the MT_d. A new mechanistic proposal for Mo(VI)- and W(VI)-catalyzed alkyne metathesis was presented based on dispersion-corrected DFT calculations. Unlike the traditionally proposed [2+2]-cycloaddition/retro-[2+2] mechanism, computations provide support for a lower energy pathway involving [2+2]-cycloaddition/pseudorotation/retro-[2+2]. The metallatetrahedrane is shown to be catalytically active as well, though these barriers to product formation are higher than that of the main pathway.

Chapter 7: Iron-Catalyzed Multicomponent Cross-Coupling of Vinyl Aryl- and Alkyl Ethers with Grignard Reagents and (Fluoro)Alkyl Halides

Excerpts from this chapter were submitted to *Chem. Comm.* and the work is under review.

7.1 Abstract

An iron-catalyzed regioselective dicarbofunctionalization of alkenes is described. Specifically, aryl- and alkyl vinyl ethers were used as effective linchpins to couple alkyl or (fluoro)alkyl halides and sp^2-hybrized Grignard nucleophiles. Preliminary results demonstrate ability to engage thioethers as linchpins and to control enantioselectivity in these transformations, an area which is largely unexplored for iron-catalyzed three-component cross-coupling reactions.

7.2 Introduction

Alkenes are prevalent motifs in natural products, pharmaceuticals, and represent valuable building blocks in organic synthesis.[184] Recently, the difunctionalization of alkenes has attracted interest from the pharmaceutical community due to the potential for cost-effective, rapid, and modular synthesis of complex scaffolds.[185] In this vein, transition metal-catalyzed three-component cross-coupling reactions have been used to selectively install functional groups across the alkene scaffold, thereby building molecular complexity in one step.[186,187,188,189,190,191 ,192,193,194] However, much of the effort in the development of these reactions has been spent on electron-deficient alkenes and derivatives bearing directing groups to control reactivity and selectivity.[195] Further, fewer examples of the 1,2-dicarbofunctionalization of electron-rich alkenes have been reported [196] and most are

limited to the use of nickel and dual nickel/photoredox as catalysts (**Figure 7.1a**)[197,198,199,200].

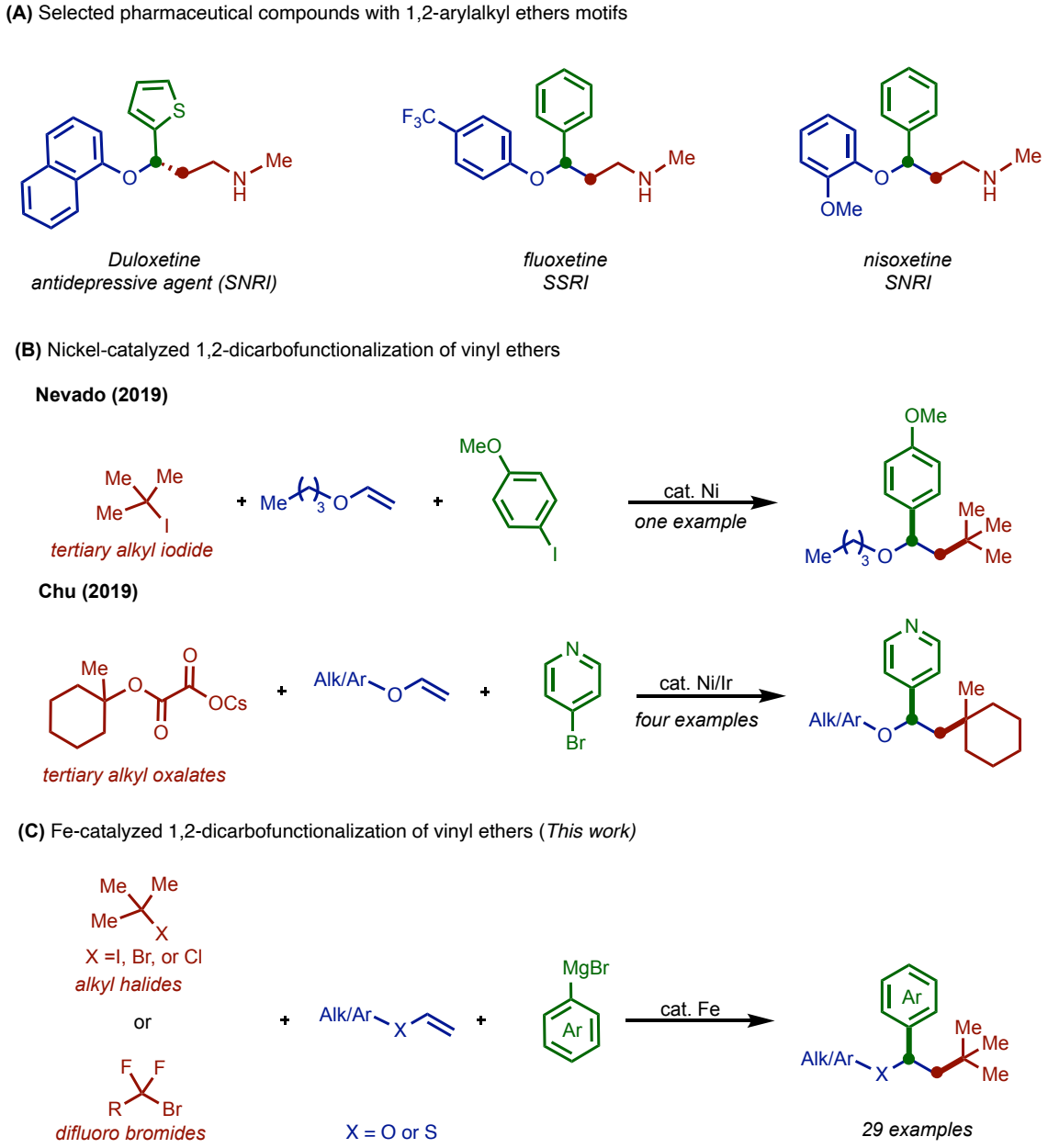


Figure 7.1 Transition-metal catalyzed 1,2-dicarbofunctionalization of electron-rich alkenes and its pharmaceutical relevance.

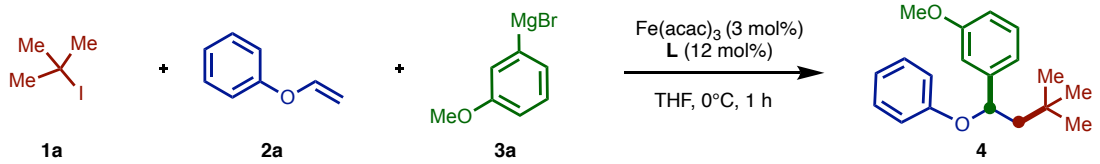
Seeking to expand the utility of Fe-catalyzed multicomponent cross-couplings, it was hypothesized that bisphosphine-iron complexes could serve as cost-effective,

practical, and sustainable catalysts to promote 1,2-dicarbofunctionalization of electron-rich vinyl ethers and, if successful, could complement existing nickel-and dual nickel/photoredox methods (**Figure 7.1b**). Herein, a three-component iron-catalyzed regioselective dicarbofunctionalization of aryl- and alkyl vinyl ethers with (fluoro)alkyl halides and sp^2-hybrized Grignard nucleophiles is reported. This method will find applications in the cost-effective synthesis of analogues of antidepressive drugs such as selective serotonin reuptake inhibitors (SSRI) and serotonin-norepinephrine reuptake inhibitors (SNRI) drug classes and, in particular, introduction of fluorine atoms into larger scaffolds with applications in pharmaceutical chemistry (**Figure 7.1c**).[201]

7.3 Results and Discussion

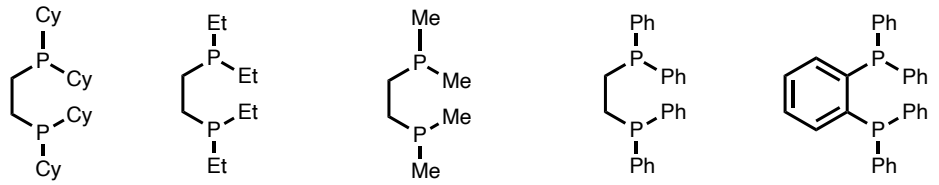
Recently an iron-catalyzed conjunctive cross-coupling was developed in the Gutierrez lab using strain-release vinyl cyclopropanes as the conjunctive reagent under exceptional rapid reaction times (< 1 hr).[202] Further, the reaction scope was extended to the use of unactivated alkenes without the use of directing groups.[203] However, the main drawback of this method is the need for high concentration of alkene (i.e., as solvent) to drive the equilibrium towards the Giese addition adduct (i.e., alkyl radicals) for effective and subsequent cross-coupling with the presumed iron-aryl species. It is hypothesized that Giese addition to vinyl ethers will lead to more stable alpha oxy radicals and provide the driving force to ensure subsequent cross-coupling. To test this hypothesis, a study of iron-catalyzed dicarbofunctionalization of vinyl ethers with commercially available phenyl vinyl ether as the alkene lynchpin was undertaken. Interestingly, under excess alkene (14 eq), the desired three-component cross-coupling product **4** was formed with a 1,2-addition of the aryl Grignard and the alkyl group in high yield (89%). However, the alkene loading

should be lowered from 14 equivalents to increase the utility of this method. Excitingly, 4 eq of phenyl vinyl ether also gave reasonably high yield (75%) but required significantly less alkene. Effectively only 1.6 eq of phenyl vinyl ether is consumed in the reaction given that we were able to recover 2.4 eq after workup. Further, screening of various iron salts and ligands revealed $Fe(acac)_3$ in combination with **L1** as the ideal candidate for this reaction. Control experiments verified that solvent, ligand, and iron catalyst were essential to the reactivity (see **Figures A7.2 – A7.4** in Appendix 7 for full details of the reaction optimization.)



1a 2a 3a 4

Entry	Deviations from standard conditions	NMR Yield [%]
1	**L1** (12 mol%)	75
2	**L2** (12 mol%)	0
3	**L3** (12 mol%)	0
4	**L4** (12 mol%)	45
5	**L5** (12 mol%)	0
6	using $FeBr_2$ (3 mol%)	63
7	using $FeCl_3$ (3 mol%)	60
8	using $Fe(OTf)_2$ (3 mol%)	63
9	neat	67
10	no **L1**	0
11	No $Fe(acac)_3$ and no **L1**	0



L1 L2 L3 L4 L5

Figure 7.2. Evaluation of Reaction Conditions. The reaction was performed with *tert*-butyl iodide **1a** (0.1 mmol, 1.0 equiv), phenyl vinyl ether **2a** (0.4 mmol, 4 equiv.) and 3-methoxyphenyl Grignard **3a** (0.15 mmol, 1.5 equiv.). Aryl Grignard **3** was added dropwise via syringe pump over 1 h. The yield was determined by ^{1}H NMR using dibromomethane as internal standard.

With the optimized conditions identified (**Figure 7.2,** entry 1), the generality of this iron-catalyzed dicarbofunctionalization reaction was studied. Initially, the diversity of Grignard nucleophiles for this reaction (**Figure 7.3**) were explored. Electron-rich Grignard reagents afforded products (**4-8**) in good yield while mildly electron-deficient Grignard reagents were tolerated as well, giving products (**11, 12**) in moderate yields. Even electron-poor Grignard reagents gave products (**9, 10,13**), albeit in lower yields.

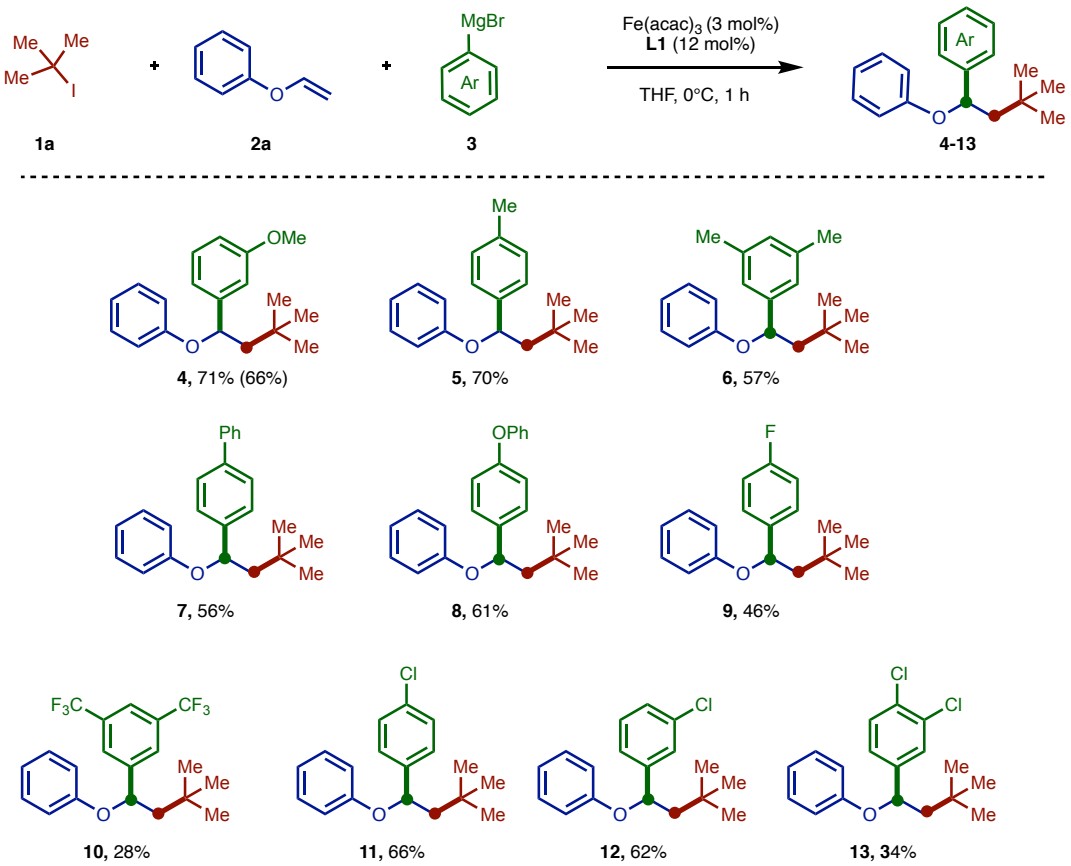


Figure 7.3. Scope of Grignard nucleophile in the 3-component conjunctive cross-coupling with *tert*-butyl iodide and phenyl vinyl ether. All reactions were performed under the optimized conditions (**Figure 7.2**, entry 1) using 0.2 mmol *tert*-butyl iodide. Isolated yields are reported.

With the scope of Grignard reagent explored, the alkyl halide scope was investigated (**Figure 7.4**). In addition to the *tert*-butyl iodide used in the optimized reaction, adamantyl (**14, 15**) and tetrafluorobutyl halides (**16**) successfully gave product in good to high yield. (Fluoro)alkyl halides were particularly high-yielding (up to 92%) in this reaction (**16-20**). This result, demonstrating the ability of this reaction to add fluoroalkyl groups to a vinyl ether, shows promise that the method can be used for pharmaceutical applications, with 20% of drugs on the market containing at least one fluorine atom.[204] In addition, 2-bromo-2-methylbutane successfully gave product in moderate yield (**21**, 51%).

Finally, *tert*-butyl chloride gave product **22** in moderate yield (39%), and albeit lower than when *tert*-butyl iodide was used as the alkyl halide (**7**, 56%). These results demonstrate that alkyl chlorides are also viable as radical precursor partners in three-component dicarbofunctionalization.

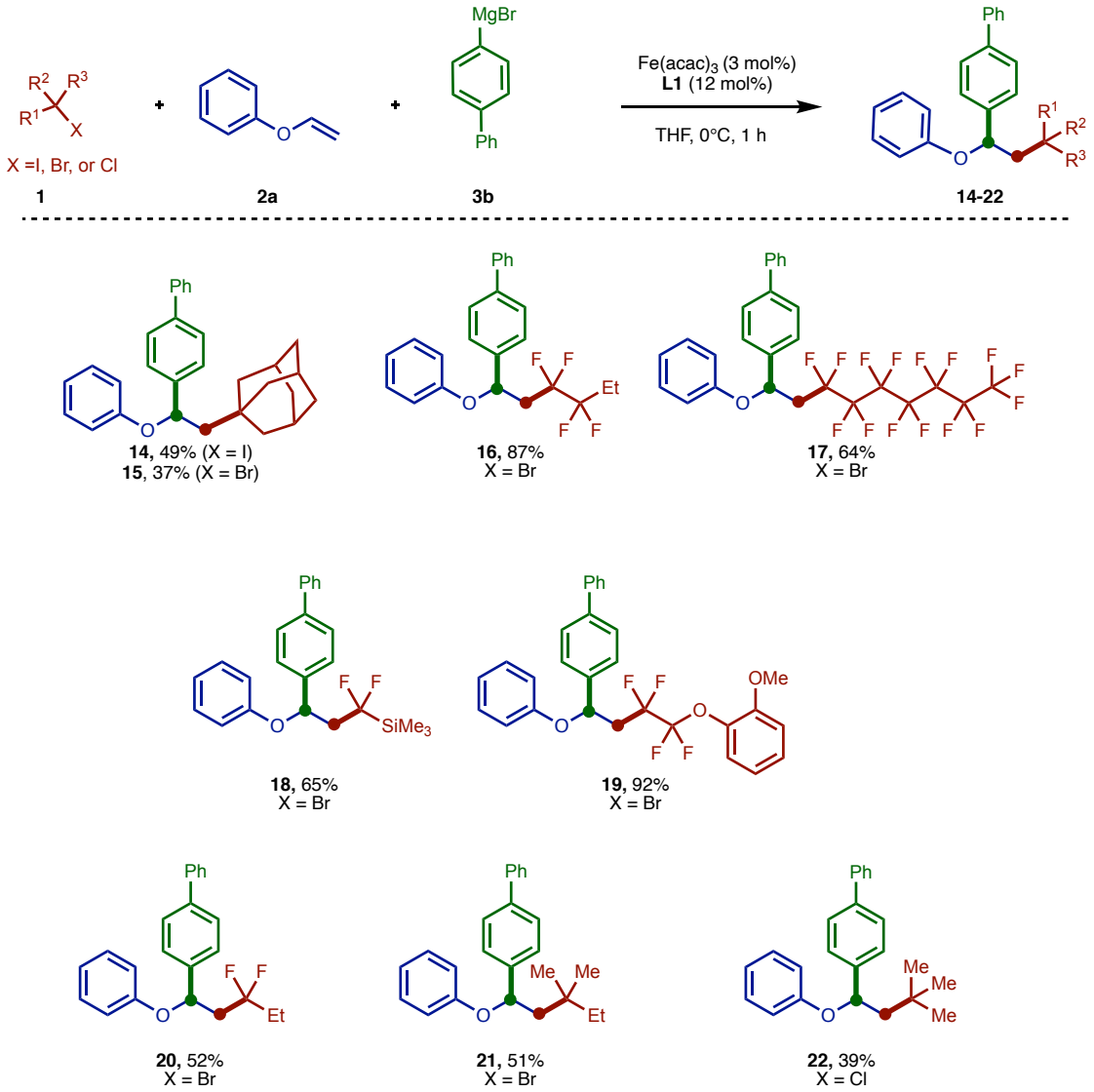


Figure 7.4. Scope of alkyl halides in the 3-component cross-coupling with phenyl vinyl ether and 4-biphenylmagnesium bromide **3b**. All reactions were performed under the optimized conditions (**Figure 7.2**, entry 1) using 0.2 mmol alkyl halide. Isolated yields are reported.

Finally, the alkene substrate scope was investigated (**Figure 7.5**). Overall, attempts to extend the reaction to primary and secondary *alkyl* vinyl ethers were successful, giving products (**23-28**) in moderate yields. These results show that alkyl vinyl ethers in addition to aryl vinyl ethers (**30, 31**) can be functionalized through this 1,2-alkylarylation method although the latter is higher yielding. Notably, tolerance of alkyl thioethers was established with compound **29**. Interestingly, even the internal alkene 3,4-dihydro-2*H*-pyran **2b** reacted in this method to give moderate yield of product **32** as the trans isomer, as determined by NOESY (Nuclear Overhauser Effect Spectroscopy; see Figures A7.1 and A7.49 in Appendix 7). The ability of this reaction to functionalize internal vinyl ethers opens the possibility for this method to be used in the formation of *C*-aryl glycosides from carbohydrate derivatives, thereby expanding the utility of this reaction.

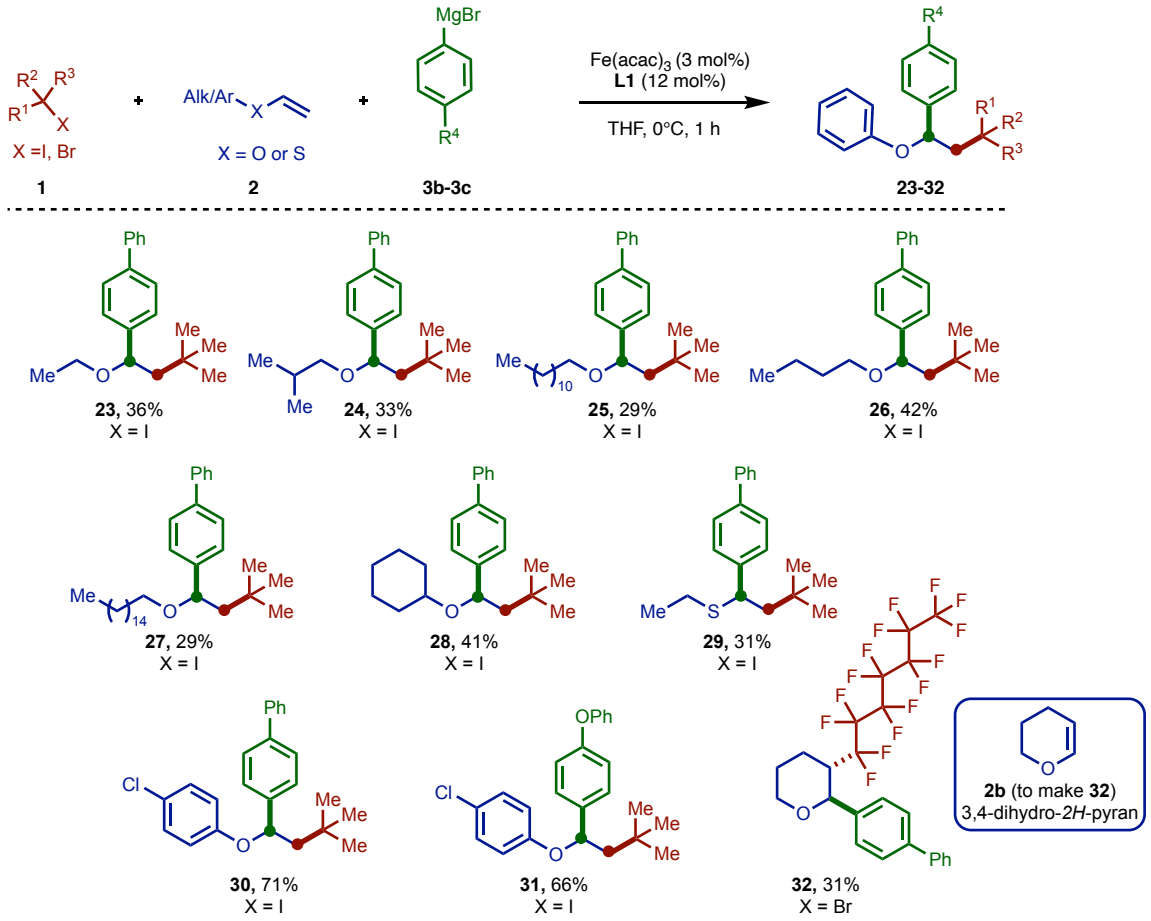


Figure 7.5. Scope of vinyl ethers in the 3-component conjunctive cross-coupling with alkyl halides and 4-biphenylmagnesum bromide **3b** or 4-phenoxyphenylmagnesum bromide **3c**. All reactions were performed under the optimized conditions (**Figure 7.2**, entry 1) using 0.2 mmol of alkyl halide. Isolated yields are reported.

With the substrate scope evaluated, the preparation of compound **4** was repeated on the gram scale (**Figure 7.6**) to demonstrate the utility of this work in a scaled-up process. Starting from 1.0 g of tert-butyl iodide, 1.02 g of the product 4 was isolated (66%) after purification by column chromatography.

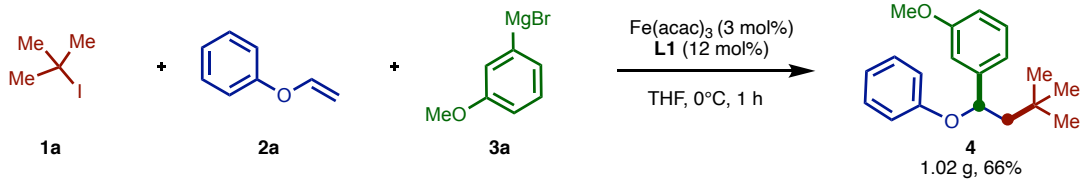


Figure 7.6. Gram-scale dicarbofunctionalization of phenyl vinyl ether (4 equiv.; 21.7 mmol) with *tert*-butyl iodide (1.0 g, 5.4 mmol) and 3-methoxyphenyl magnesium bromide (1.5 equiv.; 8.1 mmol). Isolated yield is reported.

Finally, the enantioselective version of the reaction was studied, screening five chiral phosphine ligands (see **Figure A7.5** in Appendix 7) using optimized reaction conditions previously identified in the laboratory. From this ligand screening, the (*R*,*R*)-BenzP* ligand was identified (**Figure 7.7**) as the ligand giving the most promising preliminary result (75:25 er.) The development of enantioselective three-component reactions remains a considerable challenge in the field and work in this area is currently underway.[205]

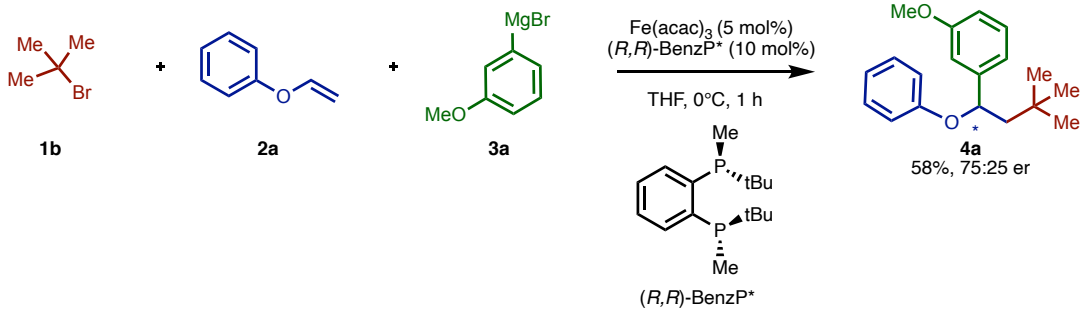


Figure 7.7. Preliminary results on the asymmetric version of the 3-component conjunctive cross-coupling. The given yield is an isolated yield and the enantiomeric ratio was determined by chiral HPLC, both determined as an average of the results from four trials.

7.4 Conclusion

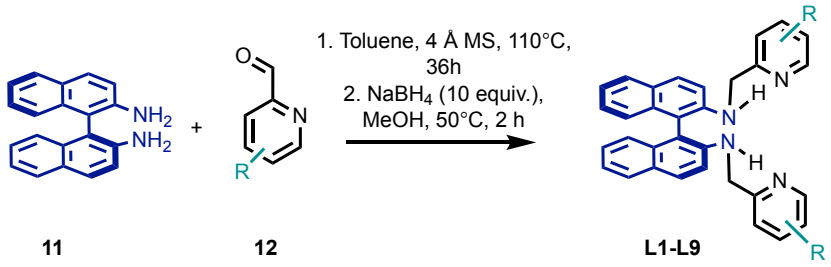
In summary, I have developed an iron-catalyzed regioselective 1,2-dicarofunctionalization of vinyl ethers with alkyl halides or (fluoro)alkyl halides and aryl Grignard reagents. This reaction successfully gives product with both electron-donating

aryl Grignard reagents and mildly electron-withdrawing aryl Grignard reagents. Further, I have shown that this method functionalizes both aryl and alkyl vinyl ethers. Notably, this method can introduce (fluoro)alkyl groups to a vinyl ether in a one-step synthesis, whereby molecular complexity can be rapidly increased. The ability to introduce (fluoro)alkyl groups to an alkene has the potential for pharmaceutical applications. Ongoing work on the asymmetric variant of this reaction is currently underway.

Appendix 1: Methods, Experimental Data, Supplementary Figures, NMR Spectra, X-ray Crystal Structures and Coordinates/Energies of Structures from Chapter 1 (Rational Design of Chiral Iron Catalysts for Asymmetric C(sp^3)-H Oxidations)

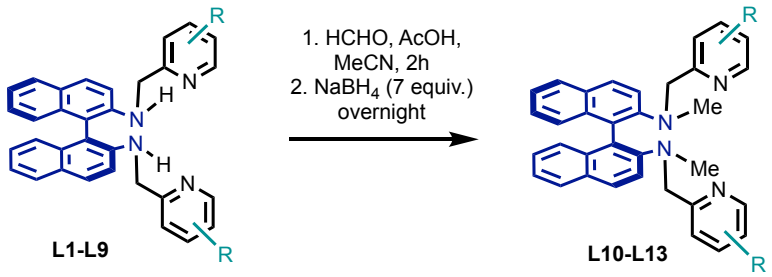
A1.1 Methods

A1.1.1 General procedure for (R)-N,N'-bis(pyridin-2-ylmethyl)-1,1'-binaphthyl-2,2'-diamine synthesis



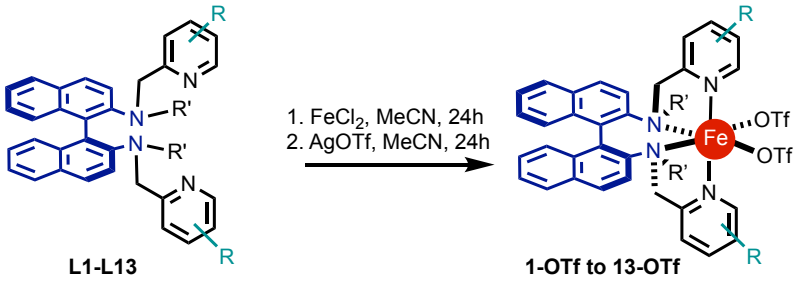
Pyridine-2-carboxaldehyde (2.2 mmol) was mixed with (R)-2,2'-diamino-1,10-binaphthyl (284 mg, 1.0 mmol) in dry toluene (4 mL). A few 4 Å molecular sieves were added, and the solution was warmed up to 110°C and kept for 36 h at this temperature, and then cooled to room temperature and methanol (4 mL) was added. $NaBH_4$ (380 mg, 10 mmol) was added in small portions at 0°C, then the solution was warmed up to 50°C and kept for 2 h at this temperature. The solvent was removed and the residue was decomposed with H_2O (20 mL), extracted with ethyl acetate (3 x 10 mL) and washed with brine (20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and the solvent was removed under reduced pressure, then purified by flash chromatography (1:1 EtOAc:hexanes).

A1.1.2 General procedure for (R)-N,N'- bis(methyl)-N,N'-bis(pyridin-2-ylmethyl)-1,1'-binaphthyl-2,2'-diamine synthesis[206]



0.25 ml of aqueous formaldehyde (37%) was added to a solution of (R)-N,N'-bis(pyridin-2-ylmethyl)-1,1'-binaphthyl-2,2'-diamine (0.2 mmol) and 0.75 ml of acetic acid in acetonitrile (5 ml), and allowed to stir for 30 min. Subsequently, 51 mg (1.34 mmol) of sodium borohydride was added and the resultant mixture was stirred overnight. All solvents were removed and 3 M aqueous sodium hydroxide (5mL) was added. This aqueous mixture was extracted with DCM (3 x 5 mL). The organic layers were combined and dried with Na_2SO_4. The solvent was removed under reduced pressure and the compound was purified by flash chromatography (1:1 EtOAc:hexanes).

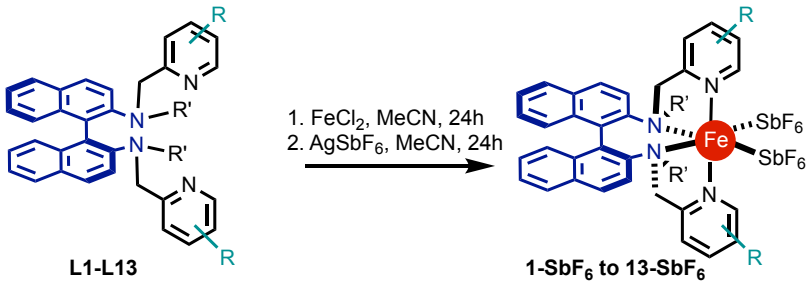
A1.1.3 General procedure for iron (II) (R)-N,N'-bis(pyridin-2-ylmethyl)-1,1'-binaphthyl-2,2'-diamine triflate complex synthesis[207]



A 25-mL round bottom flask was charged with compound **L1** (100 mg, 0.214 mmol) and iron (II) chloride powder (27 mg, 0.214 mmol) in the glove box. Anhydrous acetonitrile (2.0 mL) was added and the reaction mixture was stirred under nitrogen for 24 hours. To the solution was added silver triflate (110 mg, 0.428 mmol) and the flask was wrapped in

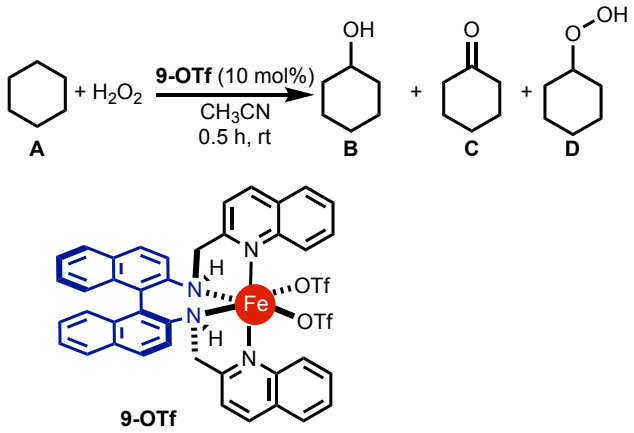
aluminum foil. After 24 hours, the silver chloride salt was removed by filtration and the filtrate was concentrated to give a dark brown powder. Single crystals suitable for x-ray crystallographic analysis (**1-OTf** and **4-OTf**) were obtained by dissolution of the powder in dichloromethane with careful layering of hexanes on top of the dichloromethane layer.

A1.1.4 General procedure for iron (II) (R)-N,N'-bis(pyridin-2-ylmethyl)-1,1'-binaphthyl-2,2'-diamine hexafluoroantimonate complex synthesis[208]



A 25-mL round bottom flask was charged with compound **L1** (100 mg, 0.214 mmol) and iron (II) chloride powder (27 mg, 0.214 mmol) in the glove box. Anhydrous acetonitrile (2.0 mL) was added and the reaction mixture was stirred under nitrogen for 24 hours. To the solution was added silver hexafluoroantimonate (147 mg, 0.428 mmol) and the flask was wrapped in aluminum foil. After 24 hours, the silver chloride salt was removed by filtration and the filtrate was concentrated to give a dark brown powder. Single crystals suitable for x-ray crystallographic analysis were obtained (**1-SbF_6**) by dissolution of the powder in dichloromethane with careful layering of hexanes on top of the dichloromethane layer.[209]

A1.1.5 General procedure for Fe-catalyzed C(sp^3)-H oxidation using an iterative addition protocol



A 5-mL screwtop vial was charged with Fe-complex **9-OTf** (9.1 mg, 0.01 mmol, 10 mol%), cyclohexane (11 μL, 0.1 mmol, 1.0 equiv.) anhydrous acetonitrile (0.5 mL) and a magnetic stir bar. The vial was placed on a stir plate and stirred vigorously at room temperature. A solution of H_2O_2 (4.0 μL, 0.12 mmol, 1.2 equiv) in CH_3CN (0.33 mL) was added dropwise via syringe over 90 seconds. After ten minutes, another aliquot of H_2O_2 (4.0 μL, 0.12 mmol, 1.2 equiv) in CH_3CN (0.33 mL) was added dropwise via syringe over 90 seconds. A third addition was done in the same manner for a total of 3.6 equiv. of H_2O_2. Each addition was allowed to stir for 10 minutes, for a total reaction time of 30 minutes. Upon completion, the mixture was extracted with EtOAc (3 x 1 mL) and filtered through a pad of silica gel. The solution was then analyzed by GC/MS using biphenyl as an internal standard to assess the yield of cyclohexanol and cyclohexanone.

A1.1.6 General procedure for spin state determination by Evan's method

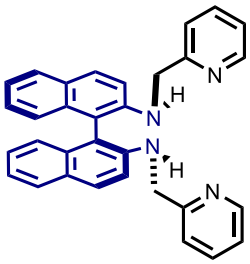
Iron (II) (R)-N,N'-bis(pyridin-2-ylmethyl)-1,1'-binaphthyl-2,2'-diamine complex (3 mg) is dissolved in 1.0 mL of $CDCl_3/CH_2Br_2$ 95/5 (v/v) solution. A portion of this solution is transferred to a capillary tube which is flame sealed and placed in an NMR tube containing

$CDCl_3/CH_2Br_2$ 95/5 (v/v). A ^1H NMR spectrum is recorded and used to calculate the magnetic moment based on the peak shift from the dibromomethane in $CDCl_3$ to dibromomethane in the presence of the iron complex using the formulas $\chi_m = \frac{3\Delta f}{1000fc}$ and $\mu_{eff} = 798\sqrt{T\chi_m}$ where χ_m is the magnetic susceptibility, Δf is the peak shift of the internal standard (dibromoethane), f is the NMR frequency, c is the molar concentration, T is temperature and μ_{eff} is the magnetic moment. In a variable temperature study, a ^1H NMR spectrum is recorded at each temperature desired in the study and the change in magnetic moment with temperature is monitored.[210]

A1.1.7 Computational Methods

All optimizations of intermediate structures were carried out in the gas phase without constraints using spin-unrestricted DFT using UB3LYP[211]/6-31G(d) method with the "opt=noeigen" and "guess=mix" keywords as implemented in Gaussian09.[212] Frequency calculations were performed at the same level to determine vibrational frequencies, obtain thermal corrections to enthalpy and free energy at 298K. To refine the energies calculated, I performed single point energy calculations on optimized geometries using implicit solvent (dichloromethane; ε = 9.04) with CPCM as the solvation model[213] in combination with the UM06L functional[214] and the 6-311+G(d,p) basis set. For comparison, we also computed single point energies of some structures using D3 dispersion correction of Grimme et al.[215] with UB3LYP (i.e., UB3LYP-D3), the UM06 functional, and the PBEPBE functional in combination the 6-311+G(d,p) basis set in solvent (dichloromethane) using the CPCM solvation model. All structural figures were generated using CYLview[216] and GaussView.[217]

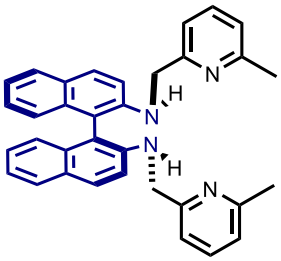
A1.2 Experimental Data



Compound **L1**

(R)-N,N'-bis(pyridin-2-ylmethyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 91%

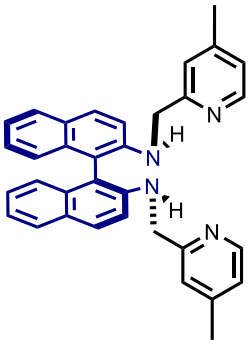
^{1}H NMR: (400 MHz, $CDCl_3$) δ 8.47 (2 H, d, J = 4.8 Hz), 7.82 (2 H, d, J = 8.8 Hz), 7.75-7.80 (2 H, m), 7.49 (2 H, td, J = 7.6 Hz, J = 2.0 Hz), 7.17-7.25 (8 H, m), 7.14 (2 H, d, J = 8.8 Hz), 7.03-7.12 (4 H, m), 4.56 (4 H, s). Spectral data matched literature.[218]



Compound **L2**

(R)-N,N'-bis((6-methylpyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 73%

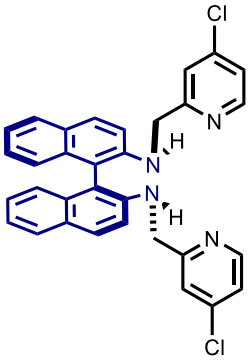
^{1}H NMR: (400 MHz, $CDCl_3$) δ 7.83 (2 H, d, J = 8.8 Hz), 7.75-7.80 (2 H, m), 7.32 (2 H, t, J = 7.4 Hz), 7.17-7.23 (4 H, m), 7.15 (2 H, d, J = 8.8 Hz), 7.04-7.10 (4 H, m), 7.00 (2 H, d, J = 7.6 Hz), 6.93 (2 H, d, J = 7.6 Hz), 4.45-4.57 (4 H, m), 2.43 (6 H, s). Spectral data matched literature.[1]



Compound **L3**

(R)-N,N'-bis((4-methylpyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 93%

^{1}H NMR: (400 MHz, $CDCl_3$) δ 8.32 (2 H, d, J = 5.2 Hz), 7.82 (2 H, d, J = 8.8 Hz), 7.75-7.80 (2 H, m), 7.17-7.24 (4 H, m), 7.14 (2 H, d, J = 9.2 Hz), 7.05-7.11 (2 H, m), 7.00 (2 H, s), 6.90 (2 H, d, J = 4.8 Hz), 4.44-4.61 (6 H, m), 2.16 (6 H, s). Spectral data matched literature.[1]



Compound **L4**

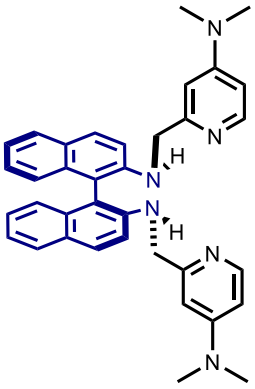
(R)-N,N'-bis((4-chloropyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 44%

^{1}H NMR: (400 MHz, $CDCl_3$) δ 8.37 (2 H, d, J = 6.5 Hz), 7.84 (2 H, d, J = 11.0 Hz), 7.77-7.82 (2 H, m), 7.21-7.29 (6 H, m), 7.06-7.14 (6 H, m), 4.50-4.64 (4 H, m). IR (neat): 3390, 3356, 3051, 2923, 1595, 1508, 1424, 1334, 1303 cm^{-1};

^{13}C NMR: (125 MHz, $CDCl_3$) δ 161.95, 150.22, 145.17, 143.43, 133.93, 130.14, 128.07, 127.34, 123.91, 122.58, 122.56, 121.33, 113.81, 112.32, 48.81;

IR (neat): 3387, 3357, 3053, 2908, 1615, 1596, 1574, 1509, 1487, 1425, 1332, 1301 cm^{-1};

HRMS: (ESI) calcd for $C_{32}H_{25}Cl_2N_4$ $[M+H]^+$: 535.1456, found: 535.1459.



Compound **L5**

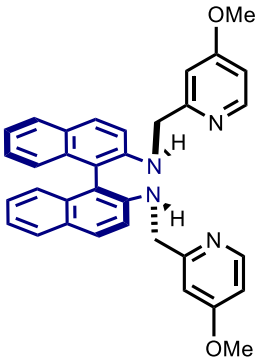
(R)-N,N'-bis((4-(dimethylamino)pyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 82%

^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.11 (2 H, d, J = 6.0 Hz), 7.81 (2 H, d, J = 9.0 Hz), 7.76 (2 H, d, J = 8.0 Hz), 7.10-7.19 (6 H, m), 7.07 (2 H, d, J = 8.0 Hz), 6.37 (2 H, d, J = 2.5 Hz), 6.29 (2 H, dd, J = 5.8 Hz, J = 2.8 Hz), 4.33-4.55 (6 H, m), 2.79 (12 H, s);

^{13}C NMR: (125 MHz, $CDCl_3$) δ 159.57, 155.10, 149.33, 144.20, 134.01, 129.74, 128.32, 127.82, 126.68, 123.78, 121.85, 114.31, 111.82, 105.13, 103.02, 49.61, 39.08;

IR (neat): 3414, 2894, 1593, 1506, 1423, 1335 cm^{-1};

HRMS: (ESI) calcd for $C_{36}H_{37}N_6$ $[M+H]^+$: 553.3080, found: 553.3082.



Compound **L6**

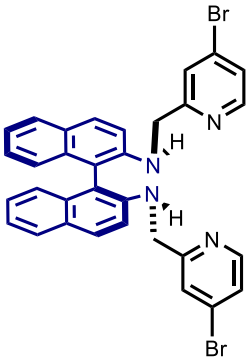
(R)-N,N'-bis((4-methoxypyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 80%

^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.30 (2 H, d, J = 5.5 Hz), 7.82 (2 H, d, J = 9.0 Hz), 7.75-7.80 (2 H, m), 7.15-7.24 (4 H, m), 7.06-7.14 (4 H, m), 6.75 (2 H, s), 6.61-6.64 (2 H, m), 4.25-4.70 (6 H, m), 3.65 (6 H, s).

^{13}C NMR: (125 MHz, $CDCl_3$) δ 166.66, 161.76, 150.48, 143.87, 133.99, 129.92, 128.36,127.94, 126.90, 123.86, 122.19, 114.11, 112.08, 108.43, 106.63, 55.12, 49.20;

IR (neat): 3408, 3049, 2954, 1730, 1591, 1500, 1422, 1333, 1297 cm^{-1};

HRMS: (ESI) calcd for $C_{34}H_{32}N_4O_2$ $[M+2H]^{2+}$: 264.1263, found: 264.1269.



Compound **L7**

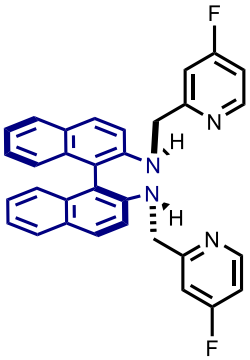
(R)-N,N'-bis((4-bromopyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 40%

^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.29 (2 H, d, J = 5.0 Hz), 7.84 (2 H, d, J = 8.0 Hz), 7.80 (2 H, dd, J = 7.5 Hz, J = 1.0 Hz), 7.43 (2 H, d, J = 1.5 Hz), 7.22-7.31(8 H, m), 7.10 (2 H, d, J = 8.5 Hz), 7.08 (2 H, d, J = 9.0 Hz), 4.51-4.62 (4 H, m);

^{13}C NMR: (125 MHz, $CDCl_3$) δ 161.80, 150.12,143.38, 133.92, 130.14, 128.40, 128.05, 127.39, 125.52, 124.30, 123.88, 122.55, 113.77, 112.26, 48.76;

IR (neat): 3387, 3050, 2908, 1614, 1568, 1488, 1333, 1151 cm^{-1};

HRMS: (ESI) calcd for $C_{32}H_{25}Br_2N_4$ $[M+H]^{+}$: 625.0426, found:625.0407.



Compound **L8**

(R)-N,N'-bis((4-fluoropyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 75%

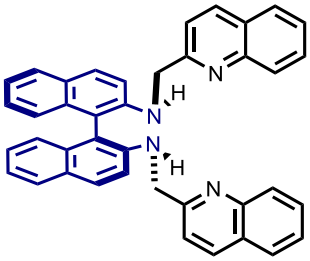
^{1}H NMR: (500 MHz, $CDCl_3$): δ 8.45-8.50 (2 H, m), 7.86 (2 H, d, J = 9.0 Hz), 7.79-7.89 (2 H, m), 7.43 (2 H, d, J = 1.5 Hz), 7.22-7.33(4 H, m), 7.09-7.17 (4 H, m), 7.03 (2 H, d, J = 10.0 Hz), 6.84-6.90 (2 H, m), 4.52-4.64 (4 H, m).

^{13}C NMR: (125 MHz, $CDCl_3$): δ 169.6 (J_{C-F} = 261.0 Hz), 163.9 (J_{C-F} = 5.9 Hz), 151.7 (J_{C-F} = 6.9 Hz), 143.6, 133.9, 130.1, 128.4, 128.1, 127.2, 124.0, 122.6, 113.9, 112.4, 110.1 (J_{C-F} = 16.8 Hz), 108.8 (J_{C-F} = 17.5 Hz), 49.1;

^{19}F NMR: (376 MHz, $CDCl_3$) δ -101.8;

IR (neat): 3398, 3346, 3056, 2908, 1595, 1577, 1510, 1335 cm^{-1};

HRMS: (ESI) calcd for $C_{32}H_{25}F_2N_4$ $[M+H]^+$: 503.2047, found:503.2026.



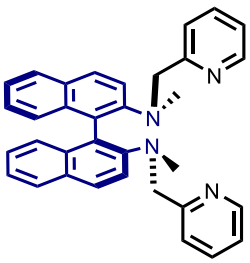
Compound **L9**

(R)-N,N'-bis(quinolin-2-ylmethyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 25%

^{1}H NMR: (400 MHz, $CDCl_3$) δ 7.91 (2 H, d, J = 8.8 Hz), 7.82-7.88 (4 H, m), 7.80 (2 H, d, J = 8.8 Hz), 7.64-7.72 (4 H, m), 7.48 (2 H, td, J = 7.6 Hz, J = 0.8 Hz), 7.28-7.33 (4 H, m), 7.22-7.27 (4 H, m), 7.15-7.21 (2 H, m), 5.13 (2 H, br), 4.66-4.78 (4 H, s).

^{13}C NMR: (100 MHz, $CDCl_3$) δ 159.63, 147.42, 144.09, 136.77, 134.14, 129.90, 129.64,128.85, 128.32, 127.99, 127.58, 127.29, 126.86, 126.20, 124.12, 122.16, 119.17, 114.36, 112.51, 49.77; IR (neat): 3411, 3332, 3051, 1616, 1594, 1503, 1423, 1295 cm^{-1};

HRMS: (ESI) calcd for $C_{40}H_{31}N_4$ $[M+H]^+$:567.2549, found:567.2551.



Compound **L10**

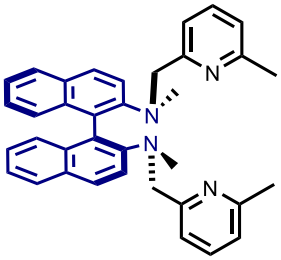
(R)-N,N'-dimethyl-N,N'-bis(pyridin-2-ylmethyl)-[1,1'-binaphthalene]-2,2'-diamine. Yield = 90%

^{1}H NMR: (400 MHz, $CDCl_3$) δ 8.32 (2 H, d, J = 5.6 Hz), 7.90 (2 H, d, J = 8.4 Hz), 7.80 (2 H, d, J = 8.0 Hz), 7.57 (2 H, d, J = 8.8 Hz), 7.27-7.33 (4 H, m), 7.14-7.20 (2 H, m), 6.94-7.00 (2 H, m), 6.29 (2 H, d, J = 7.6 Hz), 3.99-4.11 (4 H, m), 2.49 (6 H, s).

^{13}C NMR: (100 MHz, $CDCl_3$) δ 159.30, 149.48, 147.94, 136.26, 134.19, 130.45, 128.74, 128.51, 127.71, 126.18, 125.90,124.11, 121.45, 121.13, 62.5, 40.58;

IR (neat): 2991,2850, 1591, 1505, 1433, 1357 cm^{-1};

HRMS: (ESI) calcd for $C_{34}H_{31}N_4$ $[M+H]^+$: 495.2549, found: 495.2547.



Compound **L11**

(R)-N,N'-dimethyl-N,N'-bis((6-methylpyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine

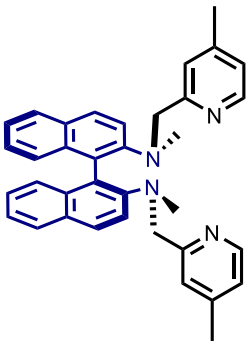
Yield = 88%

^{1}H NMR: (500 MHz, $CDCl_3$) δ 7.89 (2 H, d, J = 9.0 Hz), 7.79 (2 H, d, J = 8.0 Hz), 7.57 (2 H, d, J = 8.5 Hz), 7.25-7.30 (2 H, m), 7.13-7.20 (6 H, m), 6.81 (2 H, d, J = 7.5 Hz), 6.19 (2 H, d, J = 8.0 Hz), 4.00-4.10 (4 H, m), 2.47 (6 H, s), 2.39 (6 H, s).

^{13}C NMR: (125 MHz, $CDCl_3$) δ 159.17, 156.93, 149.79, 136.47, 134.48, 130.58, 128.87, 128.53, 127.82, 126.26, 126.20, 124.11, 121.30, 120.97, 118.41, 63.01, 40.84, 24.32;

IR (neat): 2923, 2851, 1700, 1593, 1506, 1458cm^{-1};

HRMS: (ESI) calcd for $C_{36}H_{35}N_4$ $[M+H]^+$: 523.2862, found: 523.2866.



Compound **L12**

(R)-N,N'-dimethyl-N,N'-bis((4-methylpyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine

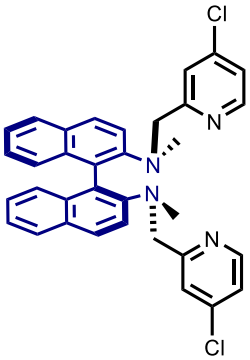
Yield = 63%

^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.13 (2 H, d, J = 5.0 Hz), 7.93 (2 H, d, J = 9.0 Hz), 7.81 (2 H, d, J = 8.0 Hz), 7.62 (2 H, d, J = 8.5 Hz), 7.28-7.33 (2 H, m), 7.13-7.23 (6 H, m), 6.75 (2 H, d, J = 4.5 Hz), 3.95-4.08 (4 H, m), 2.48 (6 H, s), 2.06 (6 H, s).

^{13}C NMR: (125 MHz, $CDCl_3$) δ 159.49, 150.04, 148.04, 147.27, 134.38,130.84, 129.60, 128.89, 127.83, 126.33, 126.25, 124.42, 122.57, 122.36, 121.41, 63.27, 40.72, 20.90;

IR (neat): 2923, 1604, 1504, 1355, 992, 819, 804 cm^{-1};

HRMS: (ESI) calcd for $C_{36}H_{35}N_4$ $[M+H]^+$: 523.2862, found:523.2846.



Compound **L13**

(R)-N,N'-bis((4-chloropyridin-2-yl)methyl)-N,N'-dimethyl-[1,1'-binaphthalene]-2,2'-diamine

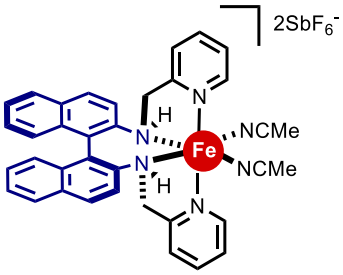
Yield = 79%

^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.13 (2 H, d, J = 5.5 Hz), 7.90 (2 H, d, J = 9.0 Hz), 7.79 (2 H, d, J = 8.0 Hz), 7.61 (2 H, d, J = 9.0 Hz), 7.27-7.32 (2 H, m), 7.14-7.21 (4 H, m), 6.94 (2 H, dd, J_1 = 5.0 Hz, J_2 = 2.0 Hz), 6.22 (2 H, d, J = 2.0 Hz), 3.96-4.05 (4 H, m), 2.59 (6 H, s).

^{13}C NMR: (125 MHz, $CDCl_3$) δ 161.70, 149.67, 149.21, 144.52, 134.23, 130.82, 129.35, 129.05, 128.04, 126.56, 125.95, 124.52, 121.90, 121.46, 120.97, 63.11, 40.97;

IR (neat): 3052, 2924, 2849, 1573, 1553, 1504, 1353 cm^{-1};

HRMS: (ESI) calcd for $C_{34}H_{29}Cl_2N_4$ $[M+H]^+$: 563.1769, found:563.1768.



(R)-N,N'-bis(pyridin-2-ylmethyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(acetonitrile) hexafluoroantimonate, **1-SbF$_6$**. Large black crystals; (44% yield).

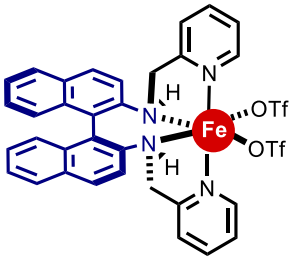
μ_{eff} (CD_3CN): 3.74μ_B.

UV (DCM) λ_{max}, nm: 332.

^{1}H NMR: (400 MHz, CD_3CN) δ 10.74, 8.88, 8.15, 7.80, 7.37, 6.31, 6.05.

IR (neat): 3562, 2981, 1611, 1441, 1252, 1022, 814, 759 cm^{-1}.

HRMS: (ESI) calcd for $C_{32}H_{28}FeN_4O_2$ $[M+H]^+$: 557.1640, found:557.3449.



(R)-N,N'-bis(pyridin-2-ylmethyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(triflate), **1-OTf**. Thin colorless crystals; (41% yield).

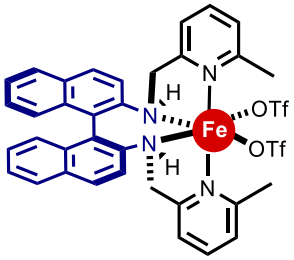
μ_{eff} (CD_3CN): 0.95μ_B.

UV (DCM) λ_{max}, nm: 336.

^{1}H NMR: (400 MHz, CD_3CN) δ 8.58, 8.44, 7.91, 7.41, 7.30, 7.14, 6.94, 4.18.

IR (neat): 3473, 2927, 1753, 1606, 1258, 1230, 1170, 1028, 814, 764 cm^{-1}.

HRMS: (ESI) calcd for $C_{32}H_{30}FeN_4O_3$ $[M+H]^+$: 575.1745, found:575.2607.



(R)-N,N'-bis((6-methylpyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(triflate), **2-OTf**. Tan powder; (49% yield).

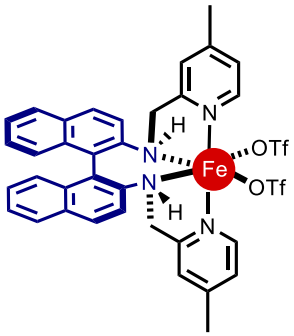
μ_{eff} (CD_3CN): 3.75μ_B.

UV (DCM) λ_{max}, nm: 349.

^{1}H NMR: (400 MHz, CD_3CN) δ 9.12, 8.85, 7.46, 7.31, 6.97, 5.23, 4.52, 2.66.

IR (neat): 3587, 3423, 3077, 2929, 2334, 1738, 1603, 1531, 1437, 1261, 1169, 1032, 828 cm^{-1}.

HRMS: (ESI) calcd for $C_{34}H_{34}FeN_4O_3$ $[M+H]^+$: 603.2059, found:603.2867.



(R)-N,N'-bis((4-methylpyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(triflate), **3-OTf**. Yellow crystalline powder; (36% yield).

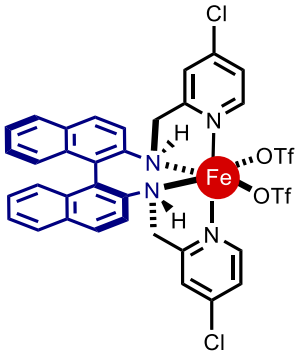
μ_{eff} (CD_3CN): 4.42μ_B.

UV (DCM) λ_{max}, nm: 347.

^{1}H NMR: (400 MHz, CD_3CN) δ 9.12, 9.02, 7.91, 7.22, 6.22, 5.78, 4.74, 2.68.

IR (neat): 3202, 1601, 1431, 1255, 1231, 1169, 1035, 765.

HRMS: (ESI) calcd for $C_{34}H_{33}FeN_4O_3$ $[M+H]^+$: 601.1902, found:601.3380.



(R)-N,N'-bis((4-chloropyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(triflate), **4-OTf.** Thin green crystals; (81% yield).

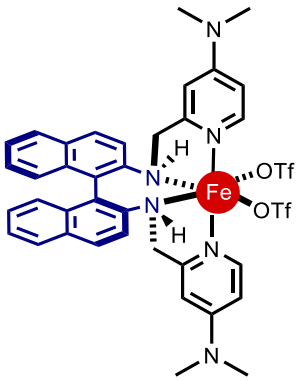
μ_{eff} (CD_3CN): 3.09μ_B.

UV (DCM) λ_{max}, nm: 332.

^{1}H NMR: (400 MHz, CD_3CN) δ 84.75, 59.43, 35.18, 14.66, 12.66, 9.99, 9.11, 7.12, 1.16.

IR (neat): 3257, 1594, 1276, 1222, 1162, 819, 752 cm^{-1}.

HRMS: (ESI) calcd for $C_{32}H_{31}FeN_4O_3$ $[M+H]^+$: 645.1123, found:645.1775.



(R)-N,N'-bis((4-(dimethylamino)pyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(triflate), **5-OTf**. Brown crystalline powder; (68% yield).

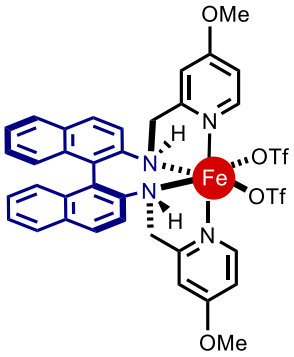
μ_{eff} (CD_3CN): 3.64μ_B.

UV (DCM) λ_{max}, nm: 352.

^1H NMR: (400 MHz, CD_3CN) δ 11.56, 7.96, 7.21, 7.19, 6.85, 4.94, 3.23.

IR (neat): 3115, 2929, 1644, 1559, 1510, 1428, 1222, 1153, 1027, 809, 751 cm^{-1}.

HRMS: (ESI) calcd for $C_{38}H_{42}FeN_7O$ $[M+H]^+$: 703.2489, found:703.4783.



(R)-N,N'-bis((4-methoxypyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(triflate), **6-OTf**. Black crystalline powder; (83% yield).

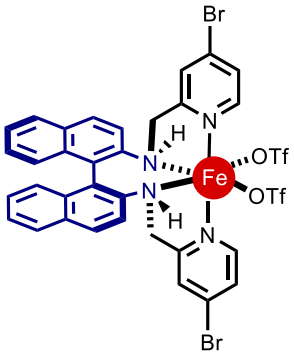
μ_{eff} (CD_3CN): 2.70μ_B.

UV (DCM) λ_{max}, nm: 347.

^1H NMR: (400 MHz, CD_3CN) δ 8.22, 7.91, 7.34, 7.14, 6.92, 4.81, 4.50, 4.04.

IR (neat): 2923, 2853, 1616, 1598, 1497, 1435, 1240, 1163, 812, 752 cm^{-1}.

HRMS: (ESI) calcd for $C_{32}H_{30}FeN_4O_3$ $[M+H]^+$: 575.1745, found:575.2607.



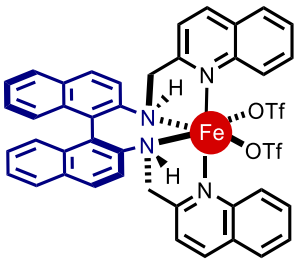
(R)-N,N'-bis((4-bromopyridin-2-yl)methyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(triflate), **7-OTf**. Blue powder; (85% yield).

μ_{eff} (CD_3CN): 4.47μ_B.

UV (DCM) λ_{max}, nm: 363.

^{1}H NMR: (400 MHz, CD_3CN) δ 12.56, 9.68, 8.05, 7.91, 7.51, 7.11, 7.03, 6.86, 4.09.

HRMS: (ESI) calcd for $C_{33}H_{25}Br_2F_3FeN_4O_3S$ $[M+H]^+$: 827.9316, found:827.4556.



(R)-N,N'-bis(quinolin-2-ylmethyl)-[1,1'-binaphthalene]-2,2'-diamine iron(II) bis(triflate), **L9-OTf**. Brown-orange crystalline powder; (79% yield).

μ_{eff} (CD_3CN): 4.40μ_B.

UV (DCM) λ_{max}, nm: 352.

^{1}H NMR:(400 MHz, CD_3CN) δ 8.94, 8.85, 8.21, 8.11, 7.99, 7.75, 7.49, 7.41, 7.19, 6.90, 6.82, 4.96.

IR (neat): 3378, 1596, 1509, 1429, 1386, 1223, 1165, 1026, 813, 751 cm^{-1}.

HRMS: (ESI) calcd for $C_{44}H_{38}FeN_6O$ $[M+OH_2]^+$: 722.2456, found:722.4336.

A1.3 Supplementary Figures

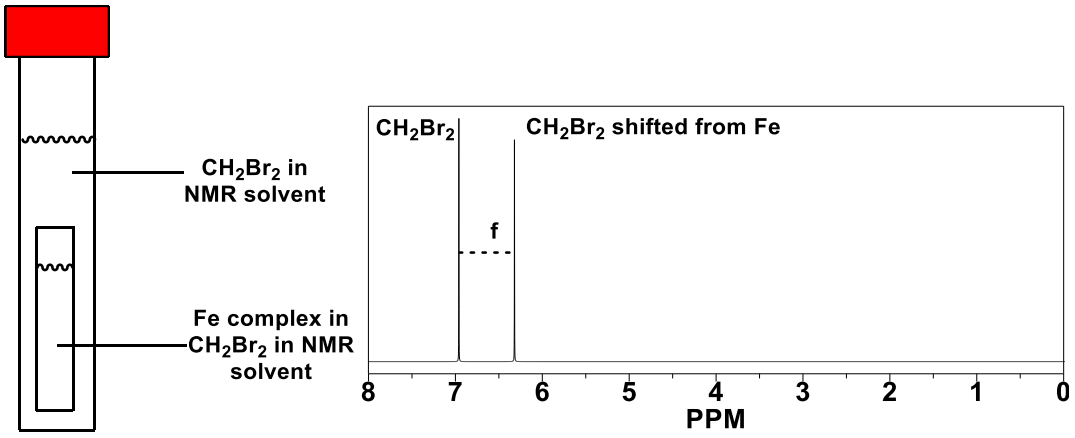


Figure A1. Experimental setup for an Evan's method NMR experiment to determine the magnetic moment of a paramagnetic species based on the peak separation, Δf.

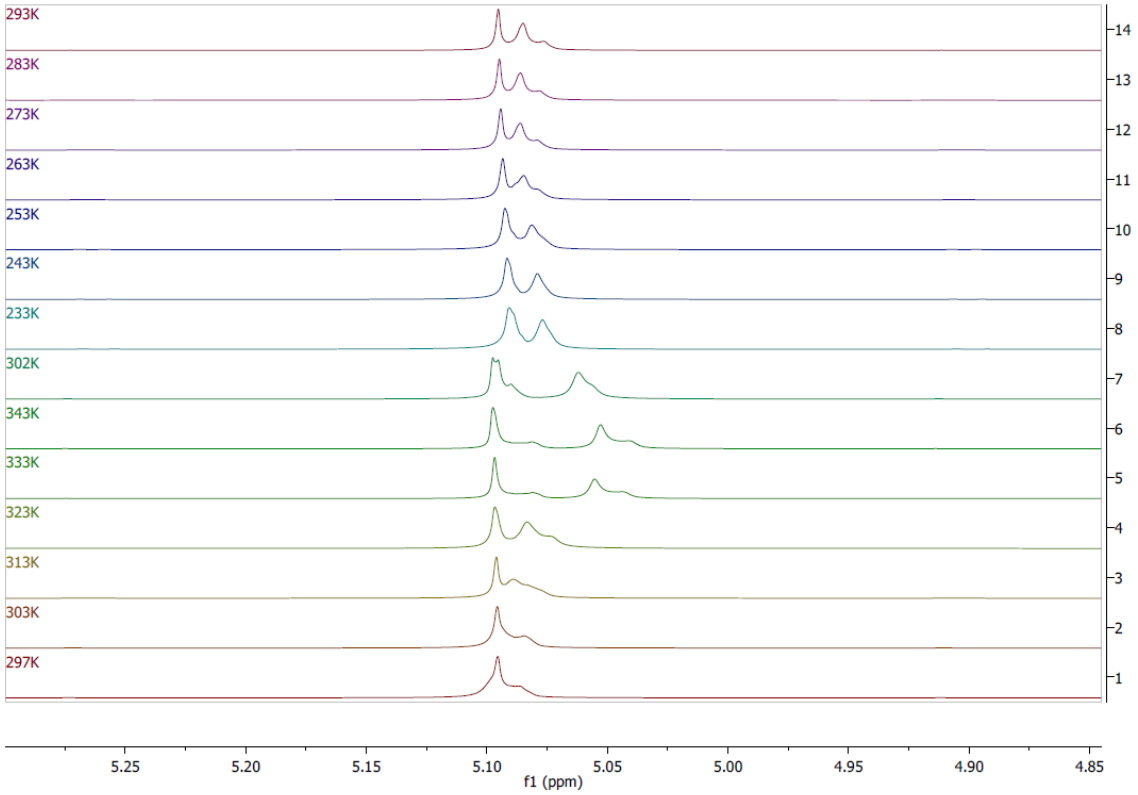


Figure A2. Variable temperature ^{1}H NMR of compound **1-OTf** in CD_3CN at temperatures -40°C to 70 °C. The CH_2Br_2 peak is shifted from the unpaired electrons in compound **1-OTf** with an increasing spin as the temperature increases. Compound **1-OTf** retains the

increased spin state at room temperature. When cooled to -40 °C, the spin state of compound **1-OTf** decreases again.

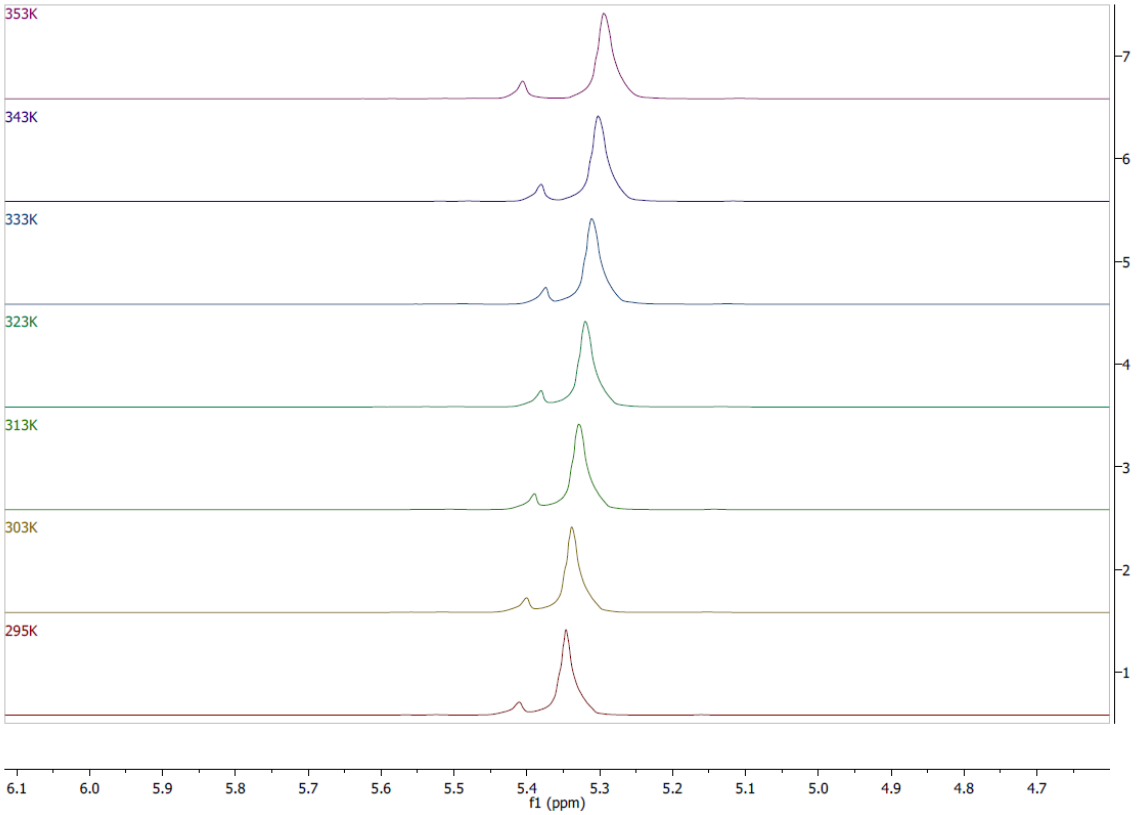


Figure A3. Variable temperature ^{1}H NMR of compound **1-OTf** in d_6-DMSO at temperatures from 23°C to 80°C. The CH_2Br_2 peak is shifted from the unpaired electrons in compound **1-OTf** with an increasing spin as the temperature increases. Compound **1-OTf** retains the increased spin state even at room temperature.

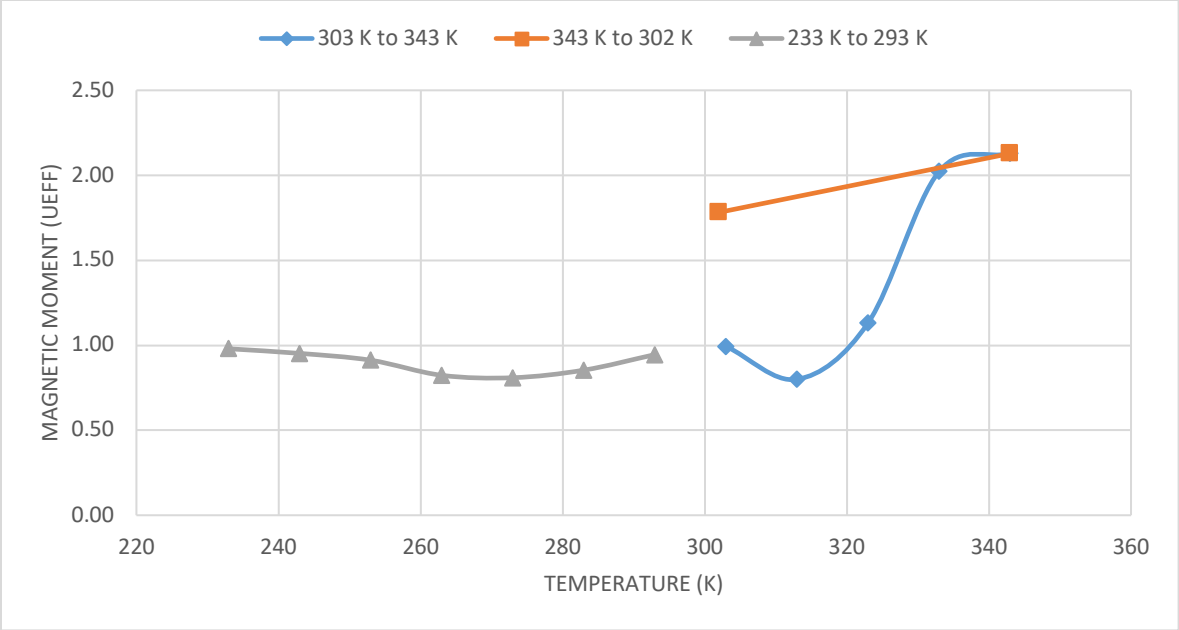


Figure A4. Magnetic moment determined from variable temperature ^{1}H NMR of compound **1-OTf** in CD_3CN at temperatures from 233 K to 343 K (-40°C to 70°C). The magnetic moment steadily increases from 0.99 to 2.13 as the temperature increases.

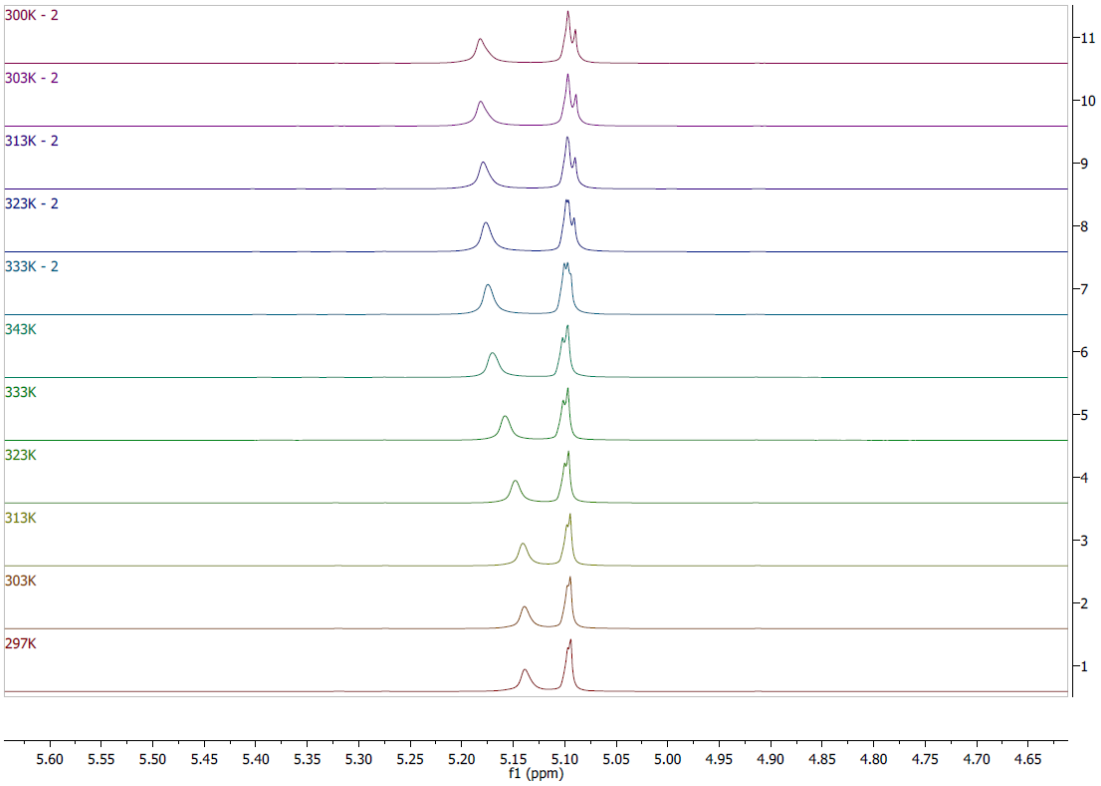


Figure A5. Variable temperature ^{1}H NMR of compound **1-SbF$_6$** in CD_3CN at temperatures from 25°C to 70°C. The CH_2Br_2 peak is shifted from the unpaired electrons in compound

1-SbF$_6$ with an increasing spin as the temperature increases. Compound **1-SbF$_6$** retains the increased spin state even at room temperature.

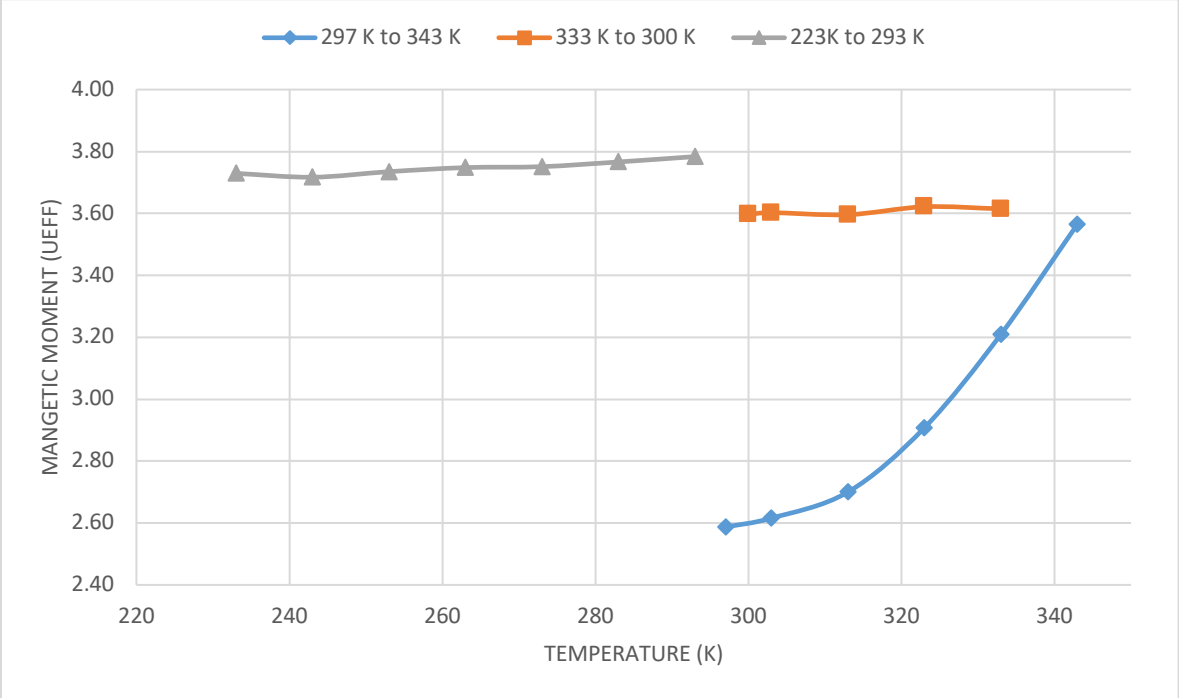


Figure A6. Magnetic moment determined from variable temperature ^{1}H NMR of compound **1-SbF$_6$** in CD_3CN at temperatures from 233 K to 343 K (-40°C to 70°C). The magnetic moment steadily increases from 2.59 to 3.60 as the temperature increases. The magnetic moment remains at 3.60 even at low temperature.

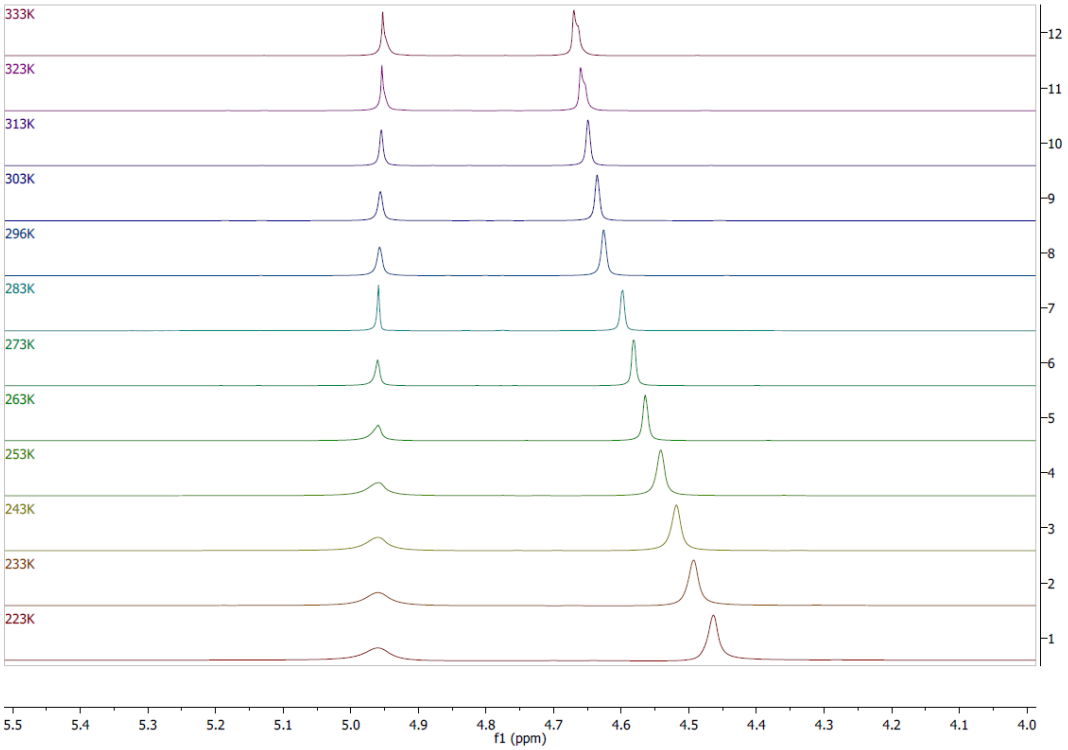


Figure A7. Variable temperature ^{1}H NMR of compound **4-OTf** in $CDCl_3$ at temperatures from -50°C to 60°C. The CH_2Br_2 peak is shifted from the unpaired electrons in compound **4-OTf** with a decreasing spin as the temperature increases. Compound **4-OTf** returns to the original spin state at room temperature.

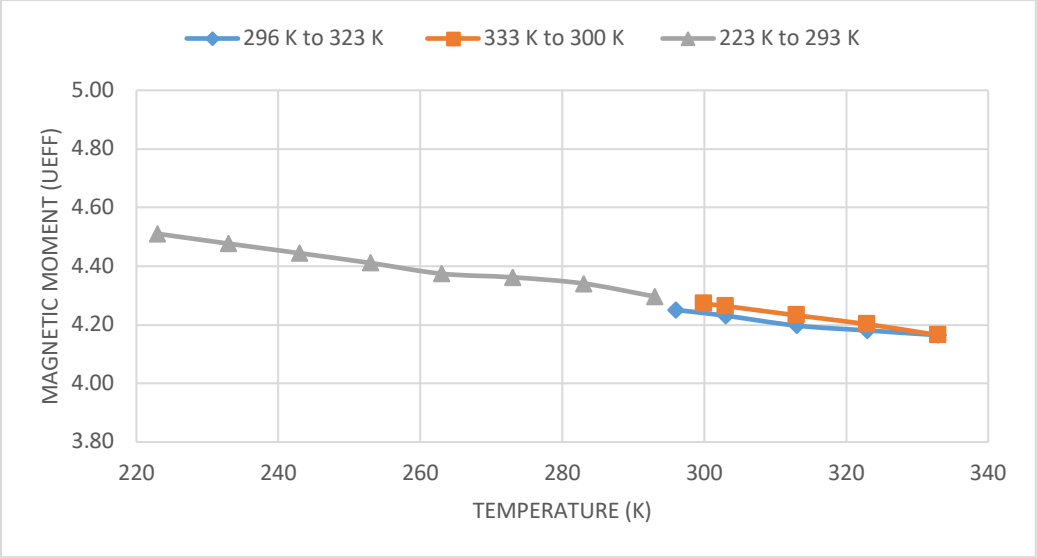


Figure A8. Magnetic moment determined from variable temperature ^{1}H NMR of compound **4-OTf** in $CDCl_3$ at temperatures from -50°C to 60°C. The magnetic moment steadily decreases from 4.51 to 4.16 as the temperature increases.

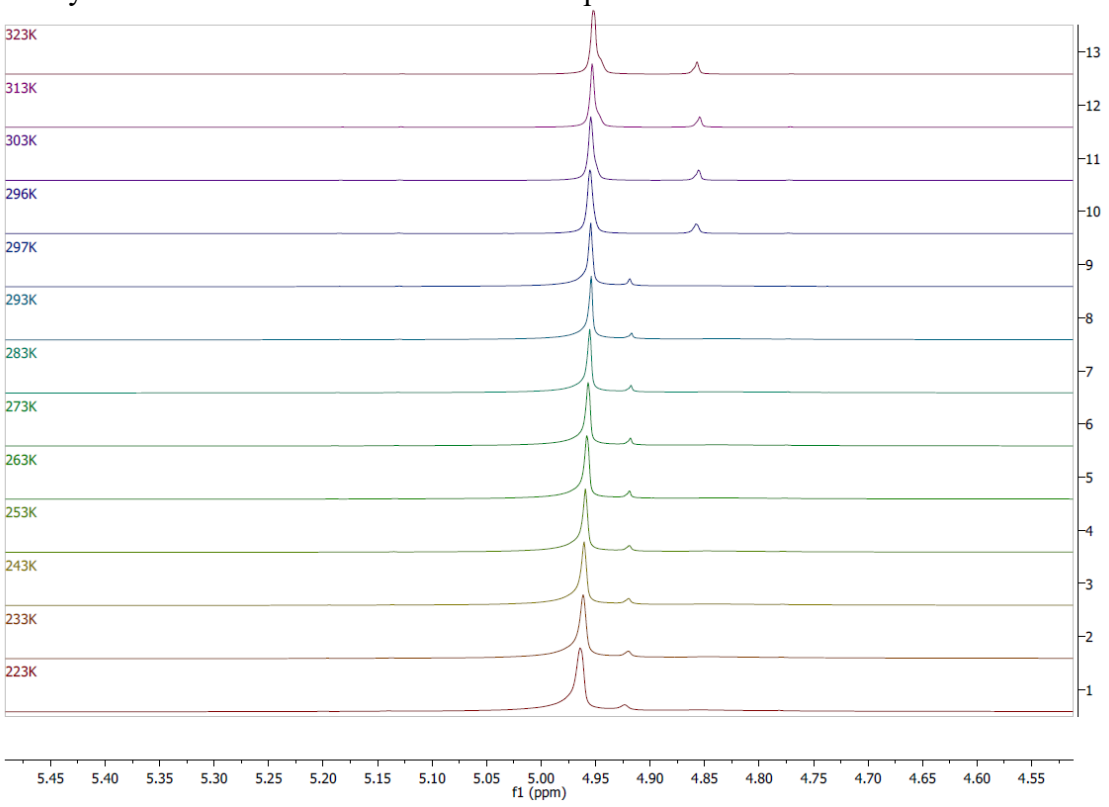


Figure A9. Variable temperature ^{1}H NMR of compound **4-SbF$_6$** in $CDCl_3$ at temperatures from -50°C to 50°C. The CH_2Br_2 peak is shifted from the unpaired electrons in compound **4-SbF$_6$** with an increasing spin as the temperature increases. Compound **4-SbF$_6$** returns to the original spin state at room temperature.

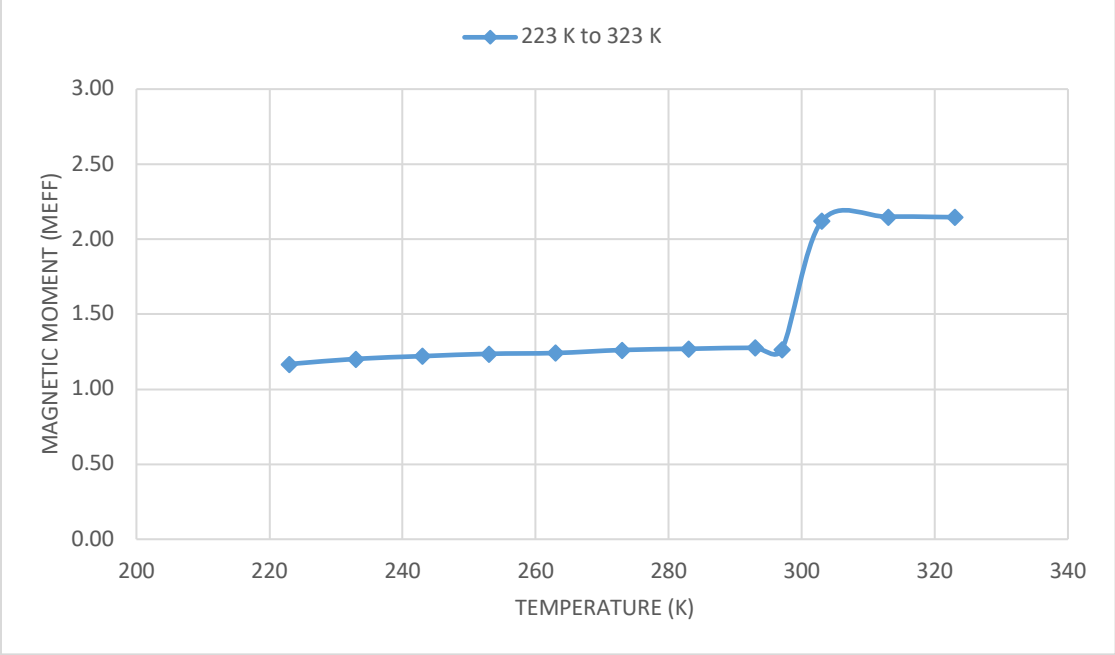
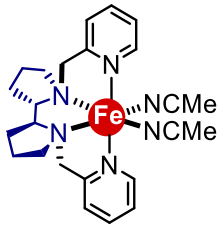


Figure A10. Magnetic moment determined from variable temperature ^{1}H NMR of compound **4-SbF_6** in $CDCl_3$ at temperatures from -50°C to 50°C. The magnetic moment begins at 1.17 in the range from -50 °C to 25°C. It increases to 2.12 at 30 °C and remains here as the temperature increases.



A

	cis-	*cis-*	*trans*
S=0	2.0	5.3	12.8
S=3/2	9.4	8.4	11.1
S=5/2	**0.0**	-1.3	1.2

(**White**. *Science*. **2007**, *318*, 783.)

uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	0.0	3.1	10.5
S=3/2	19.1	18.4	21.6
S=5/2	**21.6**	20.5	21.4

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	13.3	3.1	11.2
S=3/2	17.2	8.0	15.7
S=5/2	**0.0**	-0.6	-12.2

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

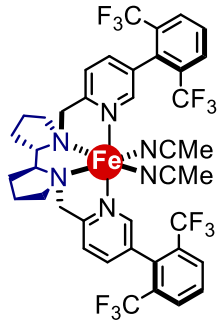
	cis-	*cis-*	*trans*
S=0	0.0	3.4	11.3
S=3/2	14.4	19.3	21.9
S=5/2	**2.4**	1.7	3.0

uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	9.1	3.2	11.2
S=3/2	16.6	8.8	11.7
S=5/2	**0.0**	-2.0	-0.9

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A11. Relative free energy values of training compound **A** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.



B

	cis-	*cis-*	*trans*
S=0	18.3	3.1	10.2
S=3/2	17.3	12.2	22.1
S=5/2	**0.0**	-1.2	-0.1

(**White.** *JACS.* **2013**, *135,* 14052.)
uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	0.0	2.3	11.6
S=3/2	18.9	18.2	22.3
S=5/2	18.3	20.1	21.6

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	12.3	14.1	25.1
S=3/2	16.2	20.2	23.8
S=5/2	-2.3	0.0	4.7

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

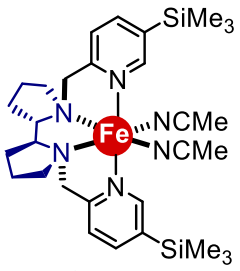
	cis-	*cis-*	*trans*
S=0	-1.5	0.7	11.7
S=3/2	12.8	18.0	17.7
S=5/2	-2.0	0.0	2.3

uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	-4.7	-2.1	8.6
S=3/2	7.0	10.9	16.5
S=5/2	-9.9	0.0	3.4

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A12. Relative free energy values of training compound **B** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.



C

	cis-	*cis-*	*trans*
S=0	6.8	9.4	17.5
S=3/2	14.1	12.7	21.4
S=5/2	0.0	3.2	5.0

(**Costas.** *ACIE.* **2016,** *55*, 5776)
uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	0.0	2.2	11.6
S=3/2	18.9	18.2	22.3
S=5/2	**18.3**	20.1	21.6

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	12.3	14.1	25.1
S=3/2	16.2	20.2	23.8
S=5/2	-2.3	0.0	4.7

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

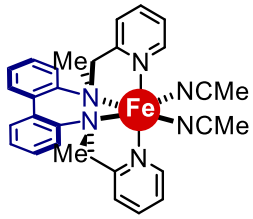
	cis-	*cis-*	*trans*
S=0	-1.5	0.7	11.7
S=3/2	12.8	18.0	17.7
S=5/2	**-2.0**	0.0	2.3

uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	2.4	4.1	16.3
S=3/2	9.8	11.2	18.4
S=5/2	**-9.7**	0.0	3.1

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A13. Relative free energy values of training compound **C** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.



D-Me

	cis-	cis-	trans
S=0	18.8	20.2	23.1
S=3/2	8.0	14.0	21.6
S=5/2	0.0	2.5	11.6

(**Britovsek**. *Dalton Trans.* **2006**,1399.)
uB3LYP/6-31G(d)-gas

	cis-	cis-	trans
S=0	0.0	1.3	46.2
S=3/2	1.4	8.0	38.8
S=5/2	5.5	8.6	16.6

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	cis-	trans
S=0	22.7	22.8	64.6
S=3/2	13.8	20.1	44.7
S=5/2	0.0	-1.7	6.1

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

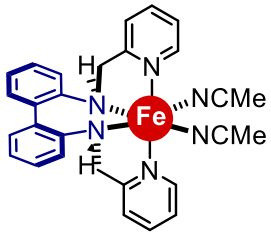
	cis-	cis-	trans
S=0	8.8	8.2	49.8
S=3/2	11.5	17.5	40.7
S=5/2	2.8	0.0	8.1

uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	cis-	trans
S=0	20.0	20.0	52.3
S=3/2	13.2	19.0	45.9
S=5/2	0.0	6.8	15.7

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A14. Relative free energy values of training compound **D-Me** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.



D-H

	cis-	*cis-*	*trans*
S=0	12.0	8.3	12.0
S=3/2	16.8	14.7	16.8
S=5/2	0.0	-0.1	0

uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	0.9	0.0	4.8
S=3/2	8.1	15.9	15.9
S=5/2	7.8	14.8	14.1

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	20.7	18.9	25.2
S=3/2	21.0	20.1	24.6
S=5/2	4.8	0.0	2.1

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

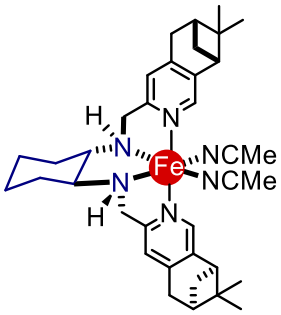
	cis-	*cis-*	*trans*
S=0	5.9	4.5	10.6
S=3/2	22.3	14.9	6.8
S=5/2	9.8	0.4	0.0

uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	17.9	16.7	22.8
S=3/2	18.3	21.7	25.3
S=5/2	4.2	0.0	9.2

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A15. Relative free energy values of training compound **D-H** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.



E-H

	cis-	*cis-*	*trans*
S=0	6.2	7.4	26.3
S=3/2	13.5	15.1	29.5
S=5/2	0.0	5.9	8.9

(**Costas.** *ACIE.* **2009,** *48*, 5720)
uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	-1.1	0.0	18.5
S=3/2	-4.2	9.1	28.2
S=5/2	4.8	22.1	23.6

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	10.1	12.7	30.0
S=3/2	17.0	15.6	28.3
S=5/2	-7.4	0.0	0.1

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

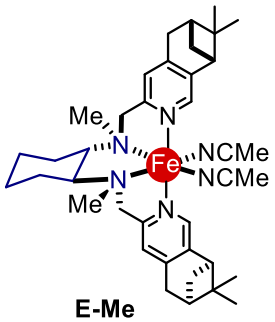
	cis-	*cis-*	*trans*
S=0	-1.1	0.0	19.7
S=3/2	16.3	13.5	23.6
S=5/2	-2.6	8.2	2.8

uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	9.0	2.4	30.2
S=3/2	16.1	9.0	30.5
S=5/2	3.6	0.0	10.9

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A16. Relative free energy values of training compound **E-H** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.



E-Me

	cis-	*cis-*	*trans*
S=0	7.2	11.5	36.2
S=3/2	14.1	18.4	16.7
S=5/2	0.0	3.7	4.8

(**Costas.** *ACIE.* **2009,** *48*, 5720)
uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	0.0	-6.3	27.9
S=3/2	18.2	11.0	21.5
S=5/2	17.3	9.9	20.3

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	11.1	17.2	40.0
S=3/2	17.0	19.6	21.8
S=5/2	-7.3	0.0	2.7

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

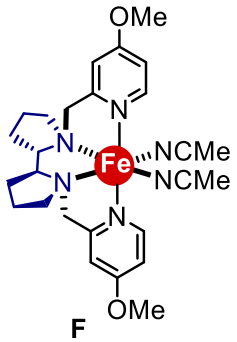
	cis-	*cis-*	*trans*
S=0	1.4	12.6	30.8
S=3/2	18.0	24.7	24.4
S=5/2	0.0	10.5	8.7

uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	10.5	6.7	40.7
S=3/2	17.1	12.8	23.8
S=5/2	4.6	0.0	11.8

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A17. Relative free energy values of training compound **E-Me** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.



F

	cis-	*cis-*	*trans*
S=0	7.2	11.5	20.2
S=3/2	14.0	13.7	16.6
S=5/2	0.0	3.4	5.7

(**Costas.** *JACS.* **2013,** *135,* 14871)
uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	0.0	3.4	12.4
S=3/2	18.1	17.8	22.1
S=5/2	17.0	17.9	19.6

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	16.9	3.4	30.0
S=3/2	20.2	31.7	32.0
S=5/2	0.0	9.3	6.7

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

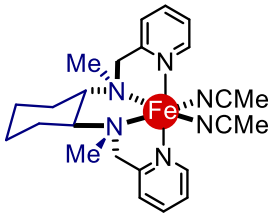
	cis-	*cis-*	*trans*
S=0	0.0	3.7	13.2
S=3/2	13.6	23.6	24.6
S=5/2	2.6	11.8	0.6

uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	5.6	9.1	18.7
S=3/2	12.5	14.1	17.4
S=5/2	0.0	-0.9	3.6

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A18. Relative free energy values of training compound **F** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.



G

	cis-	*cis-*	*trans*
S=0	3.3	6.0	14.3
S=3/2	10.2	12.7	12.8
S=5/2	-4.0	0.0	0.7

(**Que**. *JACS*. **2001**, *123*, 6722.)
uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	-12.4	0.0	8.0
S=3/2	6.0	19.1	22.5
S=5/2	5.7	18.0	17.0

uPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	12.4	16.8	25.2
S=3/2	15.7	18.4	24.8
S=5/2	-3.8	0.1	0.0

uM06/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

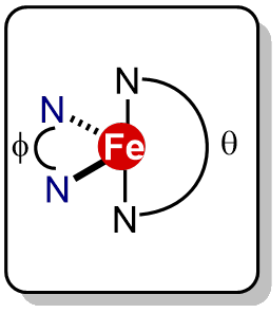
	cis-	*cis-*	*trans*
S=0	1.6	1.9	9.9
S=3/2	15.7	19.4	21.0
S=5/2	1.9	0.7	0.0

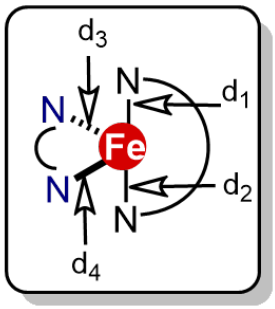
uM06L/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

	cis-	*cis-*	*trans*
S=0	-5.5	5.1	13.9
S=3/2	1.1	3.9	15.5
S=5/2	-10.9	0.4	0.0

uB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//uB3LYP/6-31G(d)-gas

Figure A19. Relative free energy values of training compound **G** in the cis-α (left), cis-β (middle), and trans (right) geometries and singlet, triplet, and quintet spin states. The compounds are optimized at the UB3LYP/6-31G(d)-gas level and free energies are refined by computing single point energy values using higher level methods. UM06L/6-311+G(d,p)-CPCM (dichloromethane)//UB3LYP/6-31G(d)-gas was identified as the best method of these four for correct prediction of experimental geometry and spin state.





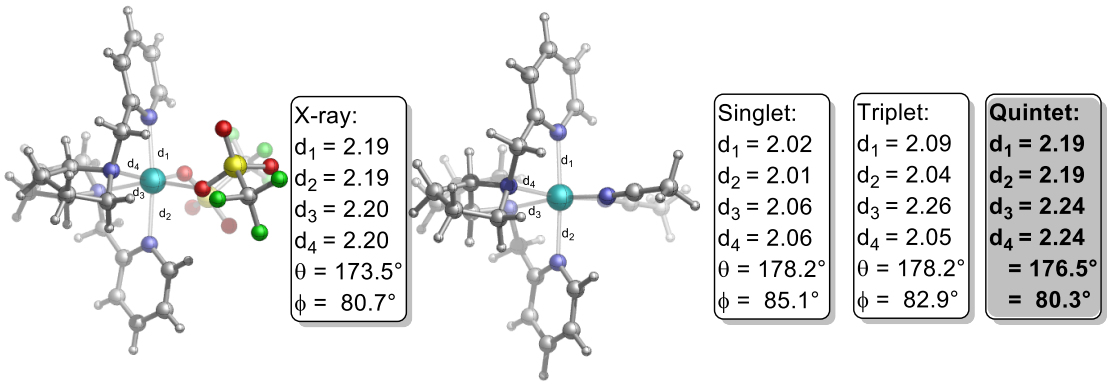


Figure A20. Experimental bond lengths (Å) and angles (°) from x-ray crystallography of compound **A** (left, triflate) compared to computed bond lengths and angles (right, acetonitrile) for the singlet, triplet, and quintet states. Based on this comparison, the experimental structure is in the quintet state.

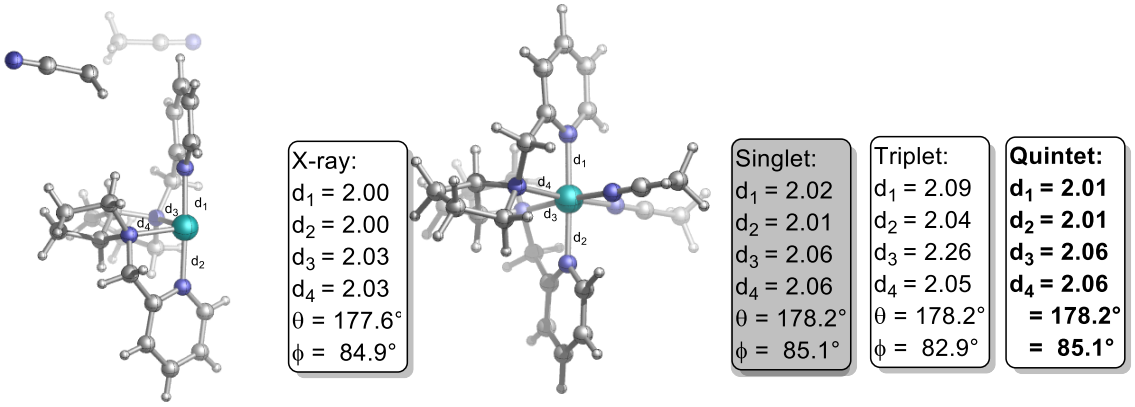


Figure A21. Experimental bond lengths (Å) and angles (°) from x-ray crystallography of compound **A** (left, acetonitrile) compared to computed bond lengths and angles (right, acetonitrile) for the singlet, triplet, and quintet states. Based on this comparison, the experimental structure is in the singlet state.

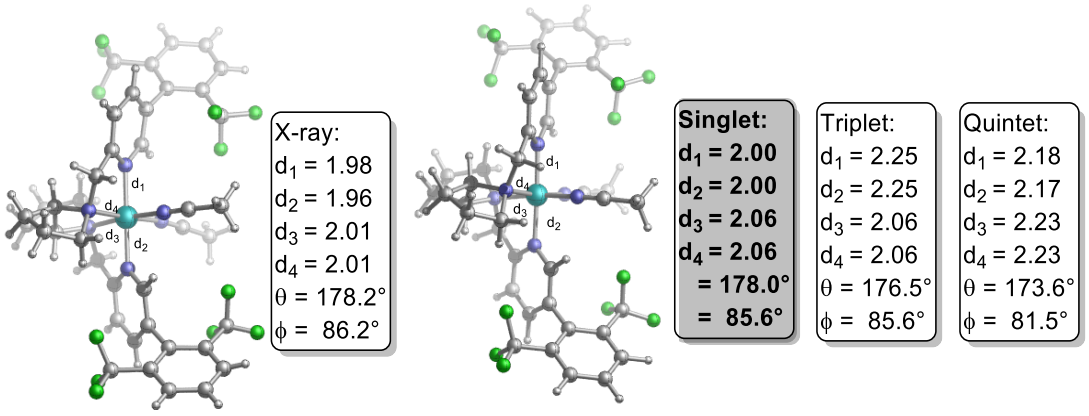


Figure A22. Experimental bond lengths (Å) and angles (°) from x-ray crystallography of compound **B** (left, acetonitrile) compared to computed bond lengths and angles (right, acetonitrile) for the singlet, triplet, and quintet states. Based on this comparison, the experimental structure is in the singlet state.

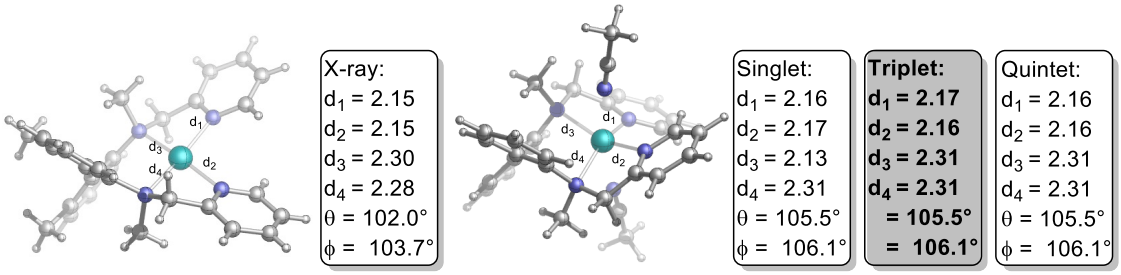


Figure A23. Experimental bond lengths (Å) and angles (°) from x-ray crystallography of compound **D-Me** (left) compared to computed bond lengths and angles (right, acetonitrile) for the singlet, triplet, and quintet states. Based on this comparison, the experimental structure is in the triplet state.

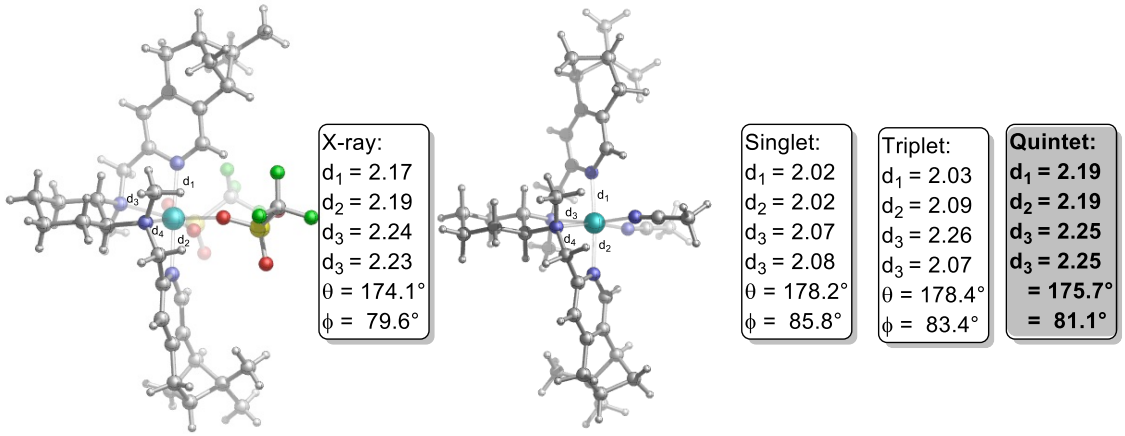


Figure A24. Experimental bond lengths (Å) and angles (°) from x-ray crystallography of compound **E-Me** (left, triflate) compared to computed bond lengths and angles (right, acetonitrile) for the singlet, triplet, and quintet states. Based on this comparison, the experimental structure is in the quintet state.

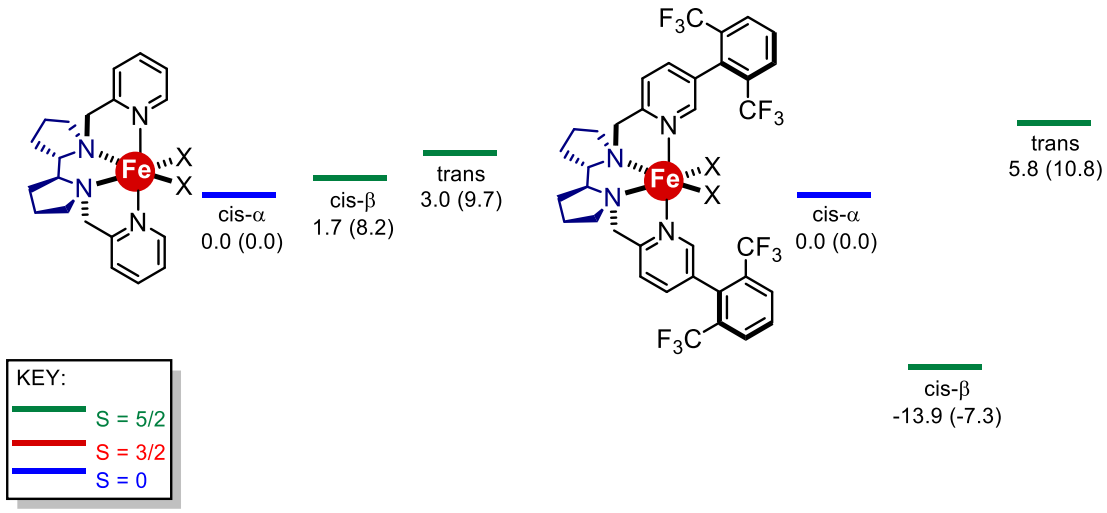


Figure A25. Relative free energies (enthalpies) for the cis-α, cis-β, and *trans* geometries computed for compound **A** (left) and compound **B** (right) at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level. The auxiliary ligand, X, is acetonitrile.

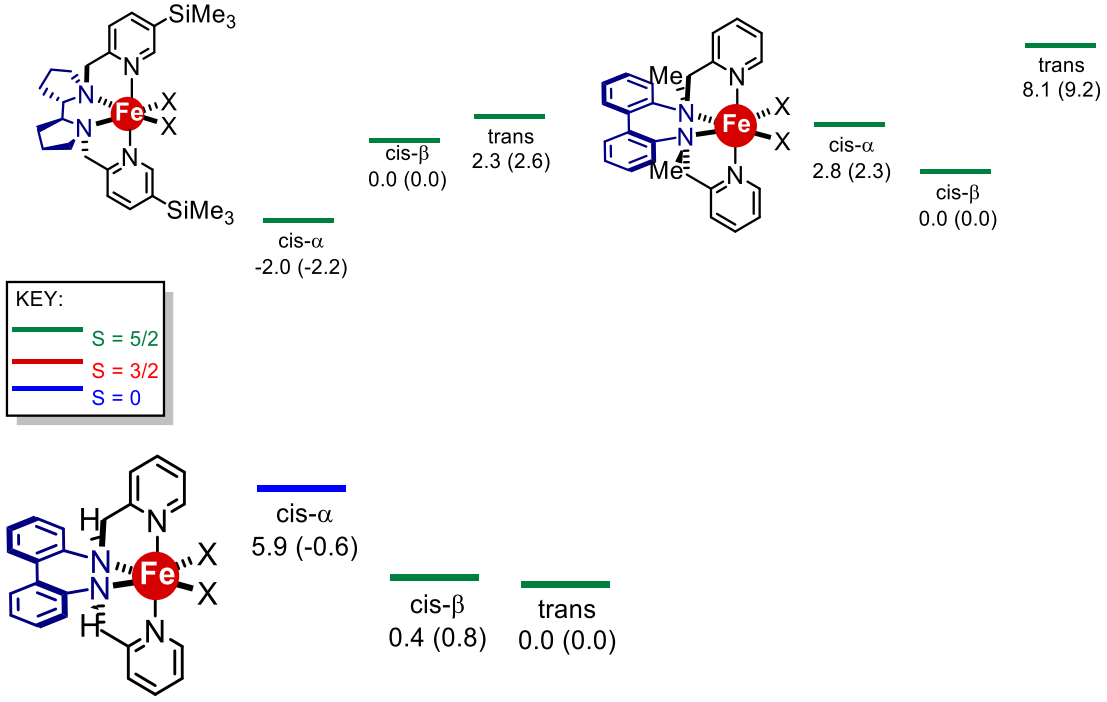


Figure A26. Relative free energies (enthalpies) for the cis-α, cis-β, and *trans* geometries computed for compound **C** (left), compound **D-Me** (right) and compound **D-H** (bottom) at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level. The auxiliary ligand, X, is acetonitrile.

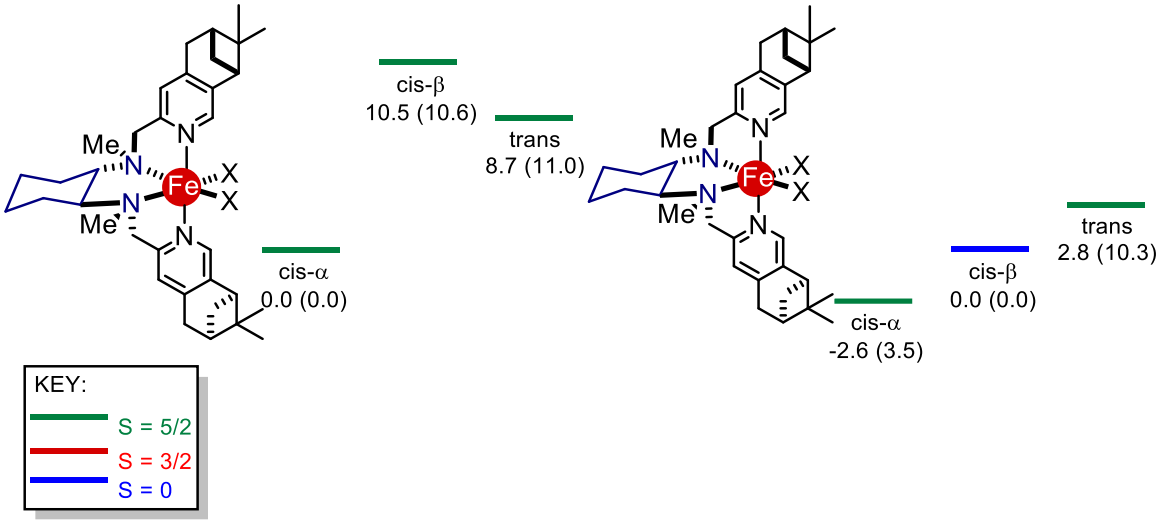


Figure A27. Relative free energies (enthalpies) for the cis-α, cis-β, and *trans* geometries computed for compound **E-Me** (left) and compound **E-H** (right) at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level. The auxiliary ligand, X, is acetonitrile.

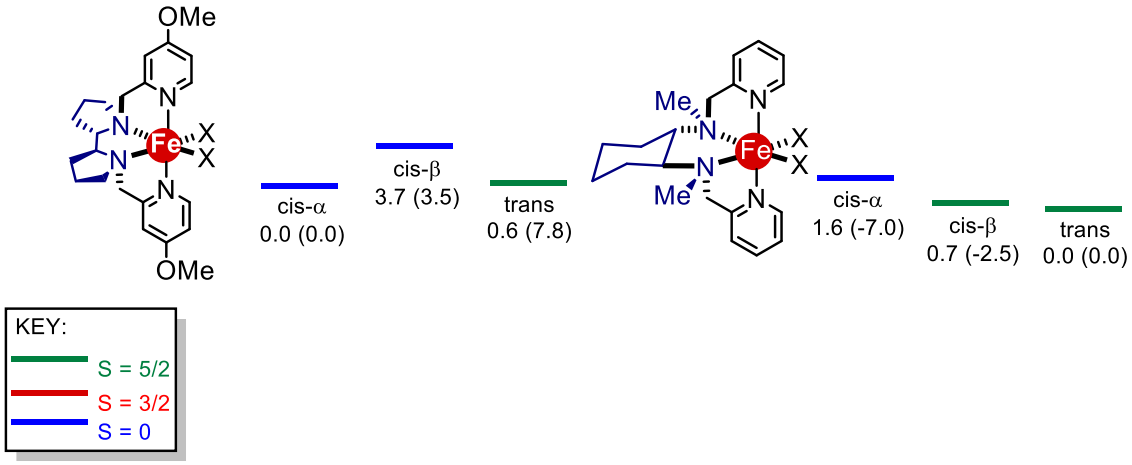


Figure A28. Relative free energies (enthalpies) for the cis-α, cis-β, and *trans* geometries computed for compound **F** (left) and compound **G** (right) at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level. The auxiliary ligand, X, is acetonitrile.

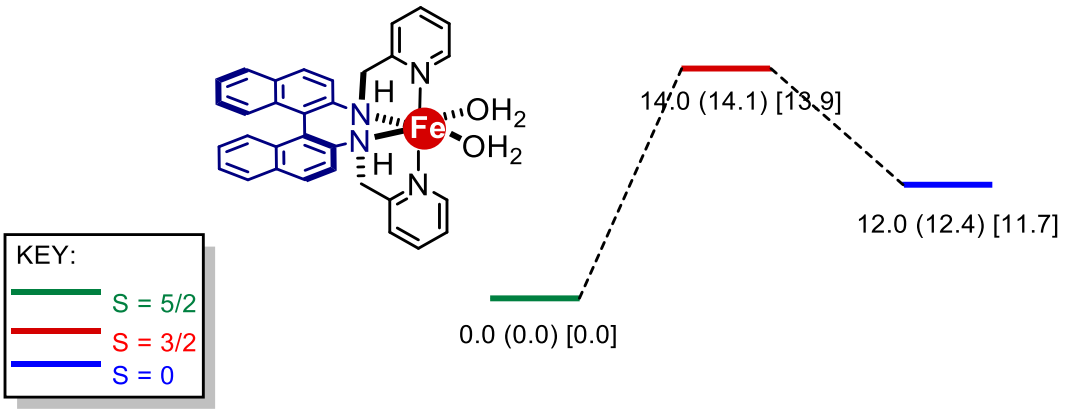
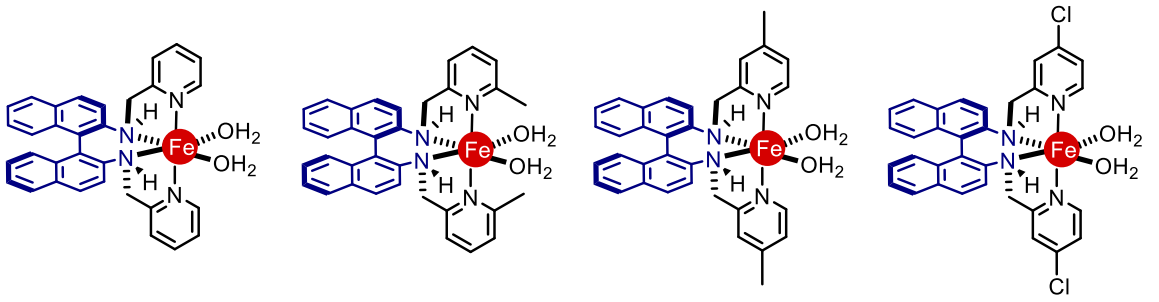


Figure A29. Relative free energies for the cis-a geometry of Complex **1-OH$_2$** computed at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level (outside parenthesis), UM06L/6-311+G(d,p)-CPCM(chloroform)//UB3LYP/6-31G(d)-gas level (parenthesis), and UM06L/6-311+G(d,p)-CPCM(acetonitrile)//UB3LYP/6-31G(d)-gas level (brackets).



Fe(L1)(OH$_2$)$_2$

	cis-	*cis-*	*trans*
S=0	12.0	12.2	16.8
S=3/2	14.0	14.3	14.8
S=5/2	0.0	-2.9	2.6

Fe(L2)(OH$_2$)$_2$

	cis-	*cis-*	*trans*
S=0	18.5	22.3	29.4
S=3/2	16.8	19.6	14.9
S=5/2	0.0	-0.7	1.9

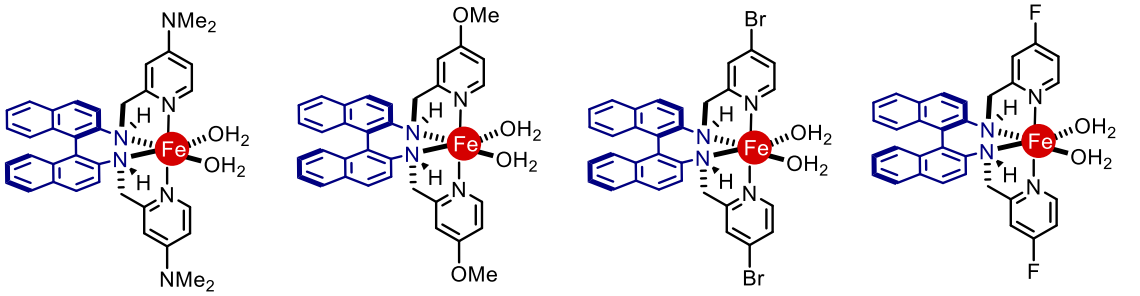
Fe(L3)(OH$_2$)$_2$

	cis-	*cis-*	*trans*
S=0	9.5	20.0	18.5
S=3/2	11.0	11.6	13.9
S=5/2	0.0	-6.2	-0.1

Fe(L4)(OH$_2$)$_2$

	cis-	*cis-*	*trans*
S=0	9.1	9.6	19.9
S=3/2	11.2	12.0	14.2
S=5/2	0.0	-5.7	0.6

Figure A30. Relative free energies for the cis-α (left), cis-β (middle), and trans (right) geometries of complexes **1-OH$_2$, 2-OH$_2$, 3-OH$_2$, and 4-OH$_2$** computed at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level.



Fe(L5)(OH$_2$)$_2$

	cis-	cis-	trans
S=0	14.7	14.0	23.3
S=3/2	16.7	14.0	15.6
S=5/2	0.0	-2.6	1.3

Fe(L6)(OH$_2$)$_2$

	cis-	cis-	trans
S=0	11.8	11.4	21.1
S=3/2	13.4	12.7	14.4
S=5/2	0.0	-4.2	-0.2

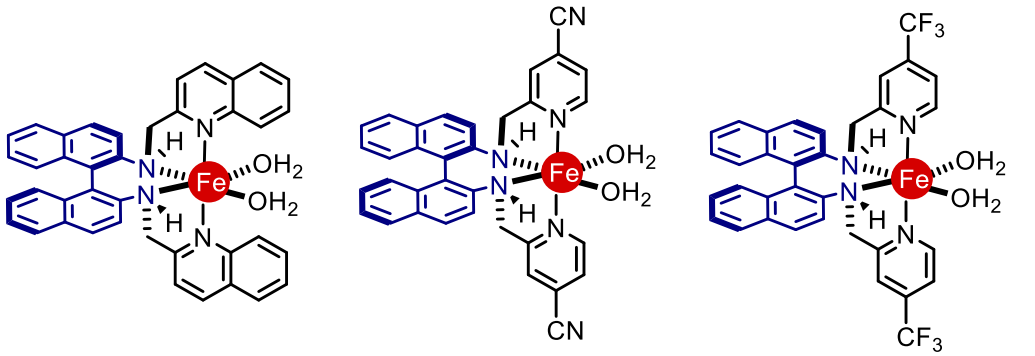
Fe(L7)(OH$_2$)$_2$

	cis-	cis-	trans
S=0	12.6	12.5	23.2
S=3/2	14.4	15.3	17.1
S=5/2	0.0	-2.9	3.6

Fe(L8)(OH$_2$)$_2$

	cis-	cis-	trans
S=0	13.0	13.2	23.5
S=3/2	14.8	15.7	17.6
S=5/2	0.0	-2.7	3.6

Figure A31. Relative free energies for the cis-α (left), cis-β (middle), and trans (right) geometries of complexes **5-OH$_2$, 6-OH$_2$, 7-OH$_2$, and 8-OH$_2$** computed at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level.



Fe(L9)(OH$_2$)$_2$

	cis-	cis-	trans
S=0	21.0	19.7	24.5
S=3/2	12.6	18.2	13.7
S=5/2	0.0	-2.4	-0.5

Fe(L-CN)(OH$_2$)$_2$

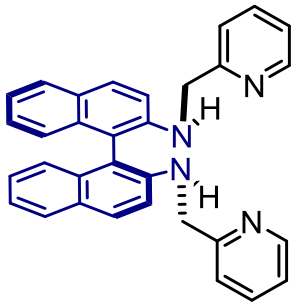
	cis-	cis-	trans
S=0	19.7	12.3	23.0
S=3/2	11.1	15.7	18.1
S=5/2	0.0	-2.5	4.3

Fe(L-CF$_3$)(OH$_2$)$_2$

	cis-	cis-	trans
S=0	19.9	11.8	23.6
S=3/2	11.7	15.8	17.8
S=5/2	0.0	-3.3	3.5

Figure A32. Relative free energies for the cis-α (left), cis-β (middle), and trans (right) geometries of complexes **9-OH$_2$, CN-OH$_2$ and CF$_3$-OH$_2$** computed at the UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas level.

A1.4 NMR Spectra



Compound **L1**

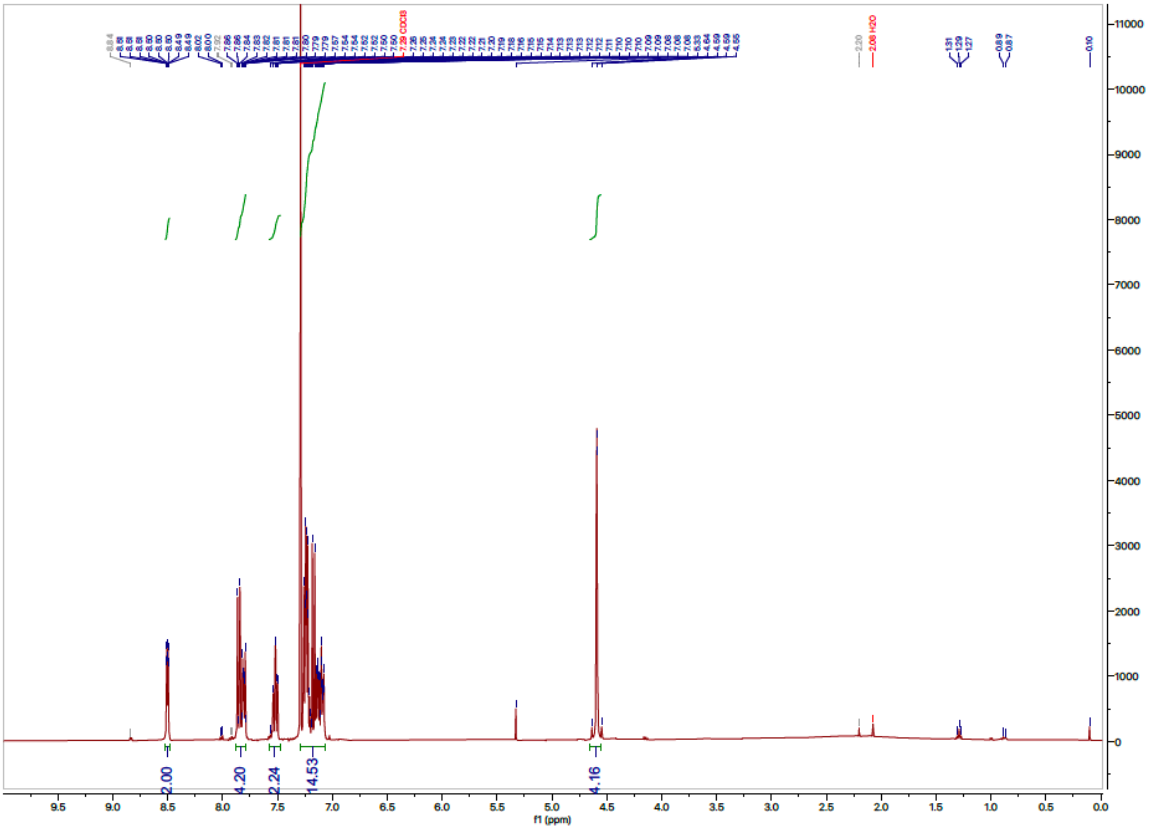
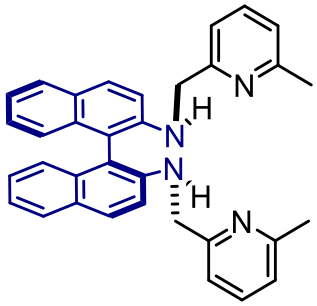


Figure A33. ^{1}H NMR ($CDCl_3$) of compound **L1.**



Compound **L2**

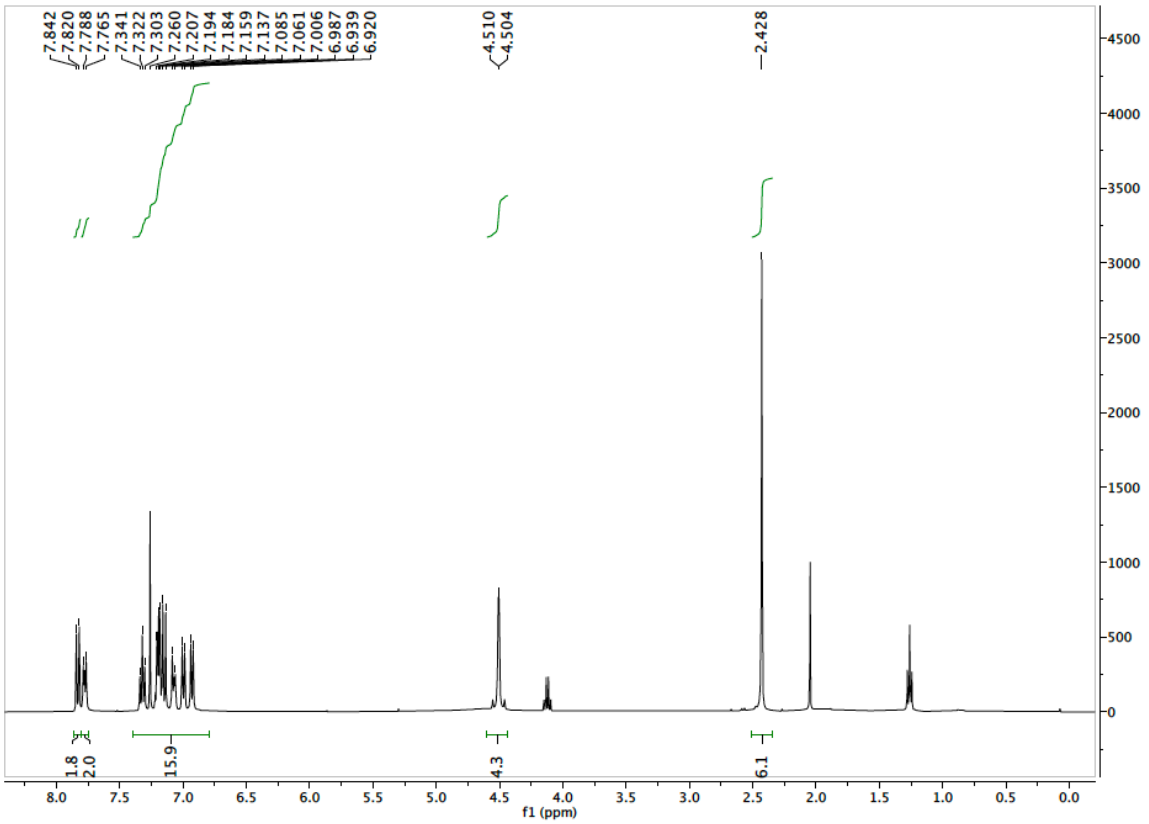
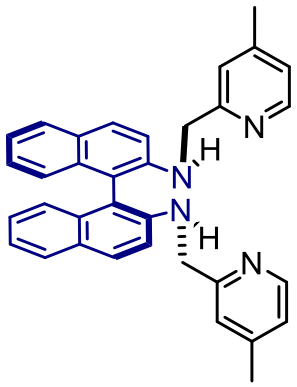


Figure A34. ^{1}H NMR ($CDCl_3$) of compound **L2**.



Compound **L3**

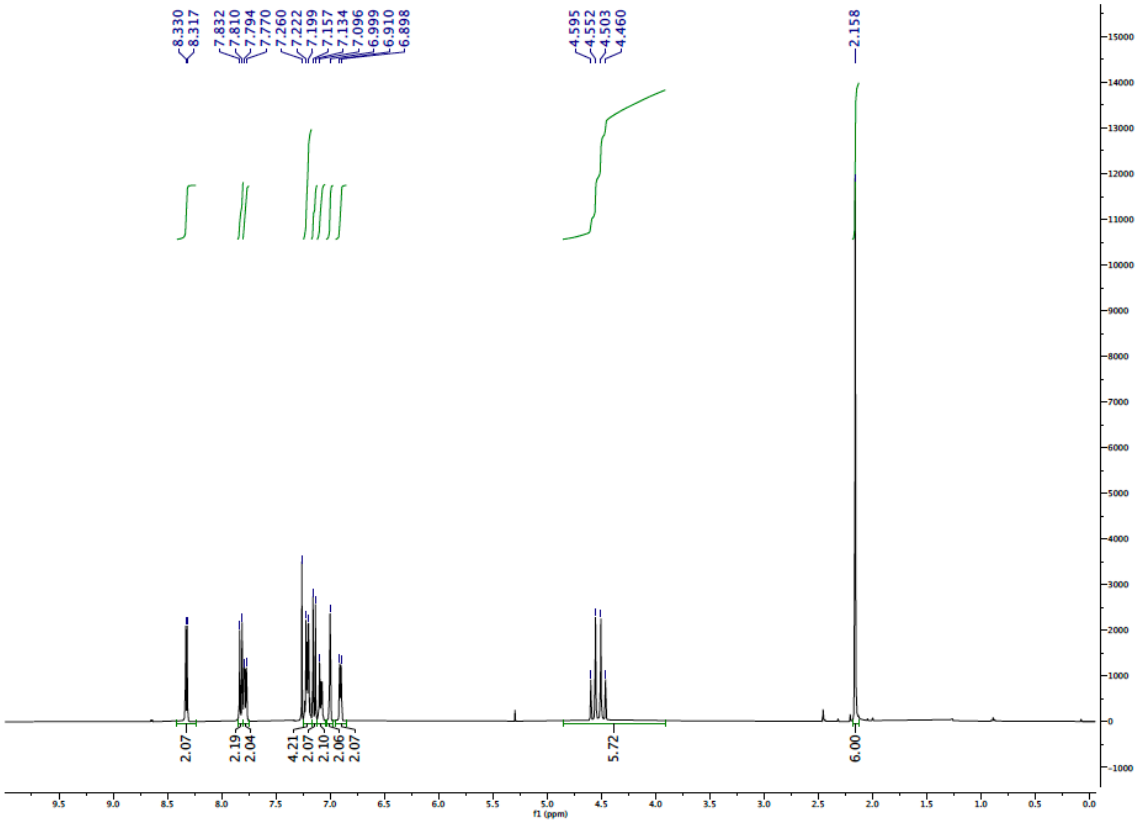
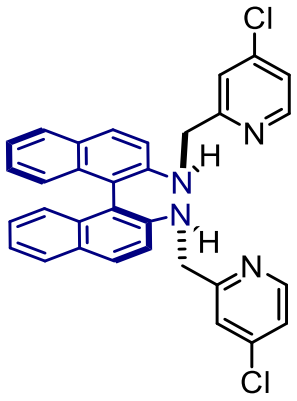


Figure A35. ^{1}H NMR ($CDCl_3$) of compound **L3**.



Compound **L4**

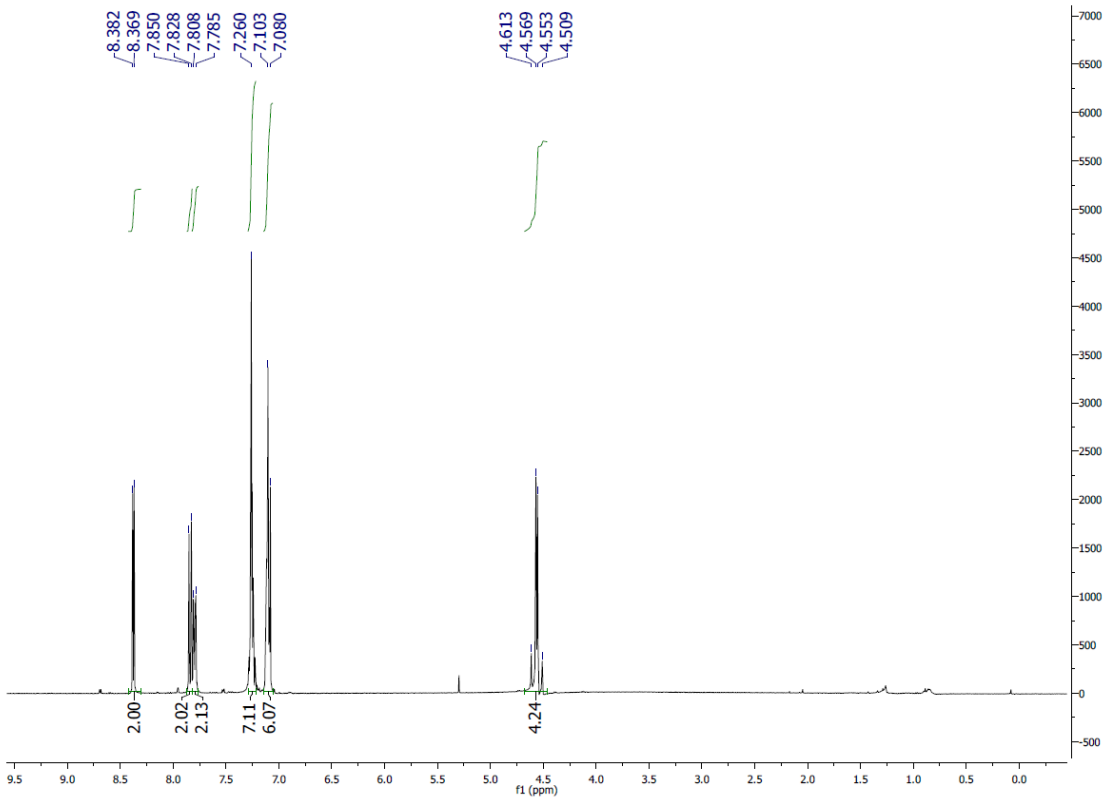
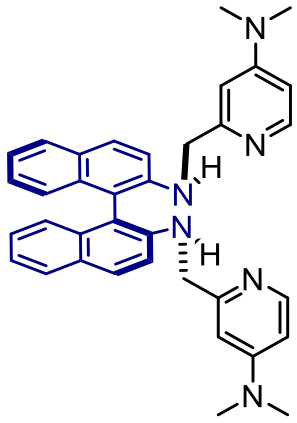


Figure A36. ^{1}H NMR ($CDCl_3$) of compound **L4**.



Compound **L5**

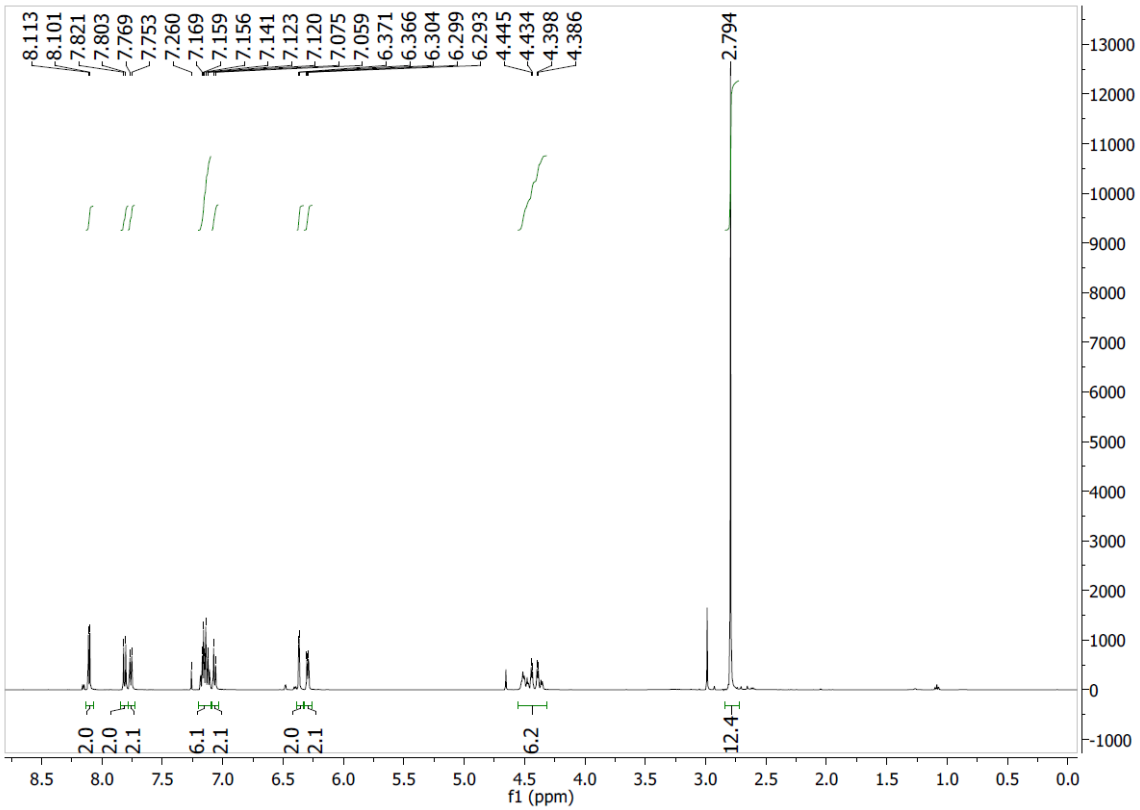


Figure A37. ^{1}H NMR ($CDCl_3$) of compound **L5**.

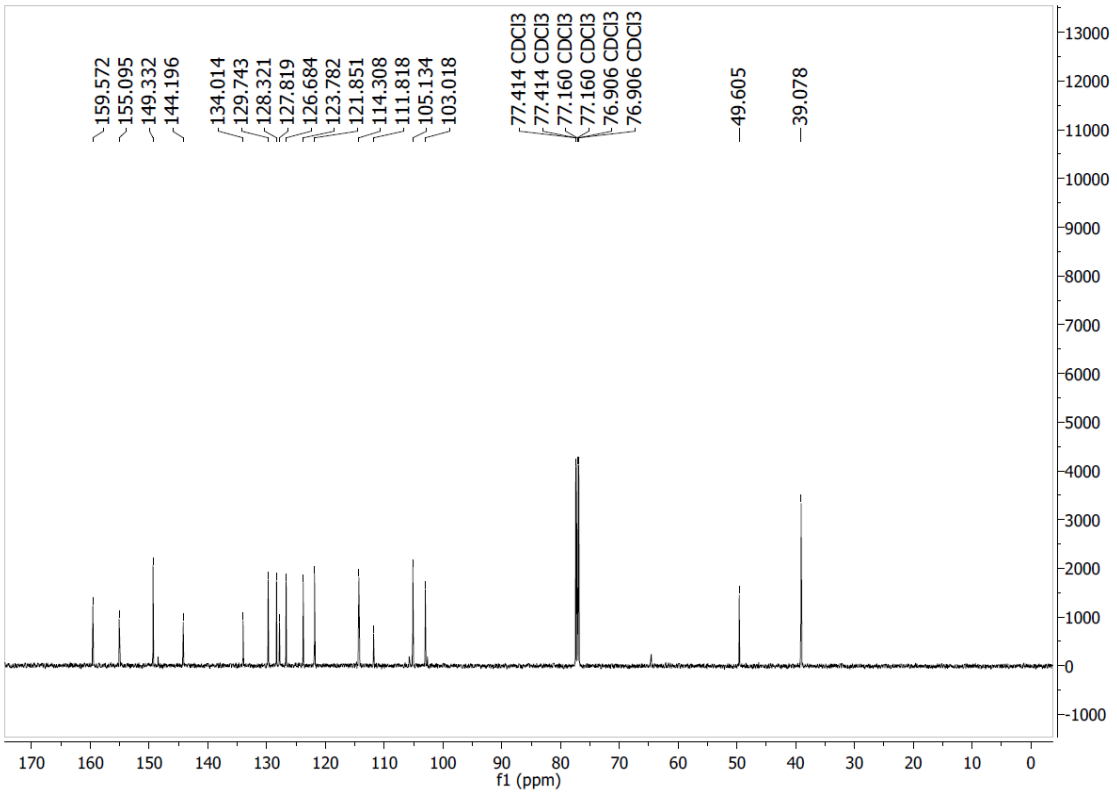
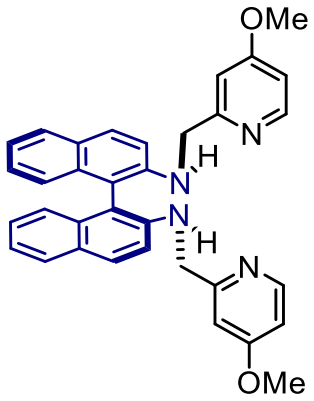


Figure A38. ^{13}C NMR ($CDCl_3$) of compound **L5**.



Compound **L6**

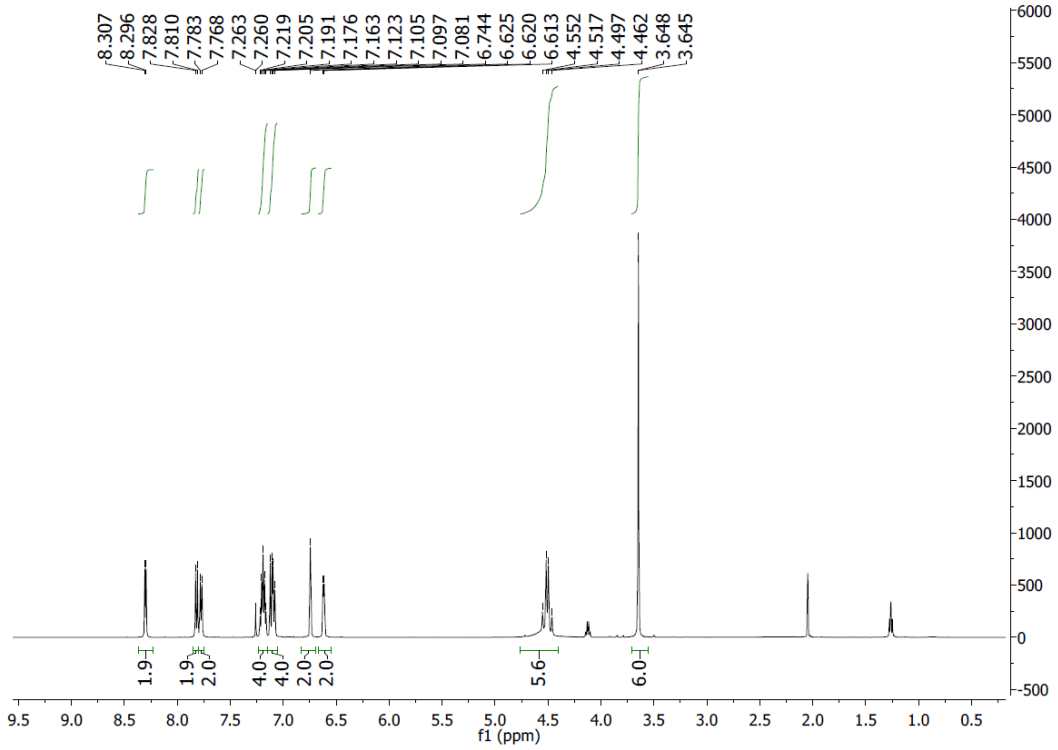


Figure A39. ^{1}H NMR ($CDCl_3$) of compound **L6**.

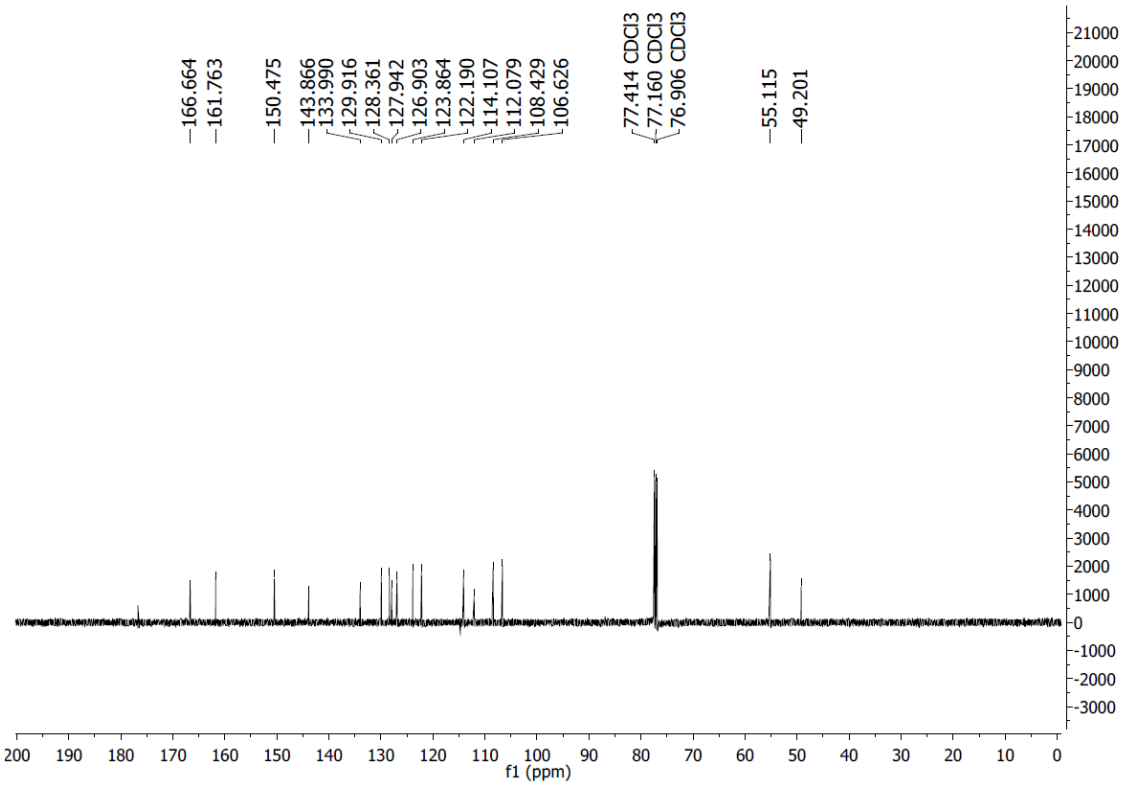
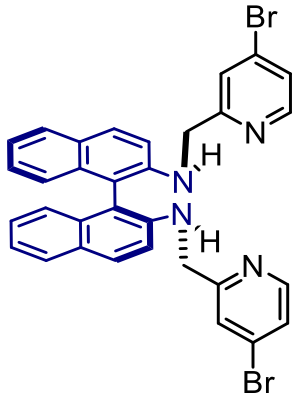


Figure A40. ^{13}C NMR ($CDCl_3$) of compound **L6**.



Compound **L7**

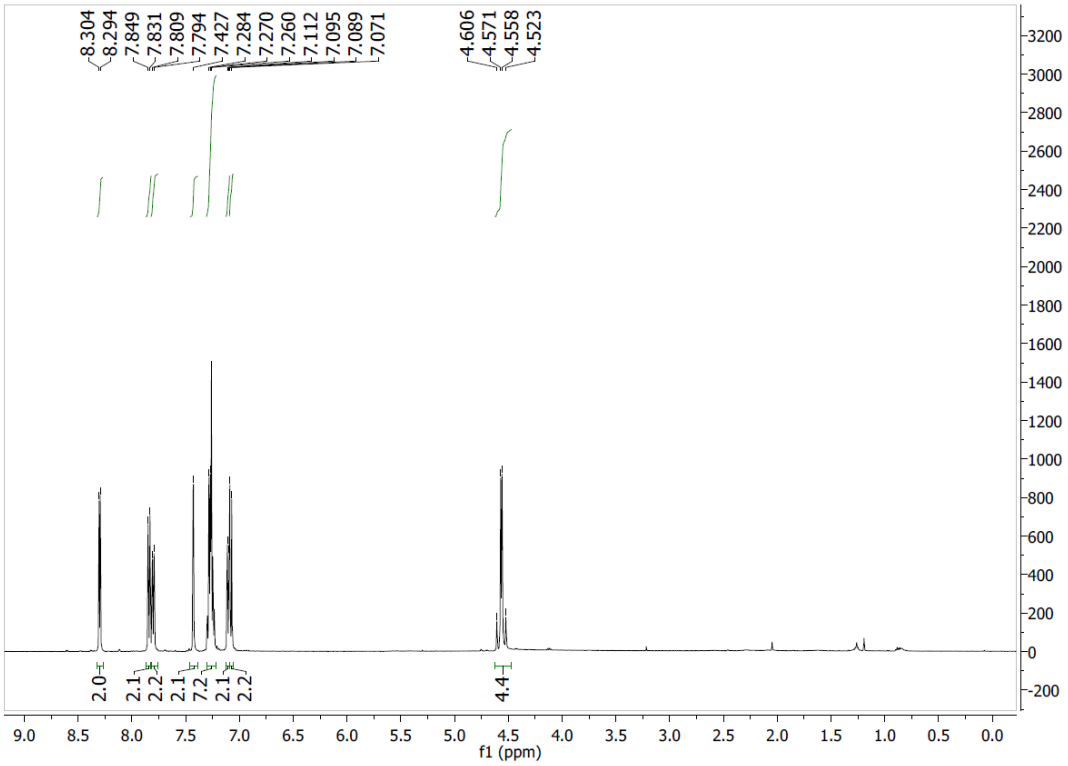


Figure A41. ^{1}H NMR ($CDCl_3$) of compound **L7**.

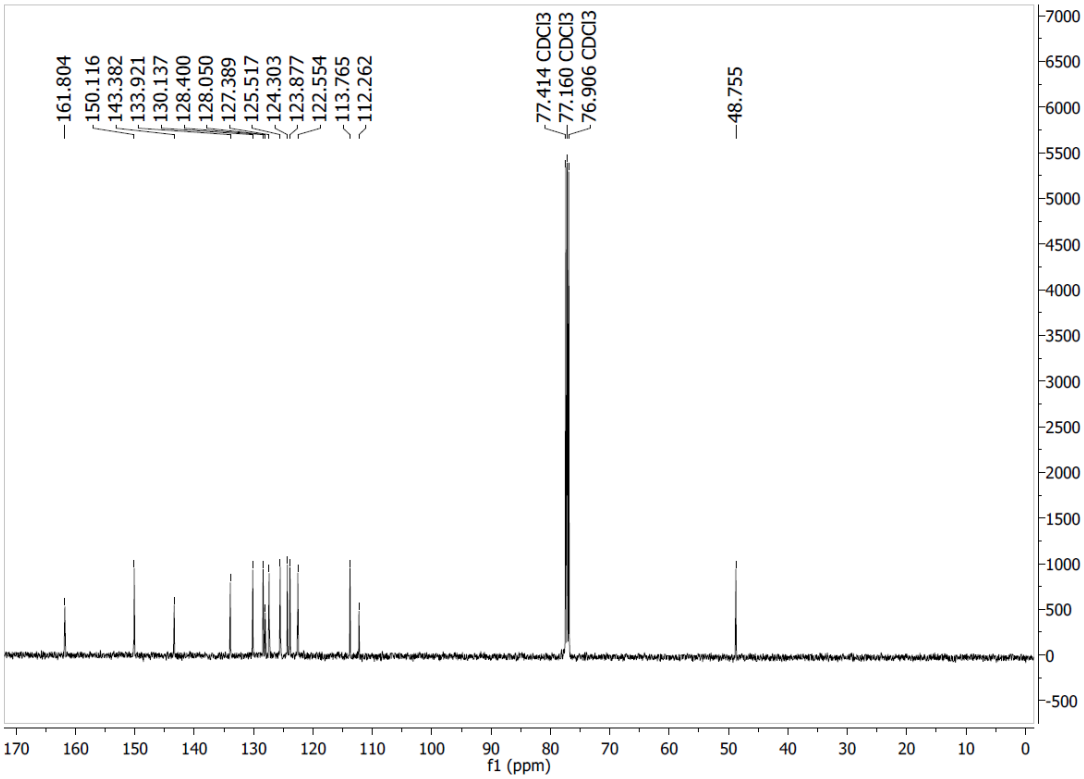
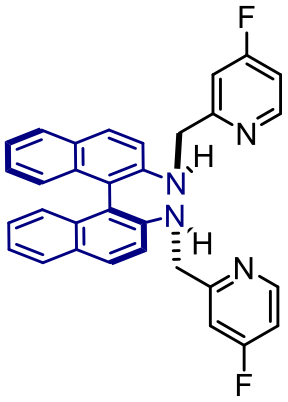


Figure A42. ^{13}C NMR ($CDCl_3$) of compound **L7**.



Compound **L8**

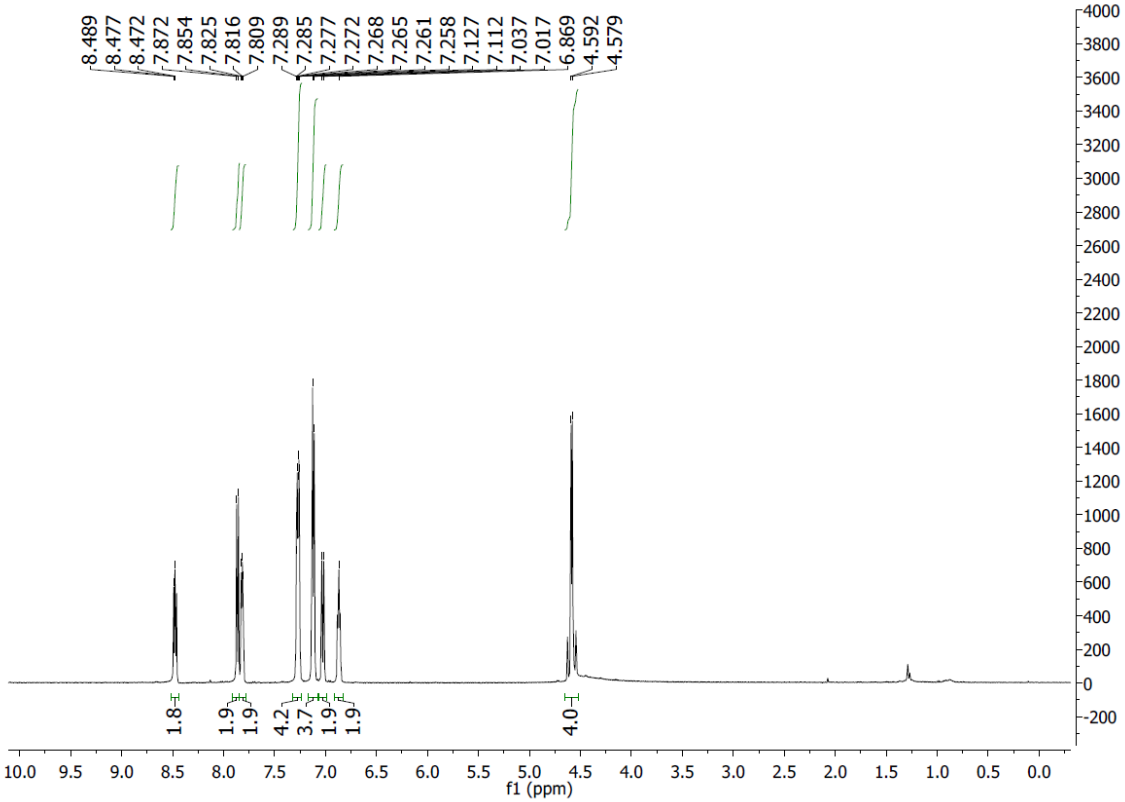


Figure A43. ^{1}H NMR ($CDCl_3$) of compound **L8**.

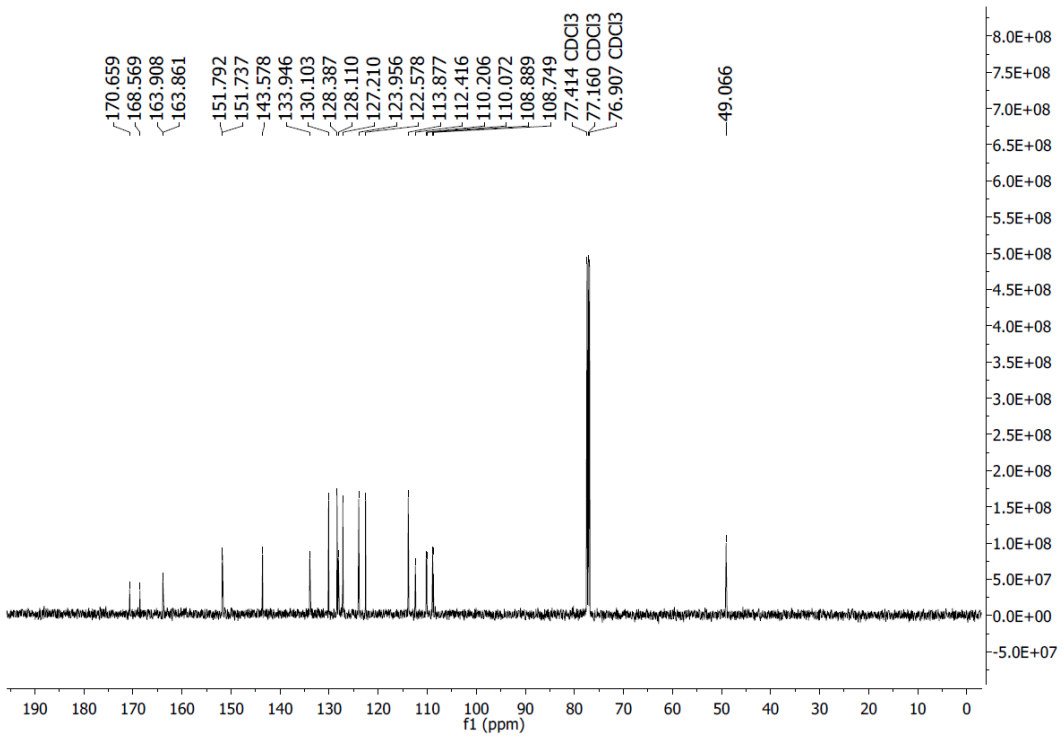
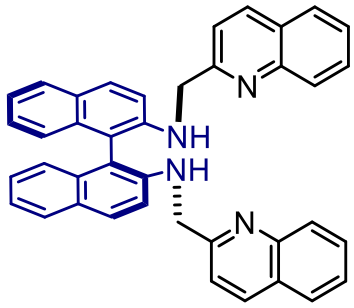


Figure A44. ^{13}C NMR ($CDCl_3$) of compound **L8**.



Compound **L9**

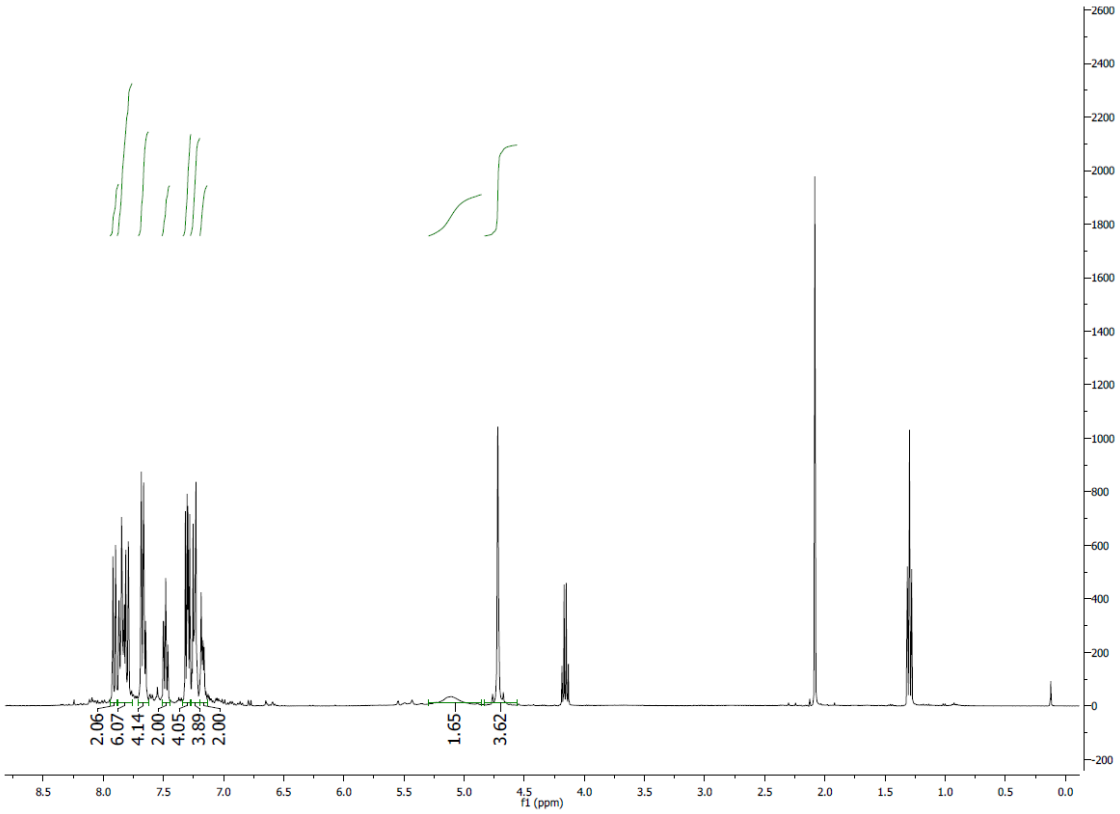


Figure A45. ^{1}H NMR ($CDCl_3$) of compound **L9**.

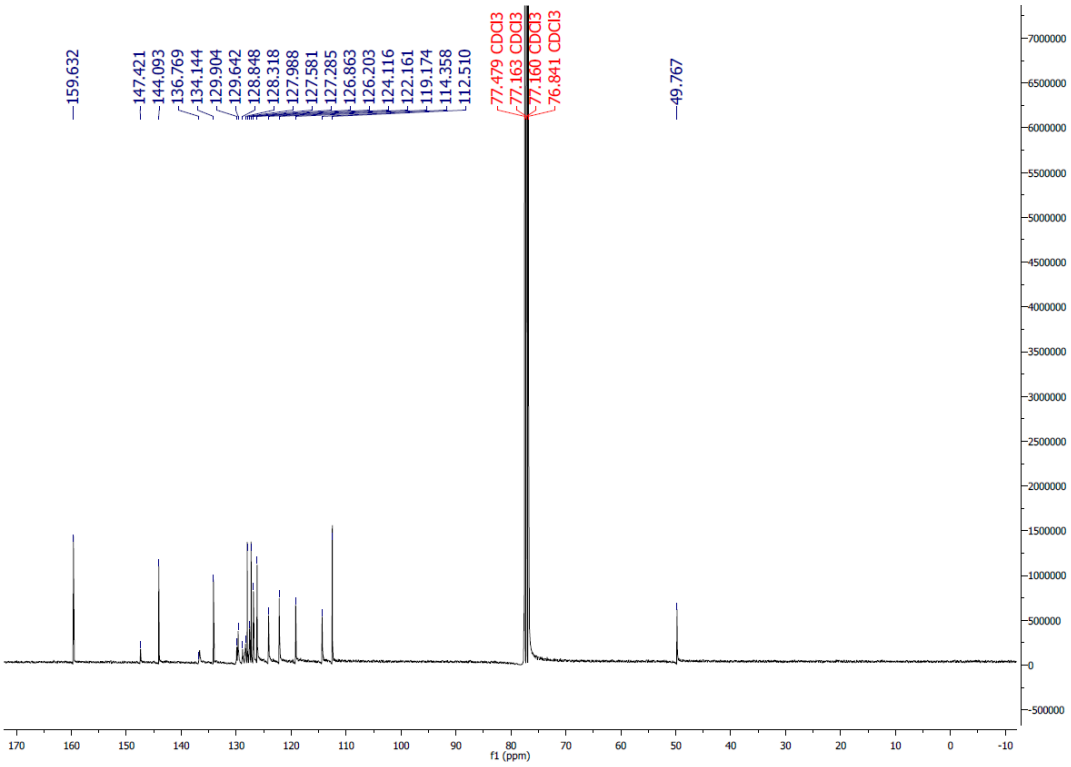
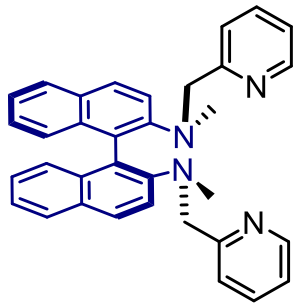


Figure A46. ^{13}C NMR ($CDCl_3$) of compound **L9**.



Compound **L10**

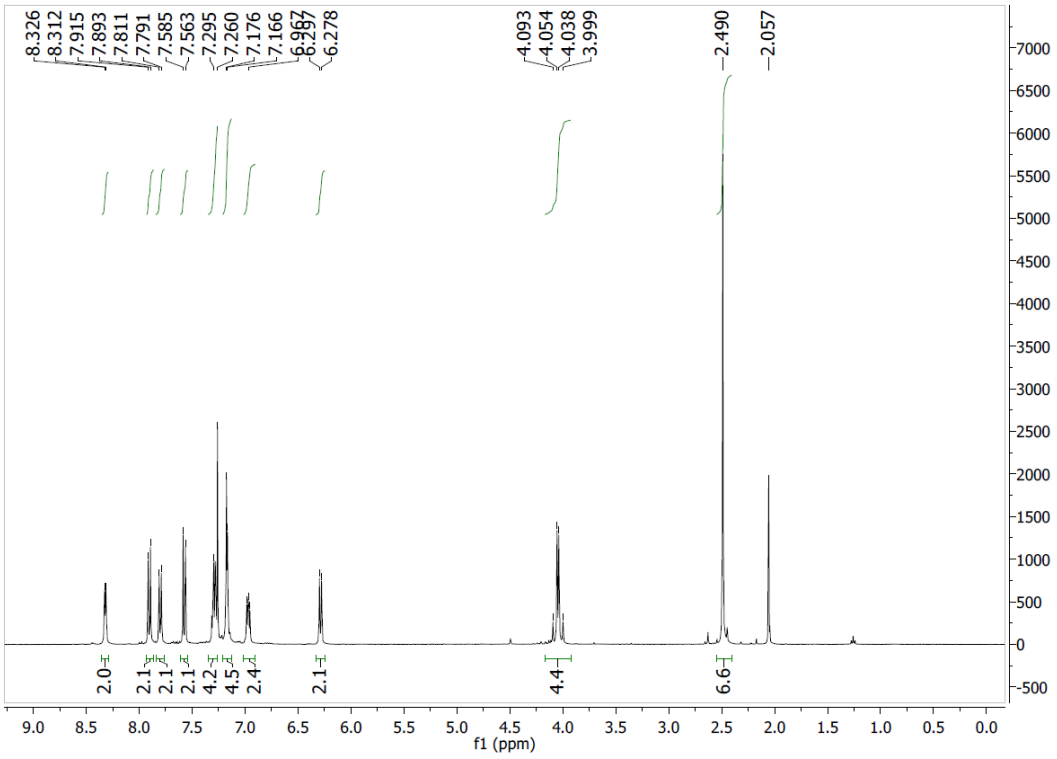


Figure A47. ^{1}H NMR ($CDCl_3$) of compound **L10.**

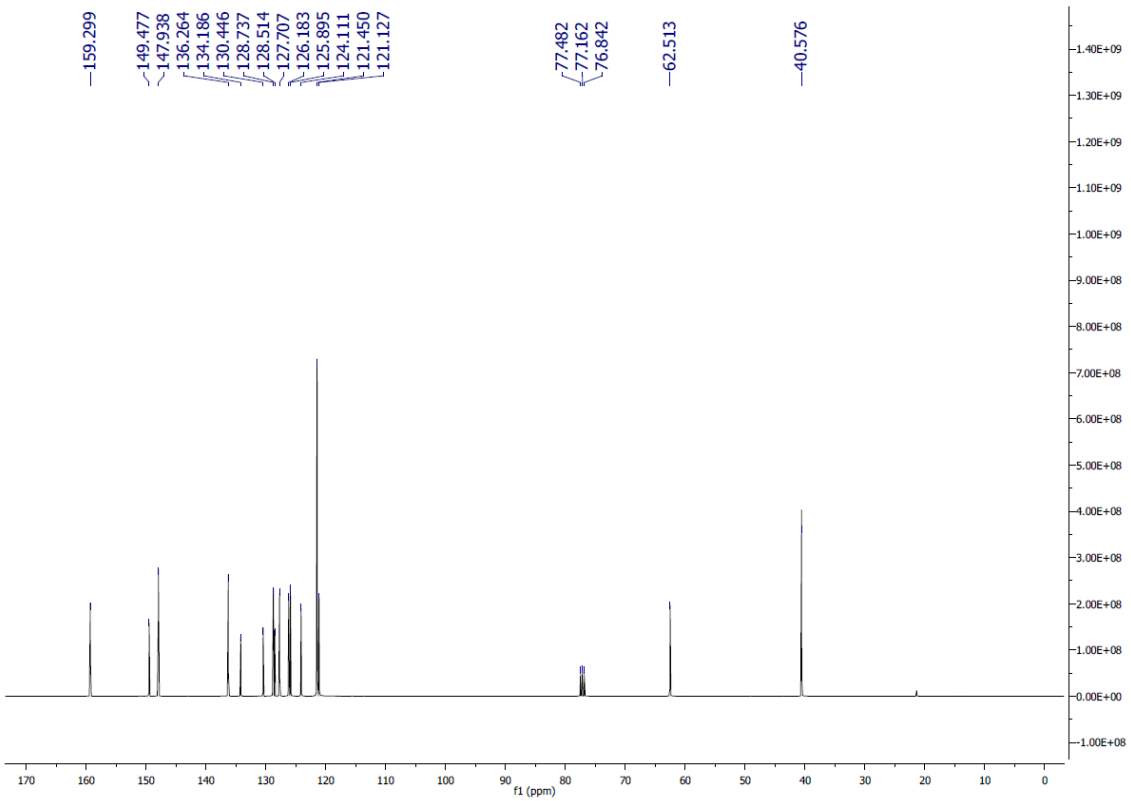
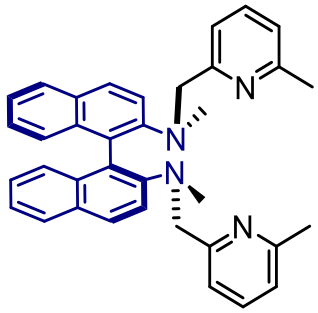


Figure A48. ^{13}C NMR ($CDCl_3$) of compound **L10**.



Compound **L11**

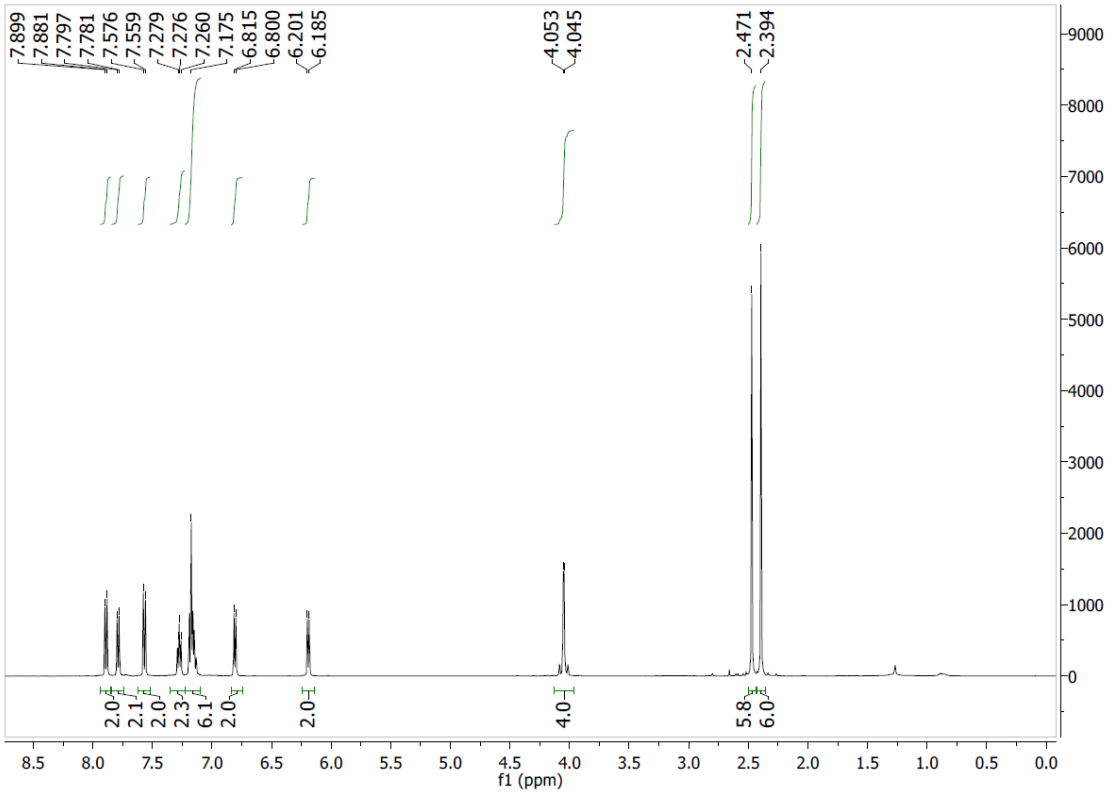


Figure A49. ^{1}H NMR ($CDCl_3$) of compound **L11**.

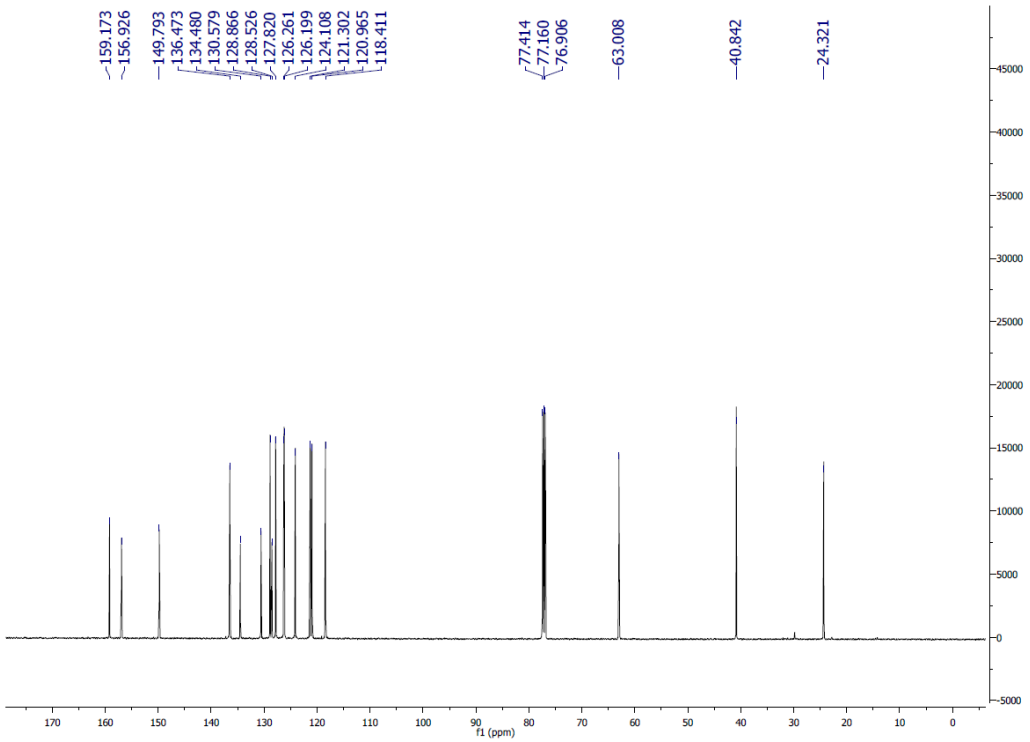
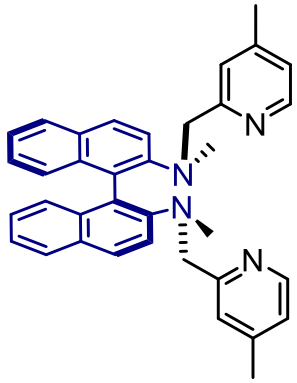


Figure A50. ^{13}C NMR ($CDCl_3$) of compound **L11**.



Compound **L12**

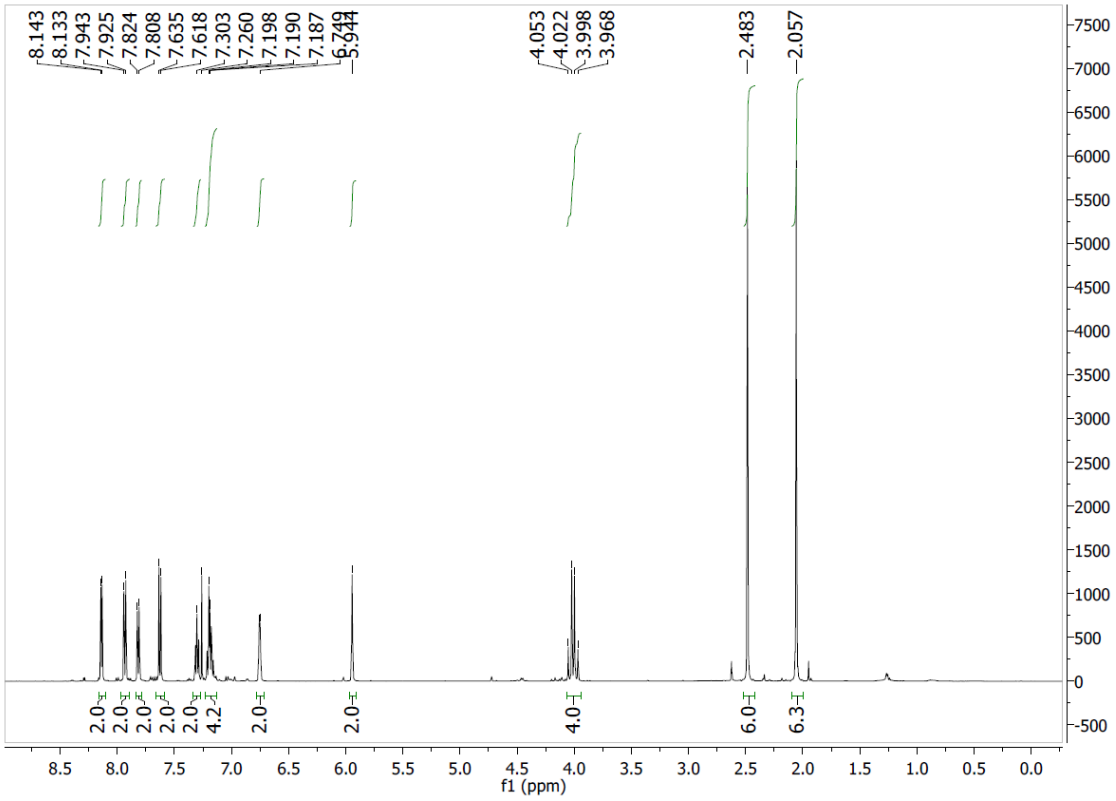


Figure A51. ^{1}H NMR ($CDCl_3$) of compound **L12**.

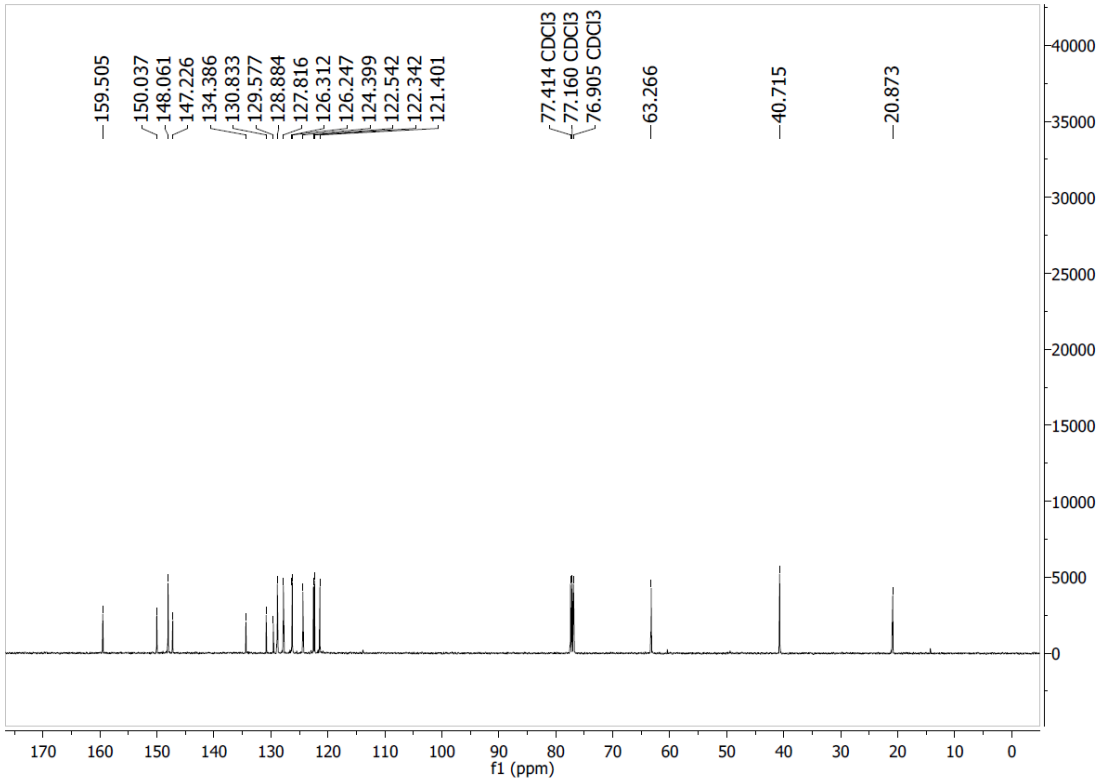
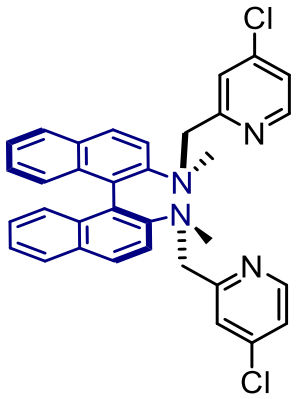


Figure A52. ^{13}C NMR ($CDCl_3$) of compound **L12.**



Compound **L13**

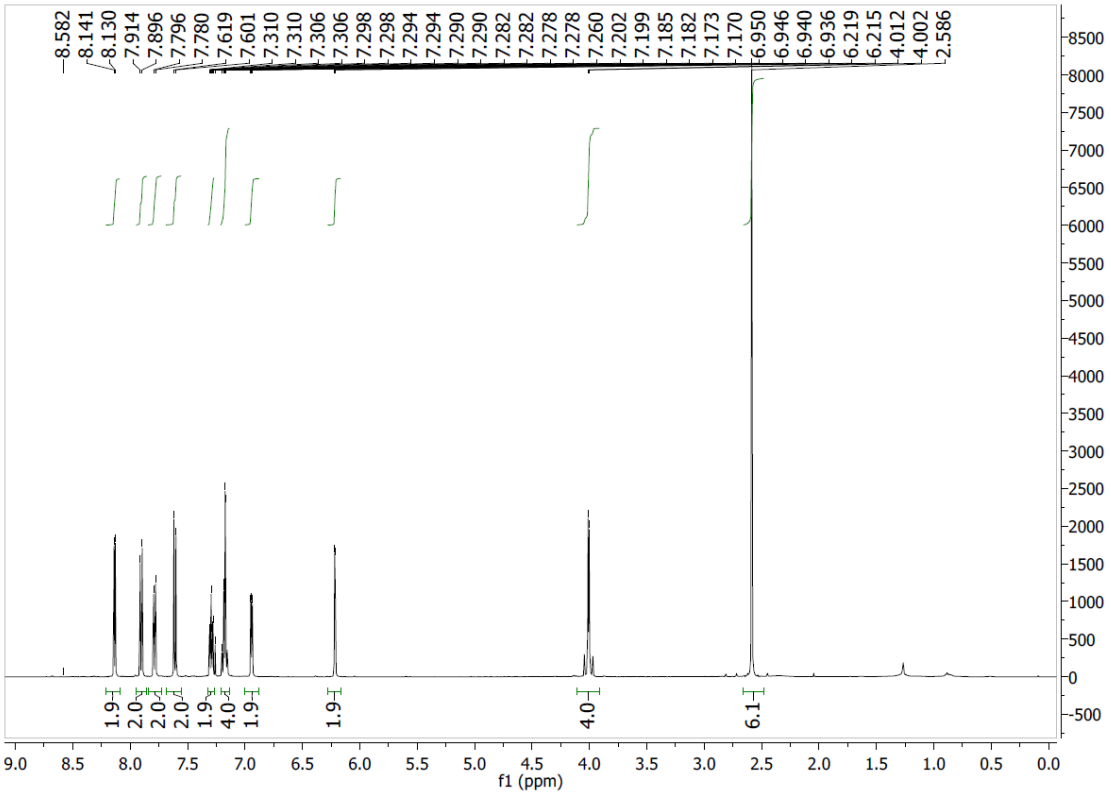


Figure A53. ^{1}H NMR ($CDCl_3$) of compound **L13.**

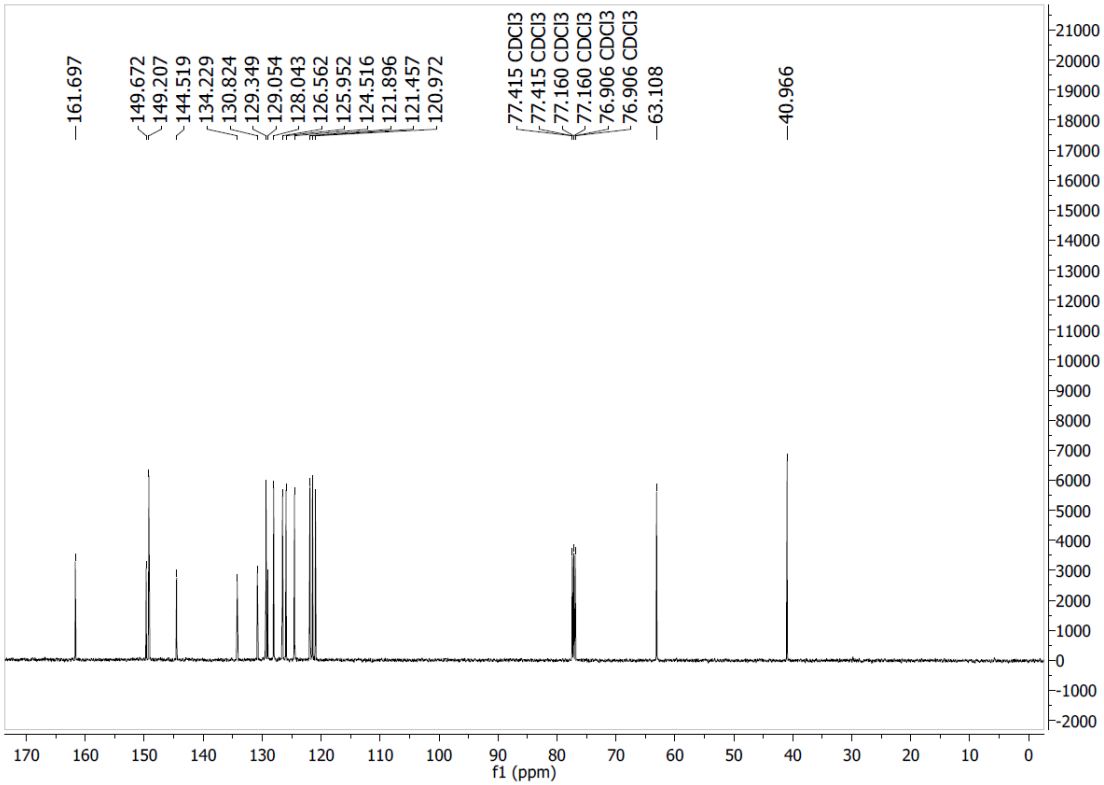
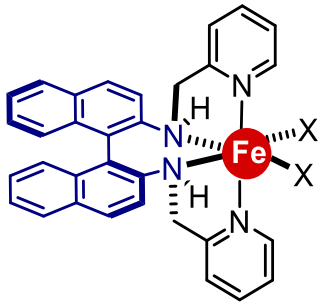


Figure A54. ^{13}C NMR ($CDCl_3$) of compound **L13**.



Compound **1-OTf**

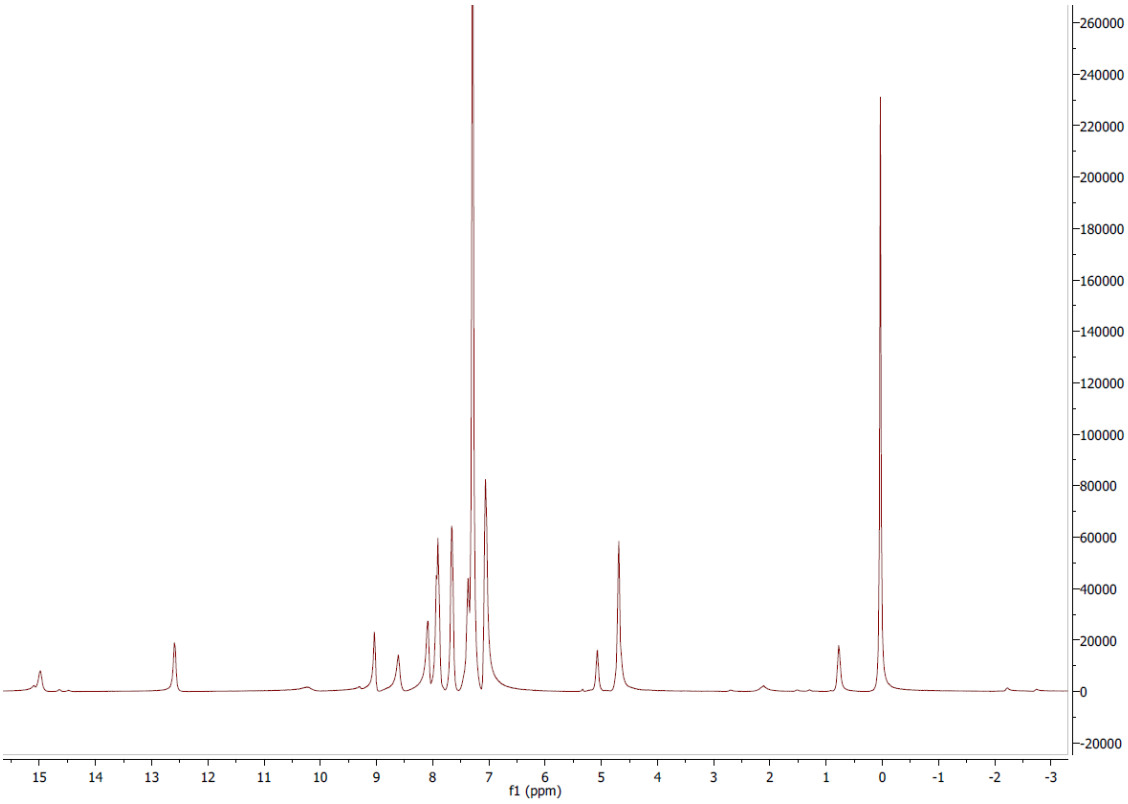
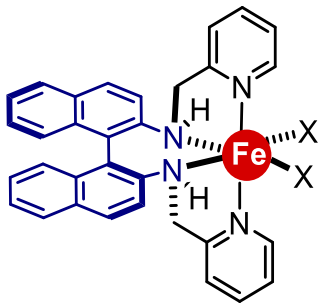


Figure A55. ^{1}H NMR ($CDCl_3$) of compound **1-OTf.**



Compound **1-SbF_6**

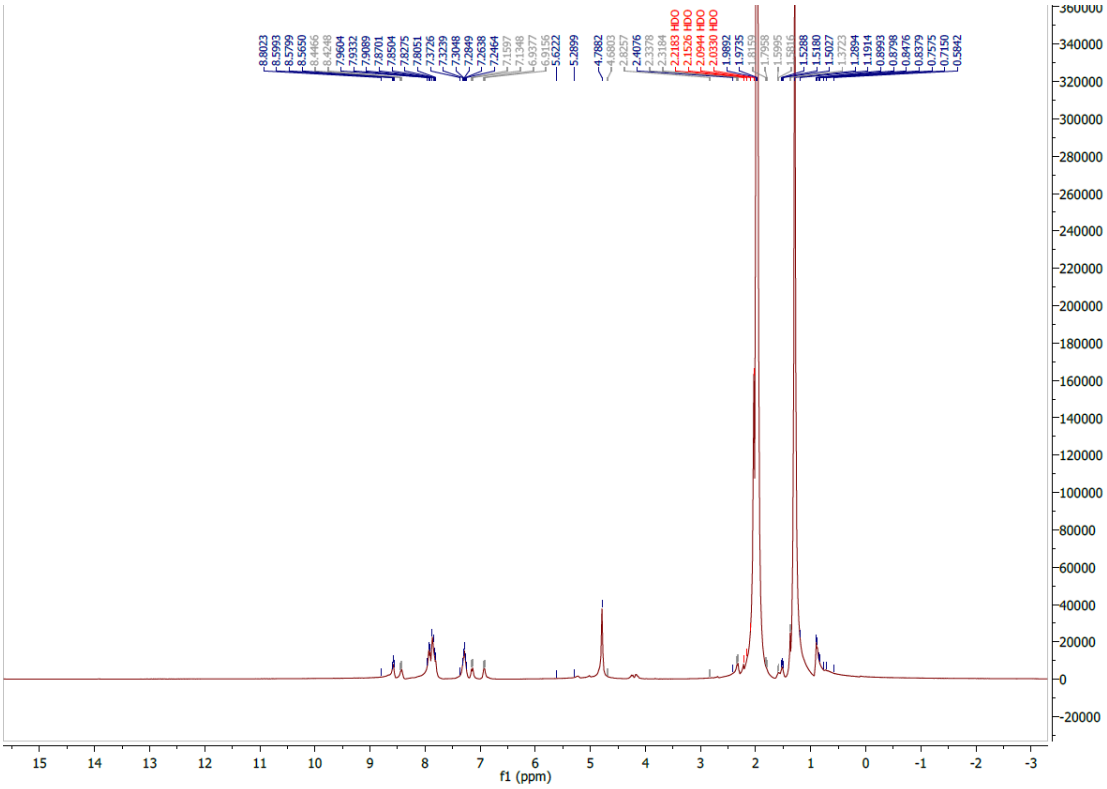
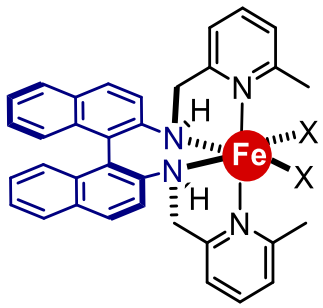


Figure A56. ^{1}H NMR ($CDCl_3$) of compound **1-SbF$_6$**.



Compound **2-OTf**

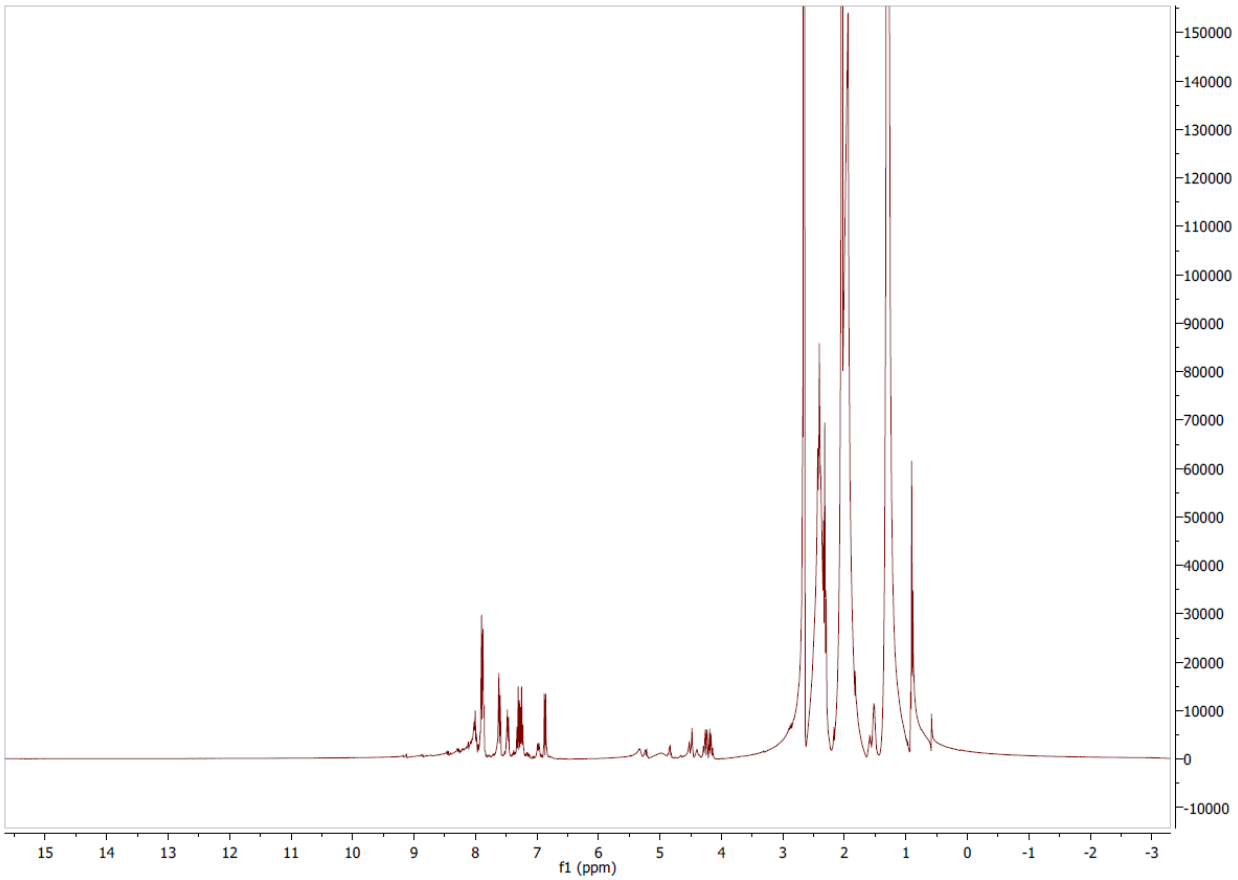
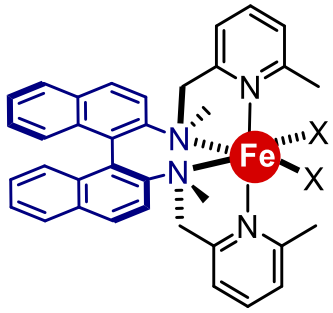


Figure A57. ^{1}H NMR ($CDCl_3$) of compound **2-OTf**



Compound **11-OTf**

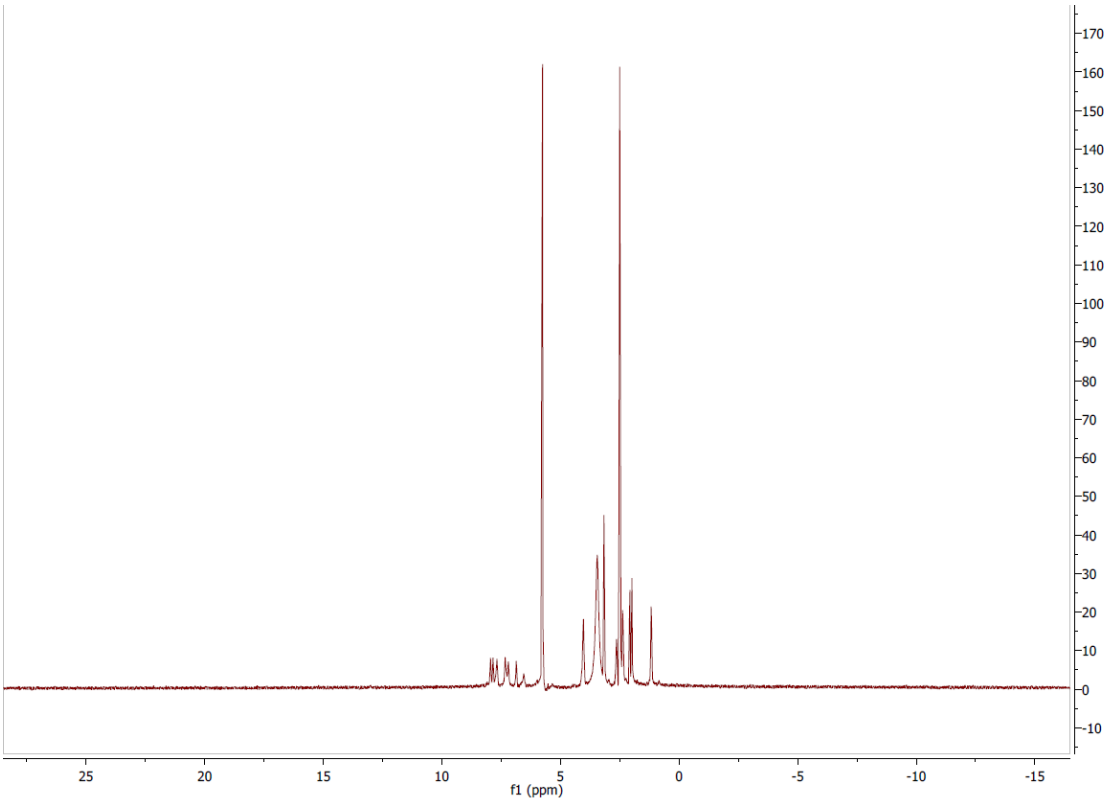
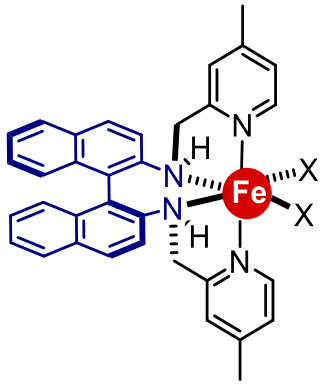


Figure A58. ^{1}H NMR ($CDCl_3$) of compound **11-OTf.**



Compound **3-OTf**

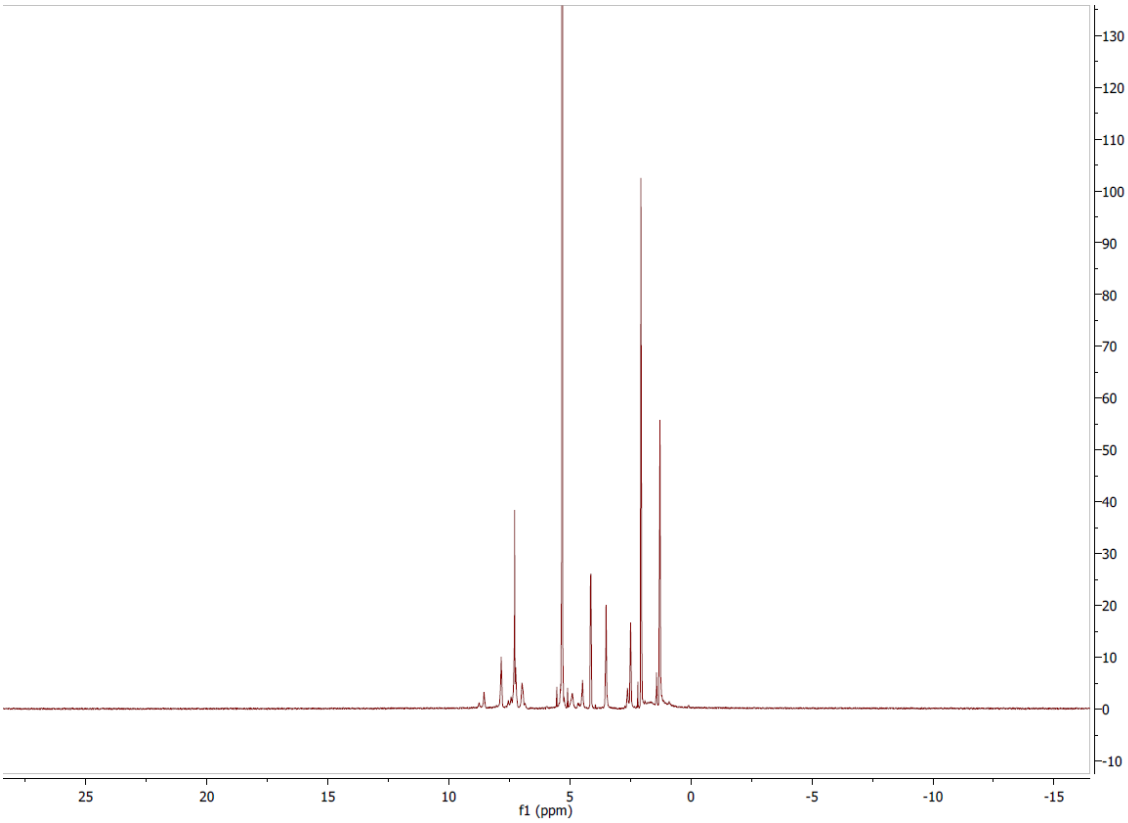
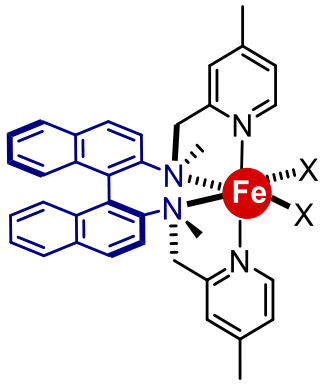


Figure A59. ^{1}H NMR ($CDCl_3$) of compound **3-OTf**



Compound **12-OTf**

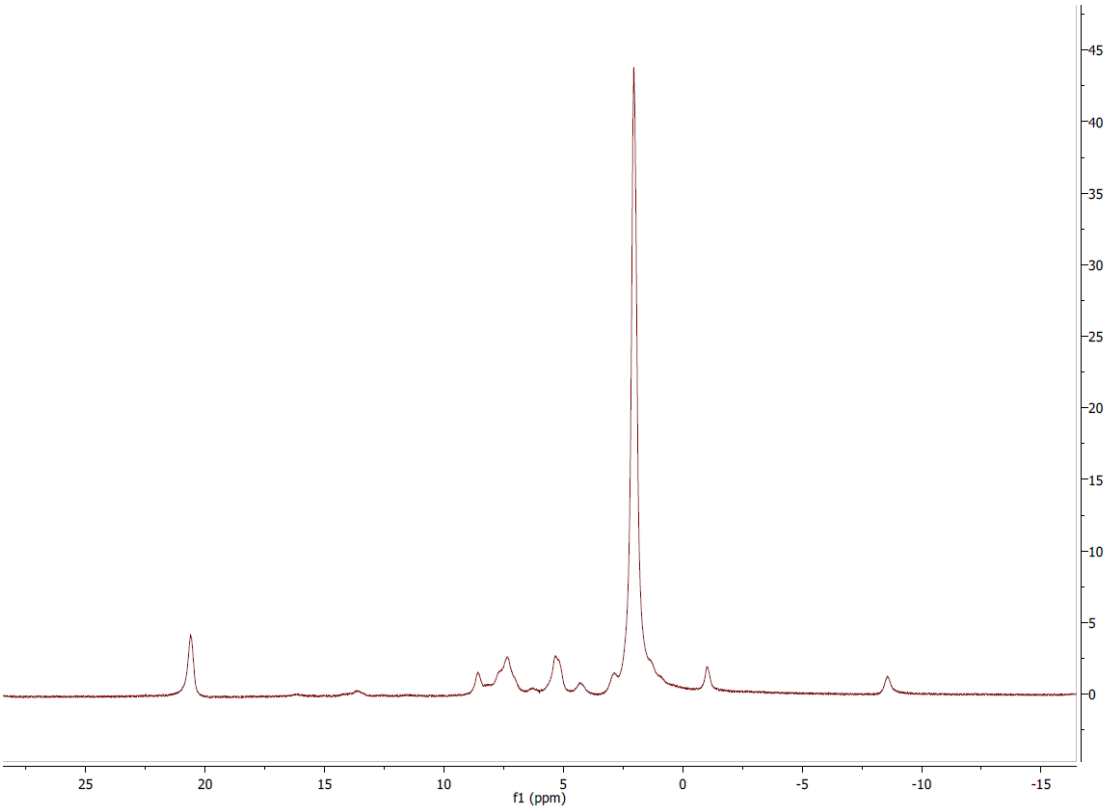
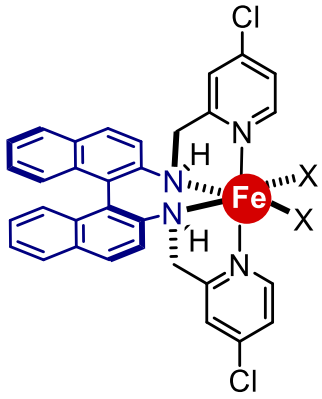


Figure A60. ^{1}H NMR ($CDCl_3$) of compound **12-OTf**



Compound **4-OTf**

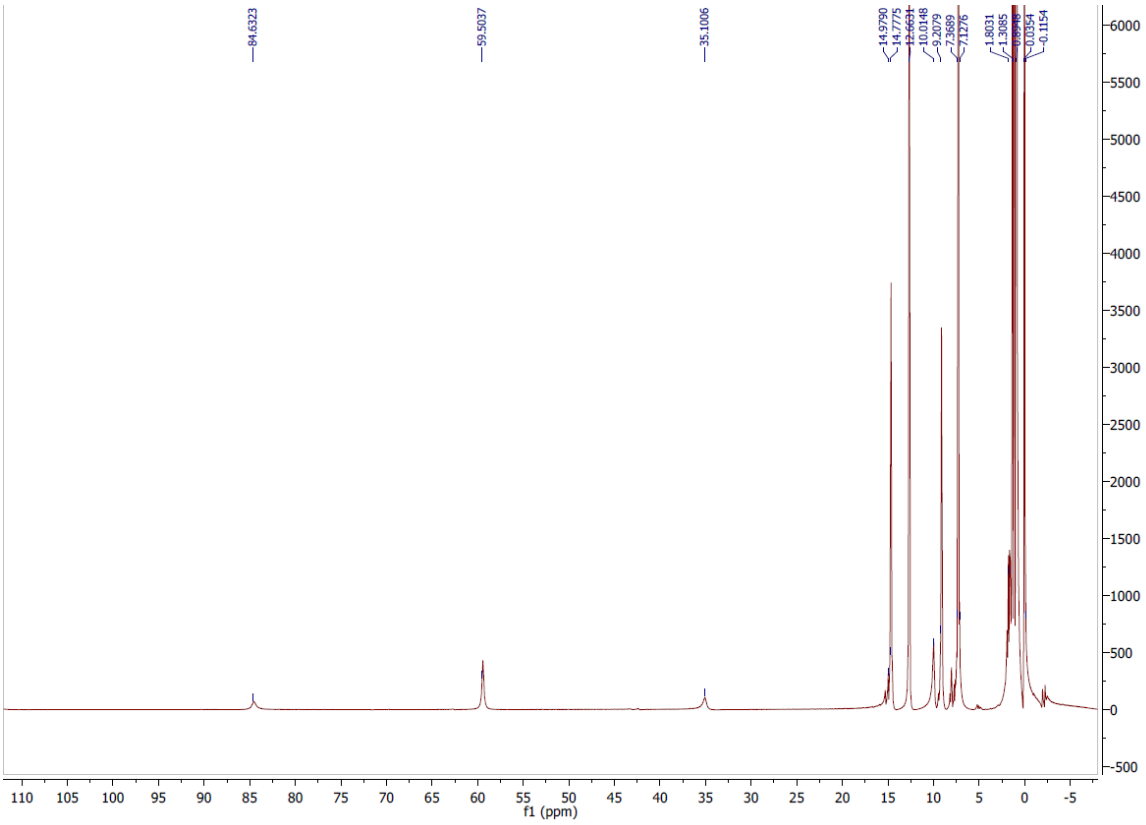
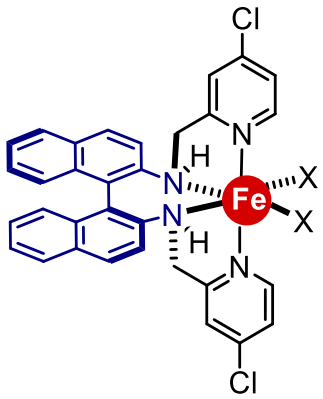


Figure A61. ^{1}H NMR ($CDCl_3$) of compound **4-OTf**



Compound **4-SbF_6**

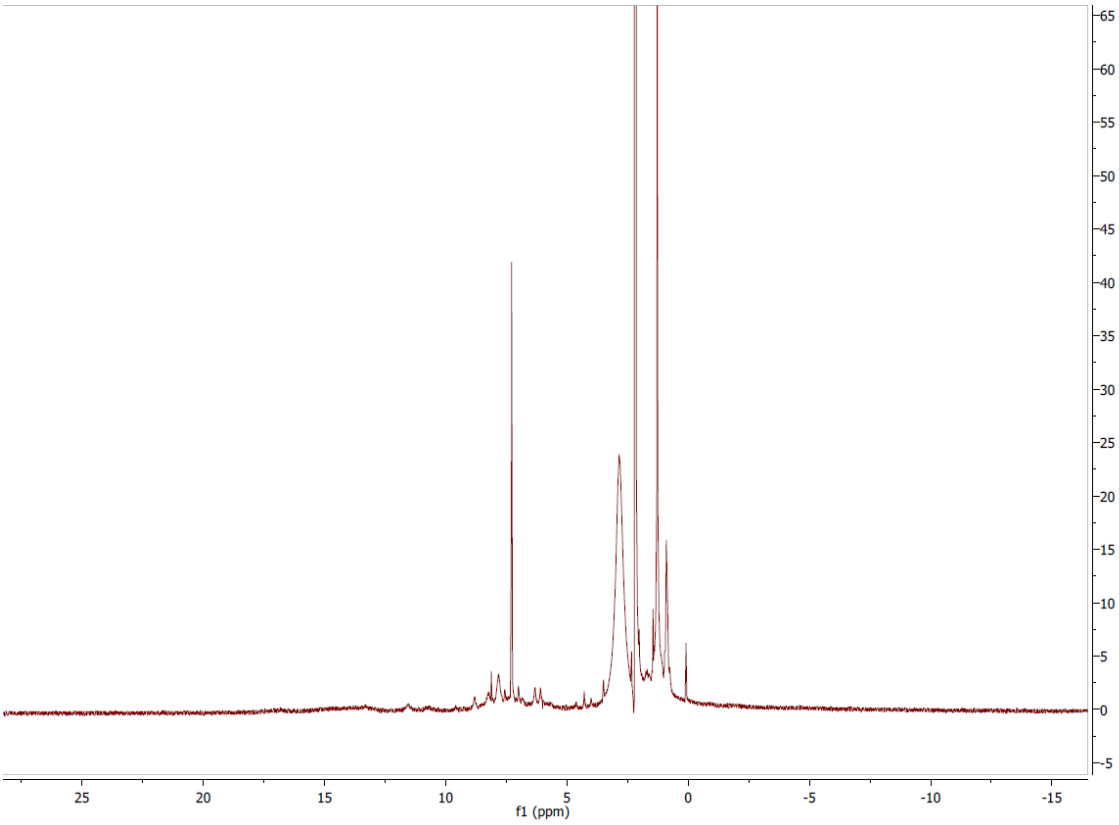
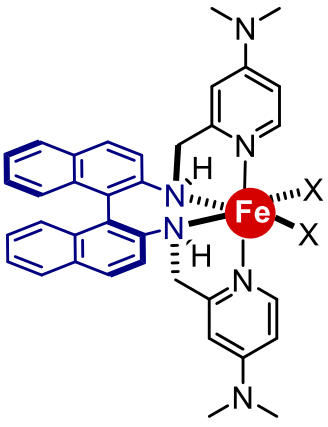


Figure A61. ^{1}H NMR ($CDCl_3$) of compound **4-SbF$_6$**



Compound **5-OTf**

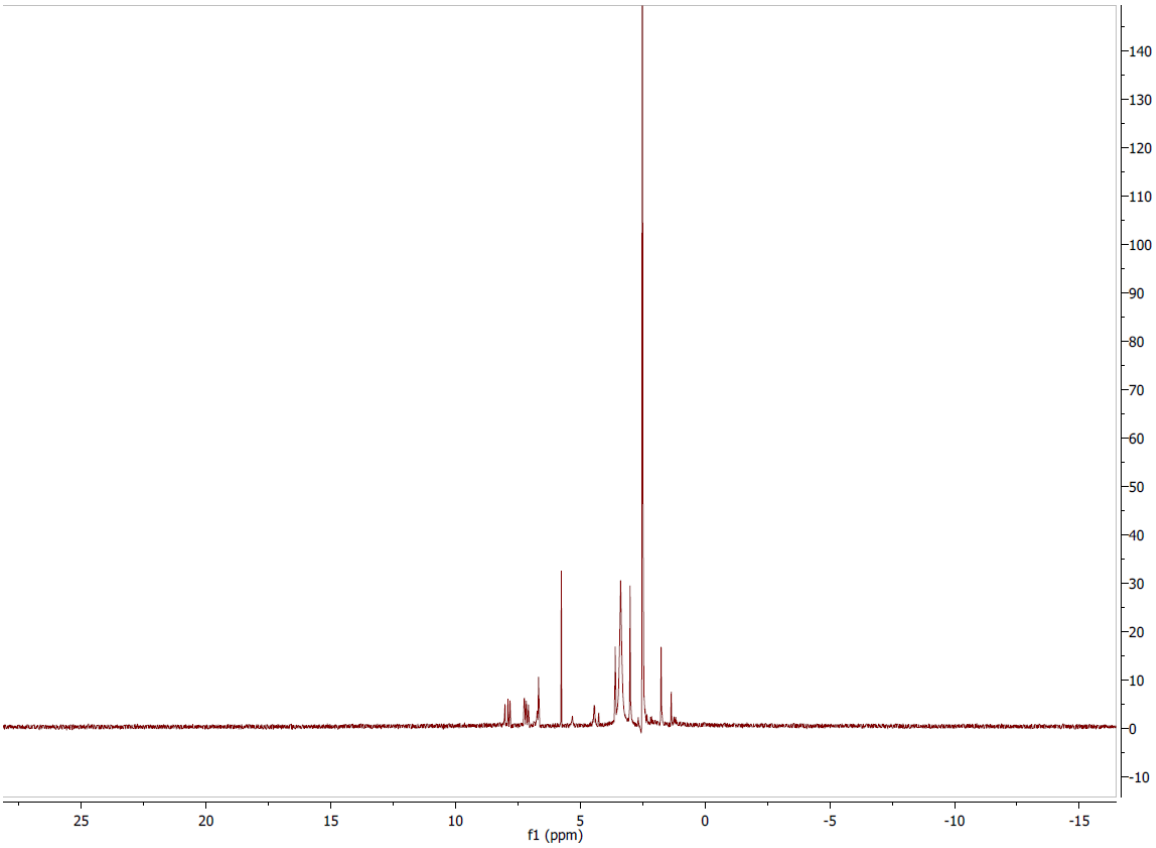
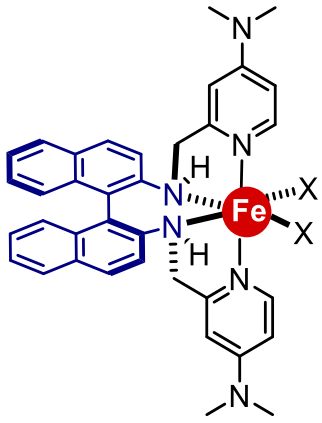


Figure A62. ^{1}H NMR ($CDCl_3$) of compound **5-OTf**



Compound **5-SbF_6**

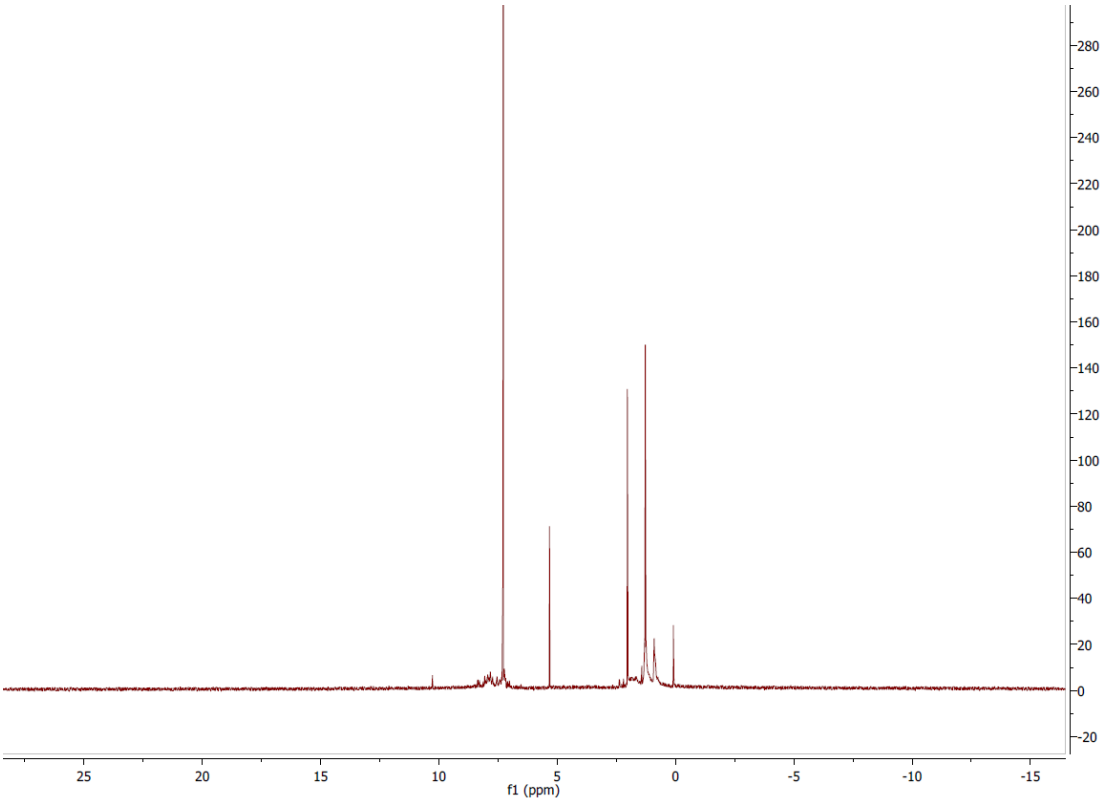
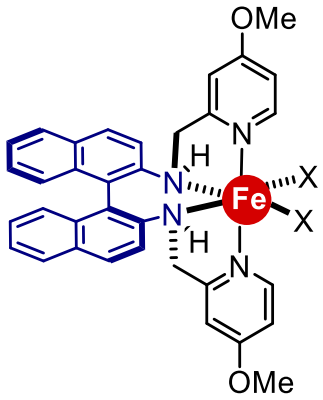


Figure A63. ^{1}H NMR ($CDCl_3$) of compound **5-SbF$_6$.**



Compound **6-SbF$_6$**

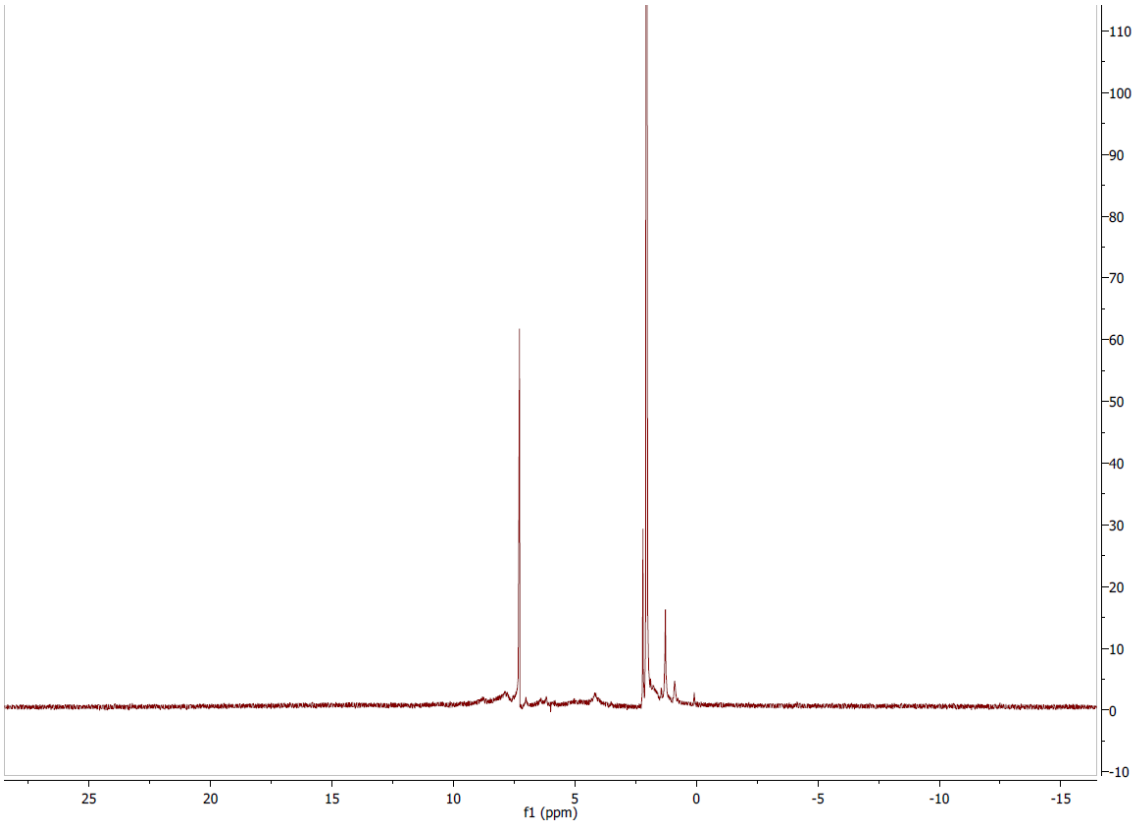
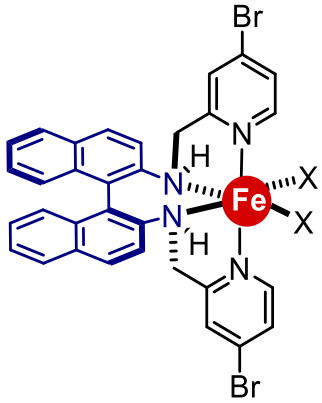


Figure A64. ^{1}H NMR ($CDCl_3$) of compound **6-SbF$_6$.**



Compound **7-OTf**

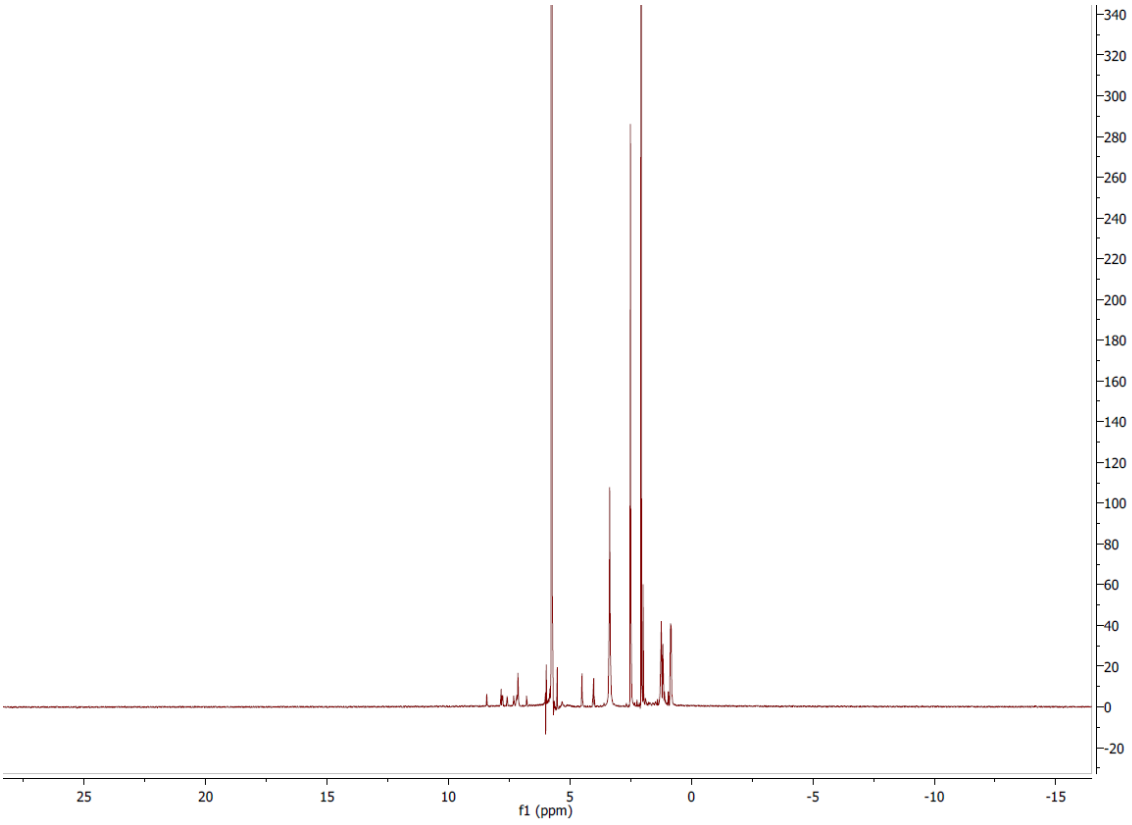


Figure A65. ^{1}H NMR ($CDCl_3$) of compound **7-OTf**

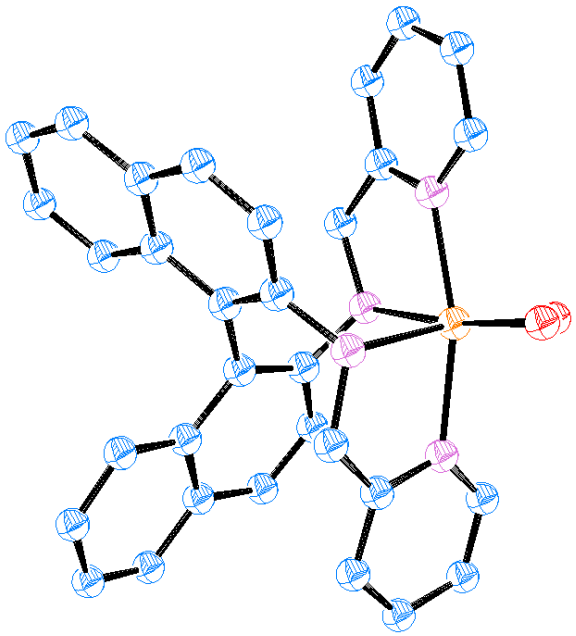


Figure A66. Solid-state structure of chiral diamine iron catalyst **1-OH$_2$** generated using ORTEP-3.[20] Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, orange, red and green ellipsoids represent C, N, Fe, O, and Cl atoms respectively.

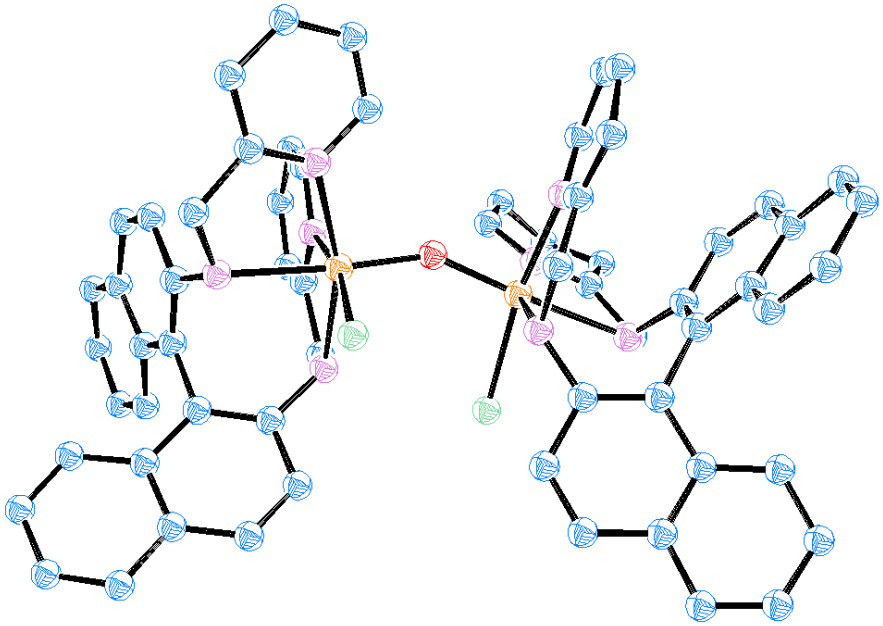


Figure A67. Solid-state structure of chiral diamine iron catalyst **1-SbF$_6$**. Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, orange, red and green ellipsoids represent C, N, Fe, O, and Cl atoms respectively.

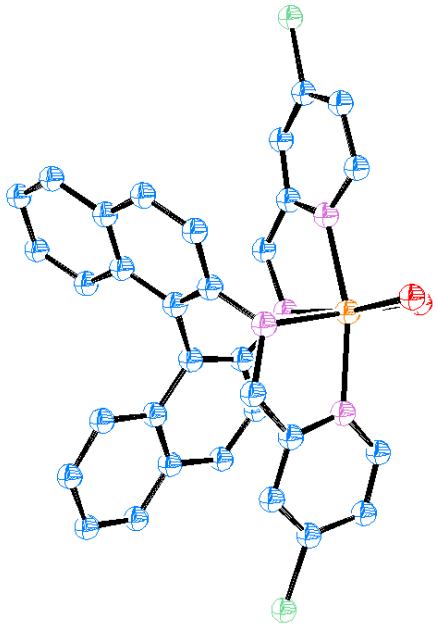


Figure A68. Solid-state structure of chiral diamine iron catalyst **4-OTf**. Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, orange, red and green ellipsoids represent C, N, Fe, O, and Cl atoms respectively.

Complex	***19a***	***Singlet***	***Triplet***	***Quintet***
Fe-N^1 (Å)	2.168	1.989	1.965	2.176
Fe-N^2 (Å)	2.141	1.987	1.973	2.177
Fe-N^3 (Å)	2.278	2.047	2.129	2.186
Fe-N^4 (Å)	2.247	2.046	2.052	2.186

N^1-Fe-	164.8(7)	178.1(8)	176.9(9)	159.2(8)
N^2 (deg)				
N^3-Fe-	91.7(7)	98.0(3)	106.0(8)	91.6(8)
N^4 (deg)				

Figure A69. Selected bond length (Å) and bond angle (deg) data from X-ray crystal structure for iron(II) complex **4-OTf$_2$** compared to the computed values (B3LYP/6-31G(d)-gas) of the complex in different spin states.

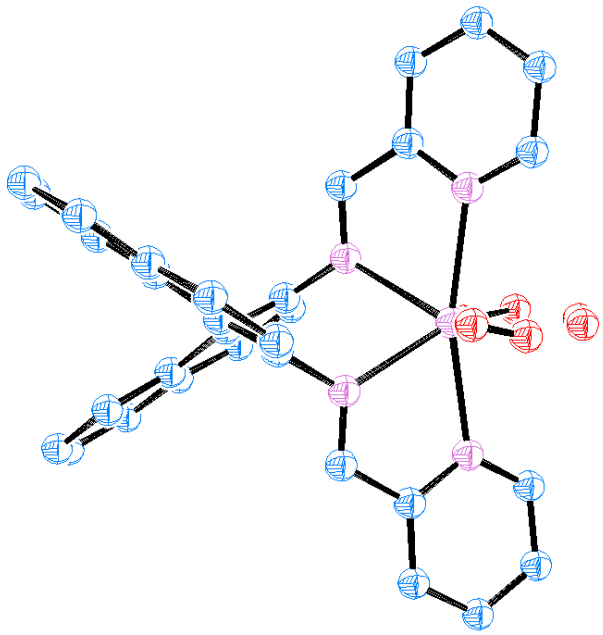


Figure A70. Solid-state structure of chiral diamine manganese catalysts **Mn-1'-OTf**. Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, brown, and red ellipsoids represent C, N, Mn, and O atoms respectively.

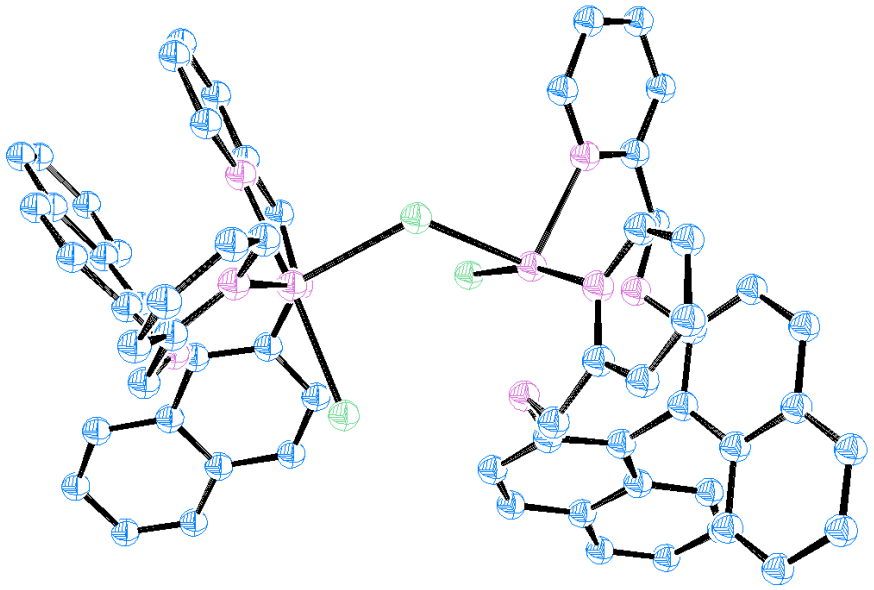


Figure A71. Solid-state structure of chiral diamine manganese catalysts **Mn-1-SbF$_6$**. Thermal ellipsoids are shown at 50% probability; hydrogen atoms are omitted for clarity. Blue, purple, brown, and green ellipsoids represent C, N, Mn, and Cl atoms respectively.

Complex	*1-OH_2*	*1-SbF_6*	*4-OH_2*	*Mn-1-OTf*	*Mn-1-SbF_6*
M	Fe	Fe	Fe	Mn	Mn
M-N^1 (Å)	2.145	2.120, 2.218	2.169	2.313	2.222, 2.222
M-N^2 (Å)	2.131	2.203, 2.113	2.141	2.313	2.236, 2.236
M-N^3 (Å)	2.241	2.220, 2.274	2.247	2.324	2.310, 2.400
M-N^4 (Å)	2.293	2,284, 2.182	2.278	2.324	2.400, 2.310
N^1-M-N^2 (deg)	164.6(7)	92.3(7), 95.1(4)	164.8(8)	165.8(9)	93.7(4), 93.7(4)
N^3-M-N^4 (deg)	92.7(8)	77.3(0), 86.8(1)	91.7(7)	77.4(4)	87.0(6), 87.0(6)

Figure A72. Selected bond length (Å) and bond angle (deg) data for iron(II) and manganese(II) diamine complexes.

A1.6 Coordinates and Energies

Compound A cis-α singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.540942 (Hartree/Particle)
Thermal correction to Energy= 0.570347
Thermal correction to Enthalpy= 0.571291
Thermal correction to Gibbs Free Energy= 0.481149
Sum of electronic and zero-point Energies= -2525.037623
Sum of electronic and thermal Energies= -2525.008218
Sum of electronic and thermal Enthalpies= -2525.007274
Sum of electronic and thermal Free Energies= -2525.097417

Fe	-0.06134	0.58352	0.32036
N	-1.66396	-0.15423	1.29318
N	0.66584	-1.30372	0.725
N	-0.51228	-0.18182	-1.54218
N	1.54876	1.26441	-0.68262
N	0.53704	1.30838	2.01578
N	-0.91238	2.28799	-0.04265
C	-2.91839	0.34204	1.30736
H	-3.09292	1.21485	0.69026
C	-3.67267	-1.3503	2.82885
H	-4.45129	-1.81861	3.42282
C	-2.381	-1.87405	2.81473
H	-2.13083	-2.75702	3.39448
C	-1.40242	-1.24806	2.046
C	0.02989	-1.70855	2.01618
H	0.58806	-1.22789	2.82605
H	0.09268	-2.79014	2.17786
C	2.14584	-1.55694	0.79401
H	2.54738	-1.15954	1.72921
H	2.61518	-1.01713	-0.03035
C	2.31812	-3.0703	0.61731
H	2.22588	-3.59206	1.57449
H	3.3043	-3.31671	0.21653
C	1.17024	-3.46483	-0.34687
H	0.66683	-4.37832	-0.02176
H	1.54994	-3.66012	-1.35431
C	0.19773	-2.25042	-0.36392
H	-0.82576	-2.55044	-0.12188
C	0.19008	-1.51631	-1.7039
H	1.2231	-1.31201	-1.99895
C	-0.57816	-2.29303	-2.81222
H	0.0336	-2.42534	-3.70766
H	-0.83797	-3.29642	-2.46144
C	-1.93406	-0.48751	-1.92119
H	-2.47029	0.44124	-2.13042
H	-2.41154	-0.96592	-1.06432
C	0.06804	0.7861	-2.52298
H	-0.62552	1.62904	-2.60714
H	0.16338	0.34512	-3.52121
C	1.40175	1.27654	-2.02798
C	2.39923	1.7417	-2.88197
H	2.24432	1.72169	-3.95622
C	3.5859	2.23084	-2.33843
H	4.3766	2.60125	-2.98337
C	3.73717	2.2278	-0.95171
C	2.70252	1.73509	-0.16536
H	2.78753	1.70885	0.91408
C	0.81427	1.80388	3.02667
C	-3.94381	-0.21874	2.05946
C	-1.35052	3.3499	-0.19946
C	-1.90303	4.68555	-0.39621
H	-2.64603	4.67495	-1.20034
H	-2.38425	5.03289	0.52388
H	-1.10481	5.38597	-0.66272
C	-1.84989	-1.45671	-3.10637
H	-2.7481	-2.07405	-3.18369
H	-1.75533	-0.91503	-4.05224
C	1.16479	2.42756	4.29794
H	1.94166	1.84615	4.8051
H	1.53819	3.44282	4.12881
H	0.28358	2.47939	4.94571
H	-4.93434	0.22248	2.03377
H	4.64349	2.59427	-0.48184

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.31477
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.13552
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.947154
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.25938

Compound A cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.538120 (Hartree/Particle)
Thermal correction to Energy= 0.569059
Thermal correction to Enthalpy= 0.570003
Thermal correction to Gibbs Free Energy= 0.473129
Sum of electronic and zero-point Energies= -2525.020527
Sum of electronic and thermal Energies= -2524.989588
Sum of electronic and thermal Enthalpies= -2524.988644
Sum of electronic and thermal Free Energies= -2525.085518

Fe	-0.12714	0.59796	0.31201
N	-1.71085	-0.13296	1.36877
N	0.60188	-1.28869	0.67174
N	-0.52378	-0.25015	-1.74215
N	1.52131	1.30088	-0.76228
N	0.78277	1.41455	2.37696
N	-0.91338	2.32702	0.02582
C	-2.96337	0.36492	1.42306
H	-3.14493	1.26663	0.8502
C	-3.68356	-1.39527	2.88029
H	-4.45091	-1.89067	3.4672
C	-2.39147	-1.91767	2.82426
H	-2.13238	-2.82328	3.36347
C	-1.42896	-1.25975	2.06315
C	0.00502	-1.70426	1.98149
H	0.57925	-1.21097	2.77256
H	0.08799	-2.7843	2.14065
C	2.08809	-1.5213	0.71633
H	2.49981	-1.10122	1.63672
H	2.53331	-0.98748	-0.12438
C	2.27695	-3.03659	0.56116
H	2.25532	-3.53866	1.53283
H	3.24289	-3.27062	0.10733

C	1.08208	-3.48079	-0.32408
H	0.57159	-4.34899	0.09988
H	1.41364	-3.77506	-1.32377
C	0.13581	-2.2496	-0.40953
H	-0.90031	-2.51624	-0.18135
C	0.17278	-1.5806	-1.79164
H	1.21642	-1.40603	-2.07001
C	-0.56687	-2.43542	-2.86851
H	0.0808	-2.65729	-3.71995
H	-0.87234	-3.39912	-2.44879
C	-1.92475	-0.55434	-2.16693
H	-2.43683	0.36561	-2.4603
H	-2.45669	-0.97211	-1.30615
C	0.11383	0.71437	-2.66746
H	-0.57816	1.55549	-2.79404
H	0.28364	0.29067	-3.66588
C	1.41774	1.23936	-2.10885
C	2.44073	1.68609	-2.94491
H	2.3283	1.60773	-4.02187
C	3.59386	2.2325	-2.38507
H	4.39962	2.58748	-3.02015
C	3.69259	2.3088	-0.99569
C	2.63988	1.8301	-0.22514
H	2.67695	1.86087	0.85754
C	0.97854	1.92957	3.39852
C	-3.97455	-0.2326	2.16547
C	-1.33063	3.3982	-0.12591
C	-1.85156	4.74664	-0.31448
H	-2.6331	4.74764	-1.0814
H	-2.27606	5.12074	0.62293
H	-1.04628	5.41795	-0.63027
C	-1.79892	-1.59564	-3.28727
H	-2.70397	-2.19961	-3.3892
H	-1.63079	-1.10673	-4.25197
C	1.23448	2.57217	4.68311
H	2.07834	2.08685	5.18392
H	1.47262	3.63	4.53328
H	0.35045	2.495	5.32397
H	-4.96732	0.20388	2.17772
H	4.57057	2.72431	-0.51298

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.27625
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.12116
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.91625
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.23950

Compound A cis-α Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.535732
(Hartree/Particle)
Thermal correction to Energy= 0.567851
Thermal correction to Enthalpy= 0.568795
Thermal correction to Gibbs Free Energy=
0.467662
Sum of electronic and zero-point Energies=
-2525.039235
Sum of electronic and thermal Energies=
-2525.007115
Sum of electronic and thermal Enthalpies=
-2525.006171
Sum of electronic and thermal Free Energies= -
2525.107304

Fe	-0.07445	0.68564	0.37548
N	-1.76668	-0.16596	1.46953
N	0.60915	-1.41082	0.75645
N	-0.44871	-0.20474	-1.64433
N	1.63058	1.42135	-0.78496
N	0.68445	1.48919	2.29095
N	-1.10205	2.59538	-0.0466
C	-3.01754	0.32797	1.54904
H	-3.19201	1.26705	1.03371
C	-3.76051	-1.52187	2.87392
H	-4.53417	-2.05519	3.41782
C	-2.47061	-2.04438	2.78762
H	-2.22055	-2.98891	3.26092
C	-1.49537	-1.3364	2.08575
C	-0.06037	-1.81402	2.02235
H	0.49969	-1.35735	2.84677
H	-0.02338	-2.89925	2.17638
C	2.08266	-1.66791	0.83892
H	2.47013	-1.31695	1.79863
H	2.56852	-1.08526	0.05145
C	2.25804	-3.17474	0.59608
H	2.18386	-3.73133	1.53512
H	3.23769	-3.40285	0.16901
C	1.0923	-3.54018	-0.35946
H	0.55984	-4.43142	-0.01854
H	1.45726	-3.76272	-1.36632
C	0.15749	-2.29264	-0.3809
H	-0.88537	-2.56623	-0.19484
C	0.23695	-1.5454	-1.72666
H	1.28988	-1.3667	-1.96432
C	-0.48393	-2.33163	-2.86424
H	0.15322	-2.42956	-3.74657
H	-0.72033	-3.34846	-2.53768
C	-1.86299	-0.50709	-2.03422
H	-2.38461	0.41785	-2.29255
H	-2.36535	-0.93968	-1.16475
C	0.16182	0.75014	-2.60839
H	-0.53314	1.59101	-2.71773
H	0.28143	0.30608	-3.604
C	1.49345	1.27946	-2.12075
C	2.50331	1.64772	-3.00937
H	2.3645	1.50883	-4.07711
C	3.68354	2.196	-2.50859
H	4.48131	2.4919	-3.18298
C	3.82318	2.3493	-1.12887
C	2.77742	1.94273	-0.30781
H	2.84632	2.03232	0.77159
C	0.95902	1.94221	3.32234
C	-4.03977	-0.30886	2.24363
C	-1.52517	3.65716	-0.24141
C	-2.05984	4.99004	-0.48889
H	-2.86467	4.93904	-1.22939
H	-2.45883	5.41027	0.43999
H	-1.26908	5.64638	-0.86625
C	-1.77174	-1.52651	-3.17961
H	-2.66093	-2.15992	-3.227
H	-1.69057	-1.02072	-4.14639
C	1.30764	2.50871	4.61899
H	2.19686	2.0103	5.0185
H	1.51742	3.57815	4.51462
H	0.47821	2.37532	5.32093
H	-5.0302	0.13188	2.28035
H	4.7258	2.76627	-0.69535

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.27132

UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.14770
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.93431
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.26496

Compound A cis-β Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.540747 (Hartree/Particle)
Thermal correction to Energy= 0.570150
Thermal correction to Enthalpy= 0.571094
Thermal correction to Gibbs Free Energy= 0.480860
Sum of electronic and zero-point Energies= -2525.032161
Sum of electronic and thermal Energies= -2525.002759
Sum of electronic and thermal Enthalpies= -2525.001815
Sum of electronic and thermal Free Energies= -2525.092049

Fe	-0.2233	0.5037	0.27004
N	0.58657	0.75275	2.0879
N	0.58822	-1.36451	0.47013
N	-0.87833	-0.1449	-1.57739
N	1.34311	1.16671	-0.78382
N	-1.86282	-0.01186	1.19526
N	-0.98116	2.27585	0.11709
C	0.85572	1.89913	2.74347
H	0.62522	2.81677	2.2136
C	1.68482	0.71553	4.65599
H	2.11689	0.6981	5.65169
C	1.41002	-0.47546	3.98351
H	1.62323	-1.43563	4.44287
C	0.85416	-0.42463	2.70816
C	0.46676	-1.66184	1.93029
H	1.08198	-2.5176	2.22718
H	-0.57284	-1.92296	2.1466
C	2.00459	-1.68304	0.05225
H	2.69987	-1.33206	0.81783
H	2.22827	-1.14332	-0.86625
C	2.03731	-3.20683	-0.18267
H	2.39131	-3.74141	0.70303
H	2.72725	-3.45606	-0.99254
C	0.5685	-3.59545	-0.51115
H	0.18762	-4.33086	0.20251
H	0.47041	-4.04429	-1.5034
C	-0.22766	-2.2738	-0.40633
H	-1.20868	-2.40942	0.05726
C	-0.40211	-1.58353	-1.77063
H	0.57144	-1.53598	-2.26556
C	-1.44822	-2.28995	-2.68008
H	-0.98693	-2.72438	-3.56998
H	-1.9237	-3.1129	-2.13558
C	-2.35332	-0.21983	-1.87094
H	-2.74591	0.78087	-2.06401
H	-2.84975	-0.61293	-0.98216
C	-0.22402	0.75104	-2.57917
H	-0.84222	1.65172	-2.66408
H	-0.18536	0.29501	-3.5747
C	1.1534	1.15495	-2.12425
C	2.14734	1.55129	-3.01703
H	1.9607	1.5121	-4.08569
C	3.36918	2.00247	-2.52034
H	4.15613	2.31999	-3.19729
C	3.55844	2.03429	-1.13879
C	2.52859	1.60353	-0.31091
H	2.64905	1.59428	0.76546
C	-2.8502	-0.14985	1.78748
C	1.3995	1.92508	4.02342
C	-1.425	3.34426	0.04149
C	-1.98032	4.68986	-0.05398
H	-2.87438	4.68627	-0.68602
H	-2.25478	5.05577	0.94079
H	-1.24276	5.37161	-0.48974
C	-2.48983	-1.20641	-3.03117
H	-3.50282	-1.60943	-3.10836
H	-2.26188	-0.72735	-3.98864
C	-4.09298	-0.32998	2.52952
H	-4.04697	0.21741	3.47664
H	-4.93904	0.04614	1.94506
H	-4.2569	-1.39124	2.74348
H	1.59765	2.87576	4.50661
H	4.49097	2.37746	-0.70394

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.30951
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.13030
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.94149
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.25403

Compound A cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.537346 (Hartree/Particle)
Thermal correction to Energy= 0.568901
Thermal correction to Enthalpy= 0.569845
Thermal correction to Gibbs Free Energy= 0.469135
Sum of electronic and zero-point Energies= -2525.018971
Sum of electronic and thermal Energies= -2524.987416
Sum of electronic and thermal Enthalpies= -2524.986472
Sum of electronic and thermal Free Energies= -2525.087182

Fe	0.31569	0.74962	0.1356
N	0.95376	0.98403	1.98802
N	0.63819	-1.20433	0.5354
N	-0.51027	0.10579	-1.60984
N	1.87479	1.33456	-1.1956
N	-3.14971	-1.07473	1.54453
N	-0.78843	2.40459	0.17956
C	1.43613	2.09826	2.57792
H	1.50718	2.97984	1.9491
C	1.71221	0.96232	4.66943
H	2.01056	0.95091	5.71312
C	1.22015	-0.19415	4.06432
H	1.12882	-1.11975	4.62359
C	0.84652	-0.15337	2.7244
C	0.26266	-1.33248	1.98051
H	0.60649	-2.28041	2.40907
H	-0.8315	-1.31062	2.04819
C	2.04149	-1.71785	0.32233

H	2.67682	-1.41173	1.15651
H	2.43896	-1.25885	-0.5849
C	1.89559	-3.24129	0.16357
H	1.99903	-3.74627	1.12828
H	2.67748	-3.64231	-0.48583
C	0.47052	-3.44982	-0.41716
H	-0.09906	-4.16465	0.18168
H	0.50128	-3.84892	-1.43507
C	-0.19615	-2.0504	-0.39082
H	-1.21419	-2.07803	0.00566
C	-0.19901	-1.37277	-1.77322
H	0.7996	-1.45191	-2.21367
C	-1.29199	-1.94564	-2.71486
H	-0.89237	-2.1486	-3.71147
H	-1.66628	-2.89875	-2.3304
C	-2.01603	0.13824	-1.67221
H	-2.35331	1.15846	-1.86411
H	-2.39668	-0.1657	-0.6935
C	0.07055	0.88953	-2.74323
H	-0.49199	1.82766	-2.8126
H	-0.05434	0.37023	-3.69981
C	1.52368	1.21773	-2.49521
C	2.42801	1.45464	-3.52837
H	2.11746	1.34366	-4.56263
C	3.73018	1.84214	-3.211
H	4.45167	2.03549	-3.99892
C	4.09109	1.97343	-1.86927
C	3.13537	1.70462	-0.89598
H	3.37571	1.78042	0.16045
C	-4.16795	-1.37606	2.01446
C	1.82347	2.12895	3.91123
C	-1.40153	3.38128	0.29742
C	-2.17549	4.60644	0.43856
H	-3.12383	4.51422	-0.10101
H	-2.38342	4.80033	1.49582
H	-1.61359	5.45046	0.02462
C	-2.41027	-0.87035	-2.75996
H	-3.40081	-1.29015	-2.56948
H	-2.45142	-0.39129	-3.74273
C	-5.448	-1.7553	2.60538
H	-5.54831	-1.31439	3.60205
H	-6.27243	-1.4017	1.97838
H	-5.51424	-2.84423	2.69314
H	2.2084	3.04717	4.34134
H	5.09314	2.27181	-1.58073

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.27343
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.11071
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.90440
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.23326

Compound A cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.535952 (Hartree/Particle)
Thermal correction to Energy= 0.567900
Thermal correction to Enthalpy= 0.568844
Thermal correction to Gibbs Free Energy= 0.468304
Sum of electronic and zero-point Energies= -2525.034940
Sum of electronic and thermal Energies= -2525.002993
Sum of electronic and thermal Enthalpies= -2525.002048
Sum of electronic and thermal Free Energies= -2525.102588

Fe	-0.26105	0.64443	0.29739
N	0.61648	0.68874	2.29048
N	0.63678	-1.40068	0.52143
N	-0.8572	-0.21588	-1.67292
N	1.35066	1.35124	-0.99706
N	-2.18454	0.03812	1.2693
N	-1.08275	2.64524	0.26855
C	0.92365	1.77719	3.02223
H	0.72139	2.73817	2.55849
C	1.69986	0.43095	4.84178
H	2.12775	0.32545	5.83408
C	1.38284	-0.69909	4.08761
H	1.55818	-1.69595	4.47997
C	0.8382	-0.53808	2.81487
C	0.42026	-1.71605	1.95575
H	0.95717	-2.6189	2.27121
H	-0.64713	-1.90766	2.10976
C	2.06721	-1.67935	0.16397
H	2.72064	-1.35779	0.97858
H	2.32802	-1.08598	-0.71396
C	2.14232	-3.19242	-0.14183
H	2.50568	-3.75598	0.72189
H	2.84081	-3.38969	-0.9589
C	0.68572	-3.60332	-0.49491
H	0.30385	-4.34155	0.21569
H	0.6127	-4.05899	-1.48598
C	-0.13425	-2.2904	-0.40123
H	-1.12962	-2.4499	0.02542
C	-0.28772	-1.62012	-1.78446
H	0.70253	-1.53077	-2.23953
C	-1.25817	-2.41995	-2.70851
H	-0.74763	-2.81116	-3.59164
H	-1.6612	-3.28289	-2.16849
C	-2.32087	-0.39576	-1.96055
H	-2.77656	0.56776	-2.20257
H	-2.79507	-0.77348	-1.05143
C	-0.24761	0.67547	-2.70414
H	-0.90388	1.54835	-2.80657
H	-0.20967	0.19195	-3.68722
C	1.13297	1.15885	-2.31477
C	2.10193	1.45625	-3.27324
H	1.89857	1.2783	-4.32472
C	3.32384	1.98806	-2.86249
H	4.09094	2.22964	-3.59178
C	3.54362	2.19909	-1.50073
C	2.53441	1.86127	-0.60591
H	2.67062	1.99158	0.46378
C	-3.17935	-0.03792	1.86117
C	1.46612	1.69528	4.29956
C	-1.47511	3.73333	0.18683
C	-1.96913	5.10073	0.08661
H	-2.88203	5.12435	-0.51737
H	-2.19638	5.48921	1.08468
H	-1.21467	5.74064	-0.38203
C	-2.39144	-1.43906	-3.07864
H	-3.36884	-1.92618	-3.12416
H	-2.2178	-0.97828	-4.05626
C	-4.43042	-0.14591	2.60178
H	-4.34183	0.37118	3.56264
H	-5.245	0.30817	2.02835
H	-4.66986	-1.19827	2.78557
H	1.70181	2.59928	4.85057
H	4.47925	2.60914	-1.13601

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.26920
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.14475
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.93164
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.24977

Compound A trans Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.540578
(Hartree/Particle)
Thermal correction to Energy= 0.569904
Thermal correction to Enthalpy= 0.570848
Thermal correction to Gibbs Free Energy=
0.480088
Sum of electronic and zero-point Energies= -
2525.019680
Sum of electronic and thermal Energies= -
2524.990354
Sum of electronic and thermal Enthalpies= -
2524.989410
Sum of electronic and thermal Free Energies= -
2525.080171

Fe	0.05955	0.36361	0.21777
N	1.11451	0.52999	1.93369
N	0.72592	-1.56166	0.34977
N	-1.48636	0.14368	1.367
C	1.6518	1.61786	2.51444
H	1.53621	2.55387	1.97788
C	2.46504	0.3364	4.36826
H	2.99	0.2577	5.31518
C	1.93095	-0.80055	3.75991
H	2.03879	-1.77855	4.21857
C	1.26026	-0.67298	2.54686
C	0.65076	-1.85208	1.81291
H	1.16621	-2.78024	2.08177
H	-0.40012	-1.97309	2.08968
C	2.09941	-1.95821	-0.1359
H	2.8555	-1.64087	0.5854
H	2.29428	-1.44043	-1.07475
C	2.02642	-3.47399	-0.36389
H	2.25104	-4.02682	0.55303
H	2.75692	-3.79594	-1.11019
C	0.56405	-3.71944	-0.81621
H	0.11118	-4.55176	-0.27204
H	0.51117	-3.97463	-1.87849
C	-0.18222	-2.38828	-0.52929
H	-1.11874	-2.55193	0.01063
C	-0.4779	-1.57954	-1.8197
H	0.45478	-1.42244	-2.36857
C	-1.5643	-2.25091	-2.70416
H	-1.24778	-2.30768	-3.74837
H	-1.74993	-3.27789	-2.37654
C	-2.50487	-0.47928	-1.33339
H	-3.04266	0.4709	-1.30992
H	-2.71486	-1.00602	-0.40261
C	-2.37426	0.19692	2.11079
C	2.32789	1.56794	3.7297
C	-2.8284	-1.3707	-2.53874
H	-3.73189	-1.9602	-2.3641
H	-3.01129	-0.77416	-3.43761
C	-3.50002	0.25494	3.03605
H	-3.61932	1.27318	3.42045
H	-4.42298	-0.0391	2.52541
H	-3.33197	-0.42245	3.87964
H	2.7398	2.47562	4.15748
C	2.63005	1.34763	-1.18226
N	1.65683	0.89518	-0.74356
C	3.85833	1.90244	-1.73945
H	4.43961	1.115	-2.23056
H	3.62248	2.67821	-2.47513
H	4.46653	2.34449	-0.94354
C	-0.99871	2.1895	-1.6483
C	-0.85878	3.28331	0.39784
C	-1.4951	3.33634	-2.26125
C	-1.3424	4.46838	-0.1485
H	-0.6137	3.21317	1.45253
H	-1.75484	3.31752	-3.31515
H	-1.46988	5.34229	0.48123
C	-1.66036	4.498	-1.50537
H	-2.04412	5.40313	-1.96571
N	-0.67389	2.16724	-0.3296
N	-1.01815	-0.22752	-1.41444
C	-0.79149	0.88195	-2.38867
H	0.23348	0.81213	-2.76267
H	-1.45847	0.82083	-3.25526

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.29702
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.11661
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.92809
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.24051

Compound A trans Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.537095
(Hartree/Particle)
Thermal correction to Energy= 0.568851
Thermal correction to Enthalpy= 0.569795
Thermal correction to Gibbs Free Energy=
0.468272
Sum of electronic and zero-point Energies= -
2525.014017
Sum of electronic and thermal Energies= -
2524.982260
Sum of electronic and thermal Enthalpies= -
2524.981316
Sum of electronic and thermal Free Energies= -
2525.082839

Fe	-0.35527	0.31748	0.73113
N	0.6548	0.39892	2.46621
N	0.67601	-1.38493	0.55481
N	-2.17487	-0.21036	1.84912
C	1.00079	1.45605	3.22658
H	0.72757	2.43331	2.84615
C	2.04136	0.05277	4.86723
H	2.57855	-0.08447	5.80047
C	1.71536	-1.04727	4.07102
H	2.00039	-2.05215	4.36618
C	1.02813	-0.8427	2.88082
C	0.64835	-1.95772	1.93114
H	1.32364	-2.81448	2.0378
H	-0.36953	-2.30783	2.1376

C	2.10583	-1.26472	0.06931
H	2.75548	-1.03494	0.91554
H	2.17188	-0.43704	-0.63951
C	2.43014	-2.60814	-0.62619
H	3.07103	-3.23848	-0.00446
H	2.9717	-2.41981	-1.55608
C	1.05808	-3.29316	-0.87946
H	0.93659	-4.17642	-0.24586
H	0.94134	-3.62978	-1.91309
C	0.01463	-2.22335	-0.5049
H	-0.90215	-2.65009	-0.08398
C	-0.33726	-1.29811	-1.68907
H	0.582	-0.99224	-2.19403
C	-1.3396	-1.94794	-2.68249
H	-0.90159	-2.06745	-3.676
H	-1.623	-2.94784	-2.33662
C	-2.47508	-0.2784	-1.36175
H	-3.01877	0.66808	-1.3151
H	-2.83176	-0.91211	-0.54631
C	-3.10736	-0.34891	2.52539
C	1.68669	1.32744	4.42998
C	-2.56785	-1.0117	-2.70077
H	-3.51067	-1.55546	-2.80079
H	-2.51434	-0.30892	-3.53867
C	-4.28253	-0.52559	3.36967
H	-4.0237	-0.34146	4.41725
H	-5.06965	0.17289	3.06789
H	-4.66067	-1.54857	3.2728
H	1.94106	2.21289	5.00225
C	3.47841	0.62904	-3.6845
N	2.63074	0.42701	-2.9175
C	4.54379	0.88371	-4.64942
H	4.14425	0.85539	-5.66794
H	4.98612	1.86864	-4.47046
H	5.32599	0.1239	-4.55644
C	-0.94828	2.40741	-1.04872
C	-1.24805	3.22503	1.11014
C	-1.30766	3.63512	-1.59575
C	-1.61352	4.47842	0.63471
H	-1.24214	3.01257	2.17368
H	-1.33736	3.75989	-2.67336
H	-1.88079	5.2649	1.33197
C	-1.63384	4.69089	-0.74384
H	-1.91475	5.65746	-1.1505
N	-0.90126	2.20784	0.29466
N	-1.00293	-0.03347	-1.14962
C	-0.57201	1.20386	-1.87934
H	0.51466	1.16113	-2.02027
H	-1.01709	1.264	-2.87874

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.26740
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.09760
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.89932
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.22789

Compound A trans Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.535789 (Hartree/Particle)
Thermal correction to Energy= 0.567819
Thermal correction to Enthalpy= 0.568763
Thermal correction to Gibbs Free Energy= 0.467840
Sum of electronic and zero-point Energies= -2525.030706
Sum of electronic and thermal Energies= -2524.998676
Sum of electronic and thermal Enthalpies= -2524.997732
Sum of electronic and thermal Free Energies= -2525.098654

Fe	0.10656	0.52009	0.31627
N	1.30597	0.28424	2.13323
N	0.74708	-1.62704	0.26091
N	-1.59807	0.40714	1.73717
C	1.89489	1.24917	2.86414
H	1.80817	2.26379	2.48476
C	2.67978	-0.3376	4.47432
H	3.21797	-0.58501	5.38426
C	2.0814	-1.34249	3.71424
H	2.14699	-2.38267	4.01786
C	1.39696	-0.99826	2.54971
C	0.68758	-2.02834	1.69137
H	1.11679	-3.02229	1.86659
H	-0.3669	-2.0784	1.98654
C	2.09878	-1.96013	-0.30217
H	2.87804	-1.69972	0.41782
H	2.25641	-1.34607	-1.19159
C	2.04309	-3.45359	-0.66264
H	2.35878	-4.07416	0.1814
H	2.71538	-3.68767	-1.49187
C	0.55432	-3.71014	-1.01211
H	0.16168	-4.57523	-0.47193
H	0.42351	-3.92212	-2.07697
C	-0.19606	-2.40791	-0.60738
H	-1.09611	-2.62367	-0.02351
C	-0.59475	-1.56555	-1.8421
H	0.29559	-1.39821	-2.45581
C	-1.73747	-2.23559	-2.65722
H	-1.52517	-2.20397	-3.72887
H	-1.84203	-3.29122	-2.39185
C	-2.58161	-0.4828	-1.18161
H	-3.12501	0.46448	-1.15502
H	-2.69937	-0.95685	-0.20481
C	-2.43133	0.53887	2.53326
C	2.58671	0.98558	4.04102
C	-3.0172	-1.43052	-2.31214
H	-3.84338	-2.07183	-1.99496
H	-3.37258	-0.87009	-3.18182
C	-3.48363	0.69686	3.52965
H	-3.04337	0.88746	4.5136
H	-4.12937	1.53888	3.26028
H	-4.09096	-0.21259	3.58184
H	3.04514	1.79631	4.59692
C	2.88549	1.71699	-1.16097
N	1.92477	1.21321	-0.75028
C	4.09467	2.34182	-1.68305
H	4.38702	1.86533	-2.62439
H	3.91892	3.40718	-1.86317
H	4.91182	2.23338	-0.96258
C	-1.16614	2.19757	-1.81077
C	-0.92609	3.53377	0.07455
C	-1.71542	3.25908	-2.52826
C	-1.45578	4.64131	-0.57792
H	-0.61206	3.59692	1.11297
H	-2.02987	3.1137	-3.55706
H	-1.55622	5.58578	-0.05416
C	-1.85718	4.49983	-1.90687
H	-2.28265	5.33915	-2.44848
N	-0.7768	2.33735	-0.52415

N	-1.11783	-0.22916	-1.40156
C	-0.94107	0.83078	-2.42937
H	0.08722	0.77116	-2.80456
H	-1.60601	0.69372	-3.29068

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2524.26740
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.14159
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.92911
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.24745

Compound B cis-α Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.721313 (Hartree/Particle)
Thermal correction to Energy= 0.774423
Thermal correction to Enthalpy= 0.775367
Thermal correction to Gibbs Free Energy= 0.631149
Sum of electronic and zero-point Energies= -4335.118088
Sum of electronic and thermal Energies= -4335.064977
Sum of electronic and thermal Enthalpies= -4335.064033
Sum of electronic and thermal Free Energies= -4335.208252

Fe	0.00554	-0.08626	-0.05428
N	-1.60013	-0.8161	0.89244
N	0.72463	-1.96849	0.35706
N	-0.43669	-0.8338	-1.91922
N	1.62078	0.57961	-1.03094
N	0.60297	0.65928	1.63147
N	-0.84978	1.62004	-0.39201
C	-2.8486	-0.31842	0.87087
H	-3.01597	0.52541	0.21641
C	-3.61814	-1.93687	2.45101
H	-4.39998	-2.37543	3.06102
C	-2.33322	-2.47325	2.46117
H	-2.09939	-3.33662	3.07604
C	-1.34509	-1.88797	1.67584
C	0.08262	-2.3628	1.64982
H	0.64557	-1.88254	2.45673
H	0.13467	-3.44447	1.81638
C	2.20281	-2.23113	0.43094
H	2.6025	-1.83935	1.36928
H	2.68491	-1.69577	-0.38806
C	2.36471	-3.74539	0.25244
H	2.26477	-4.26917	1.20788
H	3.3511	-3.99545	-0.14553
C	1.21759	-4.12993	-0.71692
H	0.70452	-5.039	-0.39425
H	1.60015	-4.32795	-1.72276
C	0.25555	-2.90728	-0.7373
H	-0.77268	-3.19833	-0.50449
C	0.2657	-2.16803	-2.0769
H	1.30278	-1.96508	-2.35858
C	-0.49175	-2.94022	-3.19571
H	0.12914	-3.06868	-4.08551
H	-0.75544	-3.94494	-2.85163
C	-1.85546	-1.13737	-2.31091
H	-2.3881	-0.20724	-2.52309
H	-2.34623	-1.61824	-1.46361
C	0.14923	0.14695	-2.88623
H	-0.54801	0.98743	-2.96506
H	0.25479	-0.283	-3.88849
C	1.47683	0.63637	-2.37394
C	2.47965	1.13752	-3.198
H	2.33684	1.16538	-4.27365
C	3.66194	1.60138	-2.62696
H	4.45357	1.99916	-3.25225
C	3.82415	1.53559	-1.23822
C	2.77326	1.01012	-0.48957
H	2.8569	0.92902	0.58501
C	0.91454	1.24485	2.5817
C	-3.89383	-0.83378	1.63452
C	5.08021	1.98892	-0.55889
C	6.25027	1.20504	-0.61353
C	5.12965	3.20901	0.14561
C	7.43305	1.64538	-0.01407
C	6.31801	3.64164	0.74138
C	7.47047	2.86673	0.65274
H	8.32145	1.02742	-0.06956
H	6.33814	4.58888	1.26735
H	8.3933	3.20977	1.1087
C	-5.25818	-0.21982	1.55505
C	-5.5424	1.01044	2.18273
C	-6.29652	-0.86143	0.85038
C	-6.8276	1.5582	2.13094
C	-7.57759	-0.30575	0.80383
C	-7.84587	0.89698	1.45113
H	-7.02858	2.49851	2.63076
H	-8.36078	-0.81701	0.25669
H	-8.84414	1.3209	1.42023
C	-1.33512	2.67093	-0.44673
C	-1.97481	3.98032	-0.4813
H	-2.43672	4.15526	-1.45818
H	-2.74683	4.0209	0.29412
H	-1.23592	4.76609	-0.29462
C	-1.76047	-2.10229	-3.4987
H	-2.65881	-2.71833	-3.58442
H	-1.65643	-1.55798	-4.44219
C	3.89313	4.06337	0.3085
C	6.24539	-0.14453	-1.30097
C	-4.46089	1.78875	2.89653
C	-6.0422	-2.15536	0.10524
F	3.24888	4.2805	-0.85651
F	4.16107	5.25477	0.8552
F	2.97999	3.45112	1.13613
F	7.39117	-0.81022	-1.11401
F	6.05012	-0.03568	-2.63484
F	5.24063	-0.93573	-0.82593
F	-3.5529	2.3036	1.9992
F	-3.74558	1.02892	3.75146
F	-4.94564	2.82947	3.58347
F	-4.98314	-2.03446	-0.74498
F	-7.09626	-2.52961	-0.62983
F	-5.74799	-3.17516	0.94384
C	1.3358	2.0091	3.7493
H	1.83422	1.35779	4.47429
H	2.03189	2.79207	3.43097
H	0.46827	2.47278	4.22955

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4333.28130
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4335.11450
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4336.51720

UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4337.10958

Compound B cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.719310
(Hartree/Particle)
Thermal correction to Energy= 0.773397
Thermal correction to Enthalpy= 0.774341
Thermal correction to Gibbs Free Energy=
0.625593
Sum of electronic and zero-point Energies= -
4335.089931
Sum of electronic and thermal Energies= -
4335.035845
Sum of electronic and thermal Enthalpies= -
4335.034901
Sum of electronic and thermal Free Energies= -
4335.183648

Fe	0.00705	-0.12673	-0.08642
N	-1.87695	-0.92503	0.85903
N	0.55846	-2.05682	0.37985
N	-0.25994	-0.83614	-2.00363
N	1.90688	0.54442	-1.08774
N	0.56845	0.62772	1.65503
N	-0.82382	1.6327	-0.44852
C	-3.11348	-0.40814	0.87756
H	-3.28914	0.43754	0.22272
C	-3.85011	-2.00943	2.48575
H	-4.6151	-2.43542	3.1253
C	-2.57407	-2.56606	2.45351
H	-2.33434	-3.42997	3.06601
C	-1.60493	-1.98908	1.63413
C	-0.17114	-2.4707	1.62114
H	0.36063	-2.02688	2.46974
H	-0.13453	-3.55785	1.75373
C	2.02725	-2.34042	0.55018
H	2.36085	-1.98553	1.52788
H	2.56577	-1.77626	-0.21283
C	2.18908	-3.85251	0.33471
H	2.07779	-4.39836	1.27599
H	3.18173	-4.09143	-0.05438
C	1.05613	-4.22343	-0.65964
H	0.48158	-5.08375	-0.30786
H	1.45648	-4.49784	-1.63985
C	0.16348	-2.95589	-0.77217
H	-0.89791	-3.19178	-0.65741
C	0.37005	-2.2096	-2.09528
H	1.44168	-2.07135	-2.26285
C	-0.31691	-2.92457	-3.29303
H	0.35824	-3.00603	-4.14831
H	-0.59594	-3.94623	-3.01954
C	-1.67159	-1.07237	-2.46983
H	-2.13909	-0.12004	-2.73059
H	-2.22948	-1.50228	-1.63623
C	0.42289	0.10237	-2.95219
H	-0.24224	0.96203	-3.08738
H	0.55243	-0.36004	-3.93711
C	1.75342	0.58852	-2.4223
C	2.73908	1.1143	-3.25632
H	2.59679	1.13468	-4.33257
C	3.90427	1.62283	-2.68775
H	4.67927	2.04488	-3.31787
C	4.07294	1.57801	-1.29735
C	3.03979	1.01547	-0.54861
H	3.12402	0.94027	0.5294
C	0.93539	1.22762	2.57559
C	-4.14133	-0.89927	1.68187
C	5.30542	2.09569	-0.62222
C	6.52299	1.38993	-0.70248
C	5.28388	3.29996	0.11193
C	7.67945	1.88903	-0.098
C	6.44672	3.79118	0.71293
C	7.64466	3.09243	0.6004
H	8.60412	1.32914	-0.17344
H	6.41129	4.72516	1.26129
H	8.54683	3.48083	1.06131
C	-5.49188	-0.25228	1.66712
C	-5.70593	1.00009	2.28027
C	-6.58742	-0.87812	1.03885
C	-6.97622	1.58422	2.28781
C	-7.85254	-0.2857	1.05093
C	-8.0498	0.93899	1.68208
H	-7.12193	2.54039	2.77643
H	-8.67923	-0.78613	0.56076
H	-9.03568	1.39179	1.69658
C	-1.36429	2.65694	-0.47786
C	-2.0635	3.93483	-0.48152
H	-2.53594	4.10865	-1.45349
H	-2.83242	3.92224	0.29807
H	-1.35846	4.74775	-0.28009
C	-1.5654	-2.06747	-3.63419
H	-2.47327	-2.66859	-3.72496
H	-1.43354	-1.54585	-4.58662
C	4.00182	4.07916	0.29814
C	6.60174	0.06108	-1.42614
C	-4.56815	1.76384	2.91855
C	-6.41539	-2.19844	0.31586
F	3.33188	4.27333	-0.85595
F	4.20668	5.27823	0.85681
F	3.13247	3.4087	1.12997
F	7.78079	-0.54535	-1.23658
F	6.42752	0.20102	-2.76107
F	5.63567	-0.79379	-0.9951
F	-3.70282	2.25134	1.96388
F	-3.81831	1.00203	3.74116
F	-4.99054	2.82366	3.61868
F	-5.38699	-2.1445	-0.57172
F	-7.51377	-2.54323	-0.36888
F	-6.13695	-3.20967	1.17153
C	1.41472	2.00675	3.70922
H	1.92504	1.35903	4.42907
H	2.11382	2.76841	3.34827
H	0.57303	2.49711	4.20881

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4333.23735
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4335.09399
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4336.47950
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4337.08117

Compound B cis-α Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.716494
(Hartree/Particle)
Thermal correction to Energy= 0.772041
Thermal correction to Enthalpy= 0.772985
Thermal correction to Gibbs Free Energy=
0.618628

Sum of electronic and zero-point Energies= -4335.117363
Sum of electronic and thermal Energies= -4335.061817
Sum of electronic and thermal Enthalpies= -4335.060873
Sum of electronic and thermal Free Energies= -4335.215229

Fe	-0.00292	-0.01574	-0.01164
N	-1.74954	-0.87281	0.95832
N	0.63021	-2.11877	0.39844
N	-0.32548	-0.86239	-2.05465
N	1.76912	0.62983	-1.09541
N	0.72962	0.85965	1.84782
N	-1.02401	1.88356	-0.34842
C	-2.98759	-0.35153	0.95818
H	-3.12951	0.5387	0.35911
C	-3.78874	-2.05681	2.42002
H	-4.58041	-2.52355	2.99566
C	-2.51284	-2.61387	2.40438
H	-2.30007	-3.51924	2.96422
C	-1.50761	-1.99721	1.66237
C	-0.08733	-2.52007	1.63748
H	0.46072	-2.09241	2.48549
H	-0.09325	-3.60834	1.77869
C	2.09199	-2.41747	0.52775
H	2.45467	-2.0906	1.50555
H	2.62637	-1.84287	-0.23357
C	2.23334	-3.92562	0.27055
H	2.10924	-4.49254	1.19817
H	3.22088	-4.17554	-0.12502
C	1.09287	-4.2434	-0.73139
H	0.52291	-5.12366	-0.42365
H	1.48875	-4.46272	-1.72717
C	0.19453	-2.96878	-0.76746
H	-0.8615	-3.21595	-0.62317
C	0.34161	-2.21308	-2.10549
H	1.40682	-2.05236	-2.29731
C	-0.34103	-2.98789	-3.27501
H	0.334	-3.09832	-4.12732
H	-0.61134	-3.99995	-2.96018
C	-1.72524	-1.1413	-2.50691
H	-2.2194	-0.20797	-2.78824
H	-2.27678	-1.56783	-1.66467
C	0.33667	0.08633	-2.98947
H	-0.3431	0.93561	-3.12713
H	0.50044	-0.35439	-3.98103
C	1.65021	0.59758	-2.43836
C	2.6764	1.05073	-3.26472
H	2.5634	1.01561	-4.34381
C	3.84512	1.54572	-2.69214
H	4.65175	1.9038	-3.32244
C	3.98078	1.56204	-1.29781
C	2.90718	1.08739	-0.54816
H	2.9577	1.06827	0.53287
C	1.09061	1.53416	2.71883
C	-4.04914	-0.89922	1.67461
C	5.22858	2.04095	-0.62147
C	6.39693	1.25239	-0.63069
C	5.27352	3.28711	0.03636
C	7.57367	1.7124	-0.03447
C	6.45603	3.73921	0.6294
C	7.60708	2.95854	0.58491
H	8.46029	1.08974	-0.05463
H	6.47295	4.70645	1.11777
H	8.52544	3.31663	1.03832
C	-5.40856	-0.27217	1.62111
C	-5.6855	0.93434	2.2969
C	-6.45163	-0.87861	0.89208
C	-6.96776	1.49074	2.26884
C	-7.72943	-0.31422	0.86962
C	-7.99068	0.86282	1.56509
H	-7.16281	2.41114	2.80658
H	-8.51563	-0.79858	0.30272
H	-8.98673	1.29286	1.55282
C	-1.56126	2.90984	-0.30343
C	-2.2609	4.18518	-0.22596
H	-2.75759	4.40432	-1.17638
H	-3.01059	4.12924	0.56998
H	-1.55395	4.9896	0.00005
C	-1.59858	-2.16052	-3.64895
H	-2.49538	-2.77843	-3.73887
H	-1.46294	-1.65462	-4.60975
C	4.03873	4.15108	0.15188
C	6.39677	-0.12281	-1.26606
C	-4.59975	1.68045	3.03777
C	-6.20755	-2.14406	0.09531
F	3.4019	4.31661	-1.02452
F	4.30647	5.36537	0.64667
F	3.11881	3.57929	1.00265
F	7.5311	-0.79056	-1.02174
F	6.24311	-0.06007	-2.60913
F	5.37166	-0.88426	-0.79288
F	-3.69896	2.23682	2.15673
F	-3.87788	0.88538	3.85262
F	-5.08036	2.69016	3.773
F	-5.13369	-2.00846	-0.72978
F	-7.25735	-2.46653	-0.67069
F	-5.94869	-3.20398	0.89634
C	1.56986	2.39697	3.79022
H	2.10236	1.80774	4.54339
H	2.25047	3.14225	3.36558
H	0.72779	2.90768	4.26777

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -4333.23708
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -4335.12629
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -4336.50306
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -4337.08117

Compound B cis-β Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.720892 (Hartree/Particle)
Thermal correction to Energy= 0.774153
Thermal correction to Enthalpy= 0.775097
Thermal correction to Gibbs Free Energy= 0.630244
Sum of electronic and zero-point Energies= -4335.112728
Sum of electronic and thermal Energies= -4335.059467
Sum of electronic and thermal Enthalpies= -4335.058522
Sum of electronic and thermal Free Energies= -4335.203375

Fe	-1.488	-0.72817	-0.57446
N	-0.63815	-0.47967	1.20956
N	-0.63218	-2.5768	-0.4095
N	-2.17698	-1.36107	-2.40902
N	0.02804	-0.01804	-1.65213

N	-3.09088	-1.28092	0.39173
N	-2.27652	1.03439	-0.64126
C	-0.37279	0.67323	1.84411
H	-0.5803	1.58159	1.29447
C	0.42525	-0.48139	3.77783
H	0.83838	-0.48773	4.78047
C	0.17434	-1.68148	3.11448
H	0.39359	-2.6316	3.5914
C	-0.36689	-1.65221	1.8342
C	-0.72929	-2.89353	1.04945
H	-0.08507	-3.73339	1.33028
H	-1.75827	-3.1877	1.2741
C	0.7869	-2.85054	-0.84872
H	1.48484	-2.48975	-0.09117
H	0.98737	-2.29499	-1.76233
C	0.85506	-4.3691	-1.10223
H	1.21723	-4.90644	-0.22124
H	1.55422	-4.59196	-1.91178
C	-0.60358	-4.78642	-1.44011
H	-0.96301	-5.55513	-0.75082
H	-0.69188	-5.2043	-2.44682
C	-1.4358	-3.49016	-1.29162
H	-2.40445	-3.66528	-0.8149
C	-1.65476	-2.77682	-2.63899
H	-0.69088	-2.68514	-3.14668
C	-2.69206	-3.50047	-3.54559
H	-2.23457	-3.88737	-4.45913
H	-3.11802	-4.35937	-3.01603
C	-3.65489	-1.48502	-2.66245
H	-4.08925	-0.49594	-2.82335
H	-4.11113	-1.91364	-1.76833
C	-1.58389	-0.41948	-3.40803
H	-2.23347	0.46209	-3.44698
H	-1.56262	-0.84903	-4.41598
C	-0.20627	0.01484	-2.9843
C	0.74891	0.47797	-3.884
H	0.5367	0.48048	-4.9485
C	1.96936	0.94457	-3.40269
H	2.72441	1.31469	-4.08766
C	2.21342	0.92739	-2.02552
C	1.21225	0.42642	-1.19505
H	1.37213	0.37287	-0.12675
C	-4.05147	-1.42256	1.02536
C	0.14812	0.73071	3.13643
C	-2.7188	2.10255	-0.56221
C	-3.26126	3.44788	-0.41742
H	-4.28391	3.49168	-0.80524
H	-3.26899	3.71748	0.64392
H	-2.64298	4.16602	-0.96533
C	-3.78735	-2.45252	-3.83953
H	-4.78534	-2.8947	-3.89561
H	-3.60816	-1.94408	-4.79221
C	-5.25693	-1.60286	1.82606
H	-5.16924	-1.04095	2.76174
H	-6.13266	-1.2417	1.27712
H	-5.40158	-2.66211	2.06236
C	0.39491	2.05584	3.78946
C	-0.67289	2.82911	4.28949
C	1.70258	2.56212	3.92671
C	-0.43262	4.04747	4.93147
C	1.93261	3.78107	4.56967
C	0.86825	4.51833	5.08017
H	-1.26611	4.62069	5.3201
H	2.94667	4.15044	4.6664
H	1.05136	5.46025	5.58656
C	2.88784	1.80478	3.36673
C	-2.10764	2.38542	4.11376
F	2.69373	1.46884	2.06129
F	3.11194	0.64956	4.03273
F	4.01768	2.52579	3.41933
F	-2.30723	1.09837	4.47116
F	-2.49185	2.47396	2.7967
F	-2.96587	3.13802	4.81165
C	3.50415	1.41022	-1.4376
C	4.65814	0.60277	-1.46699
C	3.59548	2.68279	-0.84114
C	5.86504	1.06447	-0.936
C	4.80641	3.13583	-0.3112
C	5.94079	2.33151	-0.36472
H	6.74164	0.42841	-0.97031
H	4.85866	4.1219	0.13486
H	6.88123	2.68949	0.04102
C	4.61064	-0.78761	-2.06205
C	2.38075	3.57815	-0.74232
F	4.34183	-0.76308	-3.38764
F	5.76052	-1.45111	-1.895
F	3.62766	-1.5398	-1.48506
F	2.68163	4.79391	-0.26586
F	1.76787	3.7462	-1.93499
F	1.43825	3.05049	0.09824

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4333.27679
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4335.11278
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4336.51536
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4337.10809

Compound B cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.718263 (Hartree/Particle)
Thermal correction to Energy= 0.772797
Thermal correction to Enthalpy= 0.773741
Thermal correction to Gibbs Free Energy= 0.623877
Sum of electronic and zero-point Energies= -4335.094348
Sum of electronic and thermal Energies= -4335.039814
Sum of electronic and thermal Enthalpies= -4335.038870
Sum of electronic and thermal Free Energies= -4335.188734

Fe	-1.5596	-0.61094	-0.63508
N	-0.62985	-0.46286	1.23848
N	-0.57192	-2.64769	-0.39024
N	-2.18168	-1.44098	-2.49196
N	-0.03452	0.01625	-1.71962
N	-3.15237	-1.12173	0.3229
N	-2.38332	1.40983	-0.70696
C	-0.36463	0.67969	1.89036
H	-0.55679	1.59762	1.34824
C	0.40289	-0.50542	3.81318
H	0.8097	-0.52955	4.81845
C	0.14457	-1.69346	3.13199
H	0.35021	-2.65179	3.59875
C	-0.38345	-1.6454	1.84449
C	-0.74648	-2.89453	1.05881
H	-0.15051	-3.74382	1.41626
H	-1.79587	-3.14362	1.2488
C	0.84331	-2.9365	-0.78498

H	1.52685	-2.59596	-0.00419
H	1.0834	-2.37195	-1.68702
C	0.89874	-4.45518	-1.05126
H	1.21756	-5.00099	-0.15846
H	1.62138	-4.69034	-1.83662
C	-0.55471	-4.84254	-1.43956
H	-0.94559	-5.61997	-0.77764
H	-0.61756	-5.23875	-2.45695
C	-1.37489	-3.53201	-1.28246
H	-2.35102	-3.70606	-0.81843
C	-1.5889	-2.83638	-2.64788
H	-0.61491	-2.71675	-3.12993
C	-2.57049	-3.63153	-3.56163
H	-2.07008	-4.02565	-4.44927
H	-2.97238	-4.49196	-3.01632
C	-3.64416	-1.63475	-2.77417
H	-4.11578	-0.67138	-2.98275
H	-4.10567	-2.04921	-1.87472
C	-1.59435	-0.50124	-3.49541
H	-2.2623	0.36637	-3.5558
H	-1.54846	-0.94306	-4.49741
C	-0.23074	-0.03475	-3.05912
C	0.75221	0.3728	-3.95489
H	0.5702	0.31394	-5.02324
C	1.96147	0.86219	-3.46738
H	2.73514	1.19157	-4.15201
C	2.17156	0.91643	-2.08532
C	1.14384	0.47107	-1.2554
H	1.27384	0.47235	-0.18226
C	-4.12493	-1.28274	0.93295
C	0.14341	0.71933	3.18758
C	-2.73587	2.48983	-0.47647
C	-3.1714	3.8429	-0.15696
H	-4.18673	4.01005	-0.53009
H	-3.16208	3.97094	0.93038
H	-2.49767	4.57395	-0.61464
C	-3.70369	-2.64741	-3.91931
H	-4.67896	-3.1365	-3.9854
H	-3.52256	-2.16124	-4.8834
C	-5.34592	-1.48422	1.70311
H	-5.26922	-0.96587	2.66455
H	-6.20655	-1.0876	1.1546
H	-5.50695	-2.55126	1.88839
C	0.40288	2.0335	3.85802
C	-0.65389	2.79816	4.39257
C	1.71295	2.53807	3.97594
C	-0.40018	4.0035	5.0537
C	1.95711	3.74395	4.63802
C	0.90399	4.47009	5.18662
H	-1.22552	4.56986	5.46895
H	2.97307	4.11171	4.71993
H	1.09814	5.40111	5.70884
C	2.8818	1.79695	3.36256
C	-2.09125	2.36094	4.22718
F	2.66121	1.52972	2.04505
F	3.10394	0.60812	3.96619
F	4.01992	2.50308	3.43202
F	-2.29292	1.07259	4.57437
F	-2.4854	2.46275	2.91264
F	-2.94112	3.11183	4.93719
C	3.45168	1.42058	-1.49159
C	4.616	0.62658	-1.50093
C	3.52469	2.70233	-0.91123
C	5.81282	1.10929	-0.96599
C	4.72624	3.17603	-0.3777
C	5.86997	2.38435	-0.41091
H	6.69647	0.48244	-0.98403
H	4.76394	4.16904	0.05418
H	6.80297	2.75832	-0.00243
C	4.59361	-0.77299	-2.07663
C	2.30199	3.58857	-0.83182
F	4.36271	-0.76873	-3.41002
F	5.74374	-1.42501	-1.86897
F	3.60129	-1.52267	-1.51636
F	2.59529	4.82427	-0.40416
F	1.67213	3.70664	-2.0214
F	1.37499	3.08349	0.04048

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4333.24020
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4335.11278
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4335.09951
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4337.08543

Compound B cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.716231 (Hartree/Particle)
Thermal correction to Energy= 0.771909
Thermal correction to Enthalpy= 0.772854
Thermal correction to Gibbs Free Energy= 0.618167
Sum of electronic and zero-point Energies= -4335.112153
Sum of electronic and thermal Energies= -4335.056474
Sum of electronic and thermal Enthalpies= -4335.055530
Sum of electronic and thermal Free Energies= -4335.210217

Fe	-1.59274	-0.57405	-0.60882
N	-0.71452	-0.45806	1.35011
N	-0.6275	-2.58705	-0.33316
N	-2.12065	-1.44827	-2.57125
N	0.03876	0.13435	-1.8321
N	-3.5092	-1.23191	0.35434
N	-2.46734	1.39519	-0.56313
C	-0.42927	0.67217	2.01368
H	-0.62332	1.6	1.48829
C	0.33837	-0.55365	3.908
H	0.7556	-0.59778	4.90867
C	0.05324	-1.7304	3.2161
H	0.24699	-2.69707	3.67026
C	-0.47875	-1.65412	1.93152
C	-0.85327	-2.87338	1.10687
H	-0.29159	-3.74923	1.45429
H	-1.91596	-3.09374	1.25501
C	0.81192	-2.84282	-0.66981
H	1.45256	-2.49519	0.14368
H	1.07634	-2.26207	-1.55364
C	0.91592	-4.35894	-0.94755
H	1.26301	-4.90305	-0.0646
H	1.6397	-4.55869	-1.74162
C	-0.52517	-4.79604	-1.33139
H	-0.91058	-5.53858	-0.62705
H	-0.56845	-5.25531	-2.32257
C	-1.3695	-3.4962	-1.25913
H	-2.36923	-3.66919	-0.84793
C	-1.51194	-2.83908	-2.65342
H	-0.51512	-2.72894	-3.08886
C	-2.44237	-3.67294	-3.58888

H	-1.90069	-4.07115	-4.4501
H	-2.84567	-4.53247	-3.04343
C	-3.56992	-1.6667	-2.89633
H	-4.04296	-0.71666	-3.15746
H	-4.05904	-2.05063	-1.99732
C	-1.50581	-0.53731	-3.58571
H	-2.18022	0.32037	-3.69778
H	-1.43339	-1.01604	-4.56924
C	-0.14499	-0.03104	-3.15741
C	0.84962	0.2994	-4.07496
H	0.68143	0.1585	-5.13814
C	2.06002	0.81065	-3.6119
H	2.84564	1.07204	-4.31223
C	2.26163	0.96963	-2.2355
C	1.21158	0.61442	-1.38896
H	1.32394	0.70569	-0.31461
C	-4.50148	-1.32189	0.94813
C	0.09542	0.68586	3.30341
C	-2.8386	2.46344	-0.30878
C	-3.29697	3.79918	0.04761
H	-4.326	3.94884	-0.29415
H	-3.26082	3.90643	1.13699
H	-2.65347	4.55524	-0.41311
C	-3.58231	-2.71965	-4.0069
H	-4.54728	-3.22761	-4.08183
H	-3.3837	-2.26272	-4.98173
C	-5.74854	-1.44625	1.69273
H	-5.66019	-0.93404	2.65618
H	-6.56929	-0.9963	1.12494
H	-5.97767	-2.50181	1.87079
C	0.3842	1.98725	3.98715
C	-0.64791	2.73439	4.5892
C	1.69531	2.49871	4.04324
C	-0.3667	3.92709	5.26182
C	1.96743	3.69197	4.71708
C	0.94067	4.39794	5.33772
H	-1.17291	4.48079	5.72857
H	2.98395	4.06565	4.75159
H	1.15715	5.31858	5.86949
C	2.82686	1.78699	3.33312
C	-2.08928	2.29377	4.47641
F	2.54857	1.62786	2.0082
F	3.04684	0.55065	3.83364
F	3.98032	2.46472	3.41264
F	-2.27283	1.00379	4.82607
F	-2.53044	2.39935	3.1775
F	-2.91403	3.03977	5.22019
C	3.55372	1.4724	-1.6684
C	4.69474	0.64485	-1.63259
C	3.66419	2.7791	-1.15326
C	5.90623	1.12134	-1.12561
C	4.8805	3.24649	-0.64824
C	6.00178	2.42279	-0.64184
H	6.77107	0.46879	-1.10861
H	4.94669	4.25947	-0.26932
H	6.94648	2.79185	-0.25635
C	4.63103	-0.78619	-2.12221
C	2.46538	3.70021	-1.11024
F	4.41479	-0.85921	-3.4559
F	5.75744	-1.46137	-1.86072
F	3.60986	-1.46863	-1.52811
F	2.79768	4.95128	-0.76137
F	1.82074	3.76427	-2.29502
F	1.54429	3.26983	-0.19493

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4333.23598
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4336.50925
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4337.10173

Compound B trans Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.721150
(Hartree/Particle)
Thermal correction to Energy= 0.774154
Thermal correction to Enthalpy= 0.775098
Thermal correction to Gibbs Free Energy=
0.630884
Sum of electronic and zero-point Energies= -
4335.101698
Sum of electronic and thermal Energies= -
4335.048694
Sum of electronic and thermal Enthalpies= -
4335.047750
Sum of electronic and thermal Free Energies= -
4335.191964

Fe	-0.29364	-1.3892	-0.76252
N	0.67704	-1.21746	0.98268
N	0.18411	-3.3544	-0.49581
N	-1.91573	-1.38549	0.30511
C	1.29341	-0.14916	1.50647
H	1.28813	0.75649	0.91073
C	1.91432	-1.36887	3.46557
H	2.39717	-1.43003	4.43538
C	1.2947	-2.49063	2.91482
H	1.2949	-3.43778	3.44495
C	0.68208	-2.3871	1.67141
C	-0.00625	-3.54529	0.97434
H	0.39271	-4.50183	1.32912
H	-1.07857	-3.53788	1.18846
C	1.54158	-3.89668	-0.86902
H	2.27704	-3.61057	-0.11421
H	1.84308	-3.44701	-1.815
C	1.34123	-5.40931	-1.03098
H	1.44731	-5.92975	-0.07446
H	2.08732	-5.8369	-1.70543
C	-0.10323	-5.5426	-1.57715
H	-0.66662	-6.30725	-1.0368
H	-0.10634	-5.83735	-2.6306
C	-0.7418	-4.13878	-1.39345
H	-1.72016	-4.19413	-0.90791
C	-0.88242	-3.3695	-2.73525
H	0.09502	-3.3193	-3.22295
C	-1.96454	-3.98526	-3.66337
H	-1.59302	-4.09723	-4.68486
H	-2.24684	-4.9851	-3.32127
C	-2.83037	-2.08451	-2.41838
H	-3.28661	-1.09366	-2.46841
H	-3.13239	-2.54372	-1.47727
C	-2.82904	-1.13021	0.97205
C	-3.16427	-3.00638	-3.59846
H	-4.11717	-3.5184	-3.44294
H	-3.25971	-2.44142	-4.53056
C	-3.98415	-0.78631	1.79198
H	-3.7217	-0.83903	2.85347
H	-4.3052	0.23281	1.55312
H	-4.80988	-1.47796	1.59593
C	2.45234	-0.68272	-1.97329
N	1.40341	-1.04694	-1.63985
C	3.78168	-0.23316	-2.36766
H	4.28908	-1.01001	-2.9488
H	3.70773	0.67367	-2.97642
H	4.36877	-0.01455	-1.46995

C	-1.09053	0.43113	-2.74328
C	-0.97073	1.56992	-0.71862
C	-1.47852	1.59106	-3.4034
H	-0.77871	1.51832	0.34711
H	-1.69171	1.56725	-4.46744
C	-1.60218	2.77773	-2.68163
H	-1.90631	3.69251	-3.1796
N	-0.82946	0.43104	-1.41112
N	-1.32658	-1.96043	-2.42545
C	-0.94988	-0.9159	-3.42612
H	0.0862	-1.08498	-3.73163
H	-1.56858	-0.95657	-4.32922
C	-1.49075	4.01267	-0.47228
C	-2.73933	4.38928	0.05933
C	-0.3783	4.83394	-0.20813
C	-2.87334	5.56528	0.80178
C	-0.52035	6.0096	0.53398
C	-1.76738	6.37963	1.02964
H	-3.84386	5.83999	1.198
H	0.34615	6.6343	0.71625
H	-1.8765	7.29751	1.59784
C	2.58862	1.0681	3.27428
C	1.86574	2.00299	4.03913
C	3.94859	1.32598	3.01611
C	2.49369	3.13994	4.55468
C	4.56952	2.46556	3.5339
C	3.84544	3.36584	4.3106
H	1.92168	3.84271	5.14898
H	5.61855	2.64321	3.32818
H	4.33274	4.24478	4.7196
C	1.92537	-0.16874	2.7499
C	-1.35173	2.77617	-1.3068
C	0.99612	4.44389	-0.70412
C	-3.95363	3.51106	-0.14266
C	4.75453	0.38611	2.14851
C	0.38879	1.80246	4.29607
F	-3.73373	2.25322	0.35962
F	-5.04017	3.989	0.47373
F	-4.25891	3.3465	-1.44685
F	1.40592	3.26386	-0.14439
F	1.92592	5.35837	-0.40035
F	1.02569	4.25708	-2.0414
F	-0.31806	1.78031	3.12468
F	0.13149	0.62969	4.91483
F	-0.13504	2.78095	5.04569
F	4.78393	-0.87031	2.63894
F	6.01853	0.79267	1.98756
F	4.20663	0.29319	0.89297

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4333.26600
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4335.09814
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4336.49984
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4337.09405

Compound B trans triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.715961 (Hartree/Particle)
Thermal correction to Energy= 0.770791
Thermal correction to Enthalpy= 0.771735
Thermal correction to Gibbs Free Energy= 0.620280
Sum of electronic and zero-point Energies= -4335.077366
Sum of electronic and thermal Energies= -4335.022535
Sum of electronic and thermal Enthalpies= -4335.021591
Sum of electronic and thermal Free Energies= -4335.173046

Fe	-0.2773	-1.25992	-0.68281
N	0.82628	-1.44701	1.17834
N	0.284	-3.42017	-0.6132
N	-1.98962	-1.08112	0.70856
C	1.36858	-0.443	1.88244
H	1.3051	0.54753	1.44319
C	2.05464	-1.93305	3.61507
H	2.53518	-2.12798	4.5679
C	1.5055	-2.98116	2.87907
H	1.55615	-4.00089	3.24791
C	0.88382	-2.70475	1.66371
C	0.1938	-3.76638	0.82983
H	0.61633	-4.75439	1.05056
H	-0.86694	-3.80135	1.1057
C	1.63854	-3.79203	-1.14303
H	2.4074	-3.53039	-0.41252
H	1.8279	-3.19664	-2.03947
C	1.56404	-5.29433	-1.47288
H	1.90281	-5.90197	-0.62883
H	2.21175	-5.54381	-2.31737
C	0.0646	-5.55682	-1.77614
H	-0.3285	-6.36789	-1.15806
H	-0.09211	-5.85422	-2.81656
C	-0.66035	-4.21838	-1.46229
H	-1.57975	-4.37727	-0.89009
C	-1.00448	-3.43359	-2.74911
H	-0.09992	-3.34246	-3.35827
C	-2.16812	-4.09683	-3.54003
H	-1.94431	-4.13247	-4.60943
H	-2.3217	-5.13066	-3.21848
C	-2.94546	-2.21918	-2.18138
H	-3.44055	-1.24654	-2.22417
H	-3.09836	-2.61745	-1.17582
C	-2.64653	-0.6279	1.551
C	-3.41439	-3.21709	-3.25458
H	-4.26975	-3.80079	-2.90532
H	-3.73943	-2.69709	-4.16039
C	-3.44458	-0.03605	2.61653
H	-2.7966	0.17674	3.47341
H	-3.88532	0.89917	2.25766
H	-4.24197	-0.72047	2.92237
C	2.5271	0.11063	-1.82156
N	1.62092	-0.58299	-1.61117
C	3.64922	1.00661	-2.0669
H	4.21805	0.6768	-2.94202
H	3.26838	2.01875	-2.23996
H	4.30279	1.01361	-1.1886
C	-1.38549	0.34206	-2.95329
C	-1.08091	1.76385	-1.14148
C	-1.83635	1.39938	-3.74001
H	-0.78509	1.8618	-0.10187
H	-2.14063	1.22493	-4.76698
C	-1.88486	2.67998	-3.19318
H	-2.22576	3.51774	-3.7924
N	-1.02139	0.53227	-1.66818
N	-1.46926	-2.05215	-2.39687
C	-1.22308	-1.06829	-3.48293
H	-0.19084	-1.1989	-3.83031
H	-1.87704	-1.22475	-4.34939

C	-1.50838	4.23981	-1.23172
C	-2.58173	4.65761	-0.42084
C	-0.44501	5.13937	-1.44695
C	-2.60364	5.94339	0.12733
C	-0.4745	6.42339	-0.89557
C	-1.55706	6.82857	-0.11841
H	-3.44382	6.2493	0.73985
H	0.35028	7.10232	-1.07827
H	-1.58183	7.82917	0.29975
C	2.54683	0.54234	3.86991
C	1.8083	1.14497	4.90784
C	3.81881	1.06567	3.56635
C	2.34082	2.21359	5.63473
C	4.34416	2.13461	4.29767
C	3.61033	2.70148	5.33627
H	1.75929	2.65956	6.433
H	5.32852	2.51545	4.05411
H	4.02425	3.52577	5.90756
C	1.9896	-0.626	3.11658
C	-1.49656	2.88156	-1.86293
C	0.76062	4.72457	-2.26166
C	-3.71677	3.71086	-0.10144
C	4.62912	0.4996	2.42248
C	0.41489	0.65967	5.24314
F	-3.26557	2.65186	0.64944
F	-4.68871	4.29668	0.60736
F	-4.27393	3.17705	-1.20605
F	1.33983	3.59664	-1.74226
F	1.7082	5.66962	-2.2858
F	0.44137	4.43147	-3.54034
F	-0.40248	0.71138	4.14401
F	0.40472	-0.62372	5.66176
F	-0.16786	1.40128	6.19267
F	4.79289	-0.83466	2.51348
F	5.84161	1.05761	2.328
F	3.99731	0.72689	1.22298

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4333.21179
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4336.45293
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4337.06019

Compound B trans Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.716608
(Hartree/Particle)
Thermal correction to Energy= 0.771940
Thermal correction to Enthalpy= 0.772884
Thermal correction to Gibbs Free Energy=
0.620588
Sum of electronic and zero-point Energies= -
4335.112370
Sum of electronic and thermal Energies= -
4335.057039
Sum of electronic and thermal Enthalpies= -
4335.056095
Sum of electronic and thermal Free Energies= -
4335.208390

Fe	-0.27655	-1.25965	-0.69399
N	0.83215	-1.441	1.16933
N	0.29619	-3.41522	-0.62668
N	-1.98449	-1.09369	0.7087
C	1.36163	-0.43486	1.88024
H	1.29247	0.5567	1.44409
C	2.05051	-1.92491	3.61146
H	2.52707	-2.11833	4.56689
C	1.51531	-2.97466	2.86877
H	1.57234	-3.99522	3.23399
C	0.89749	-2.69911	1.65143
C	0.2158	-3.76411	0.81589
H	0.64608	-4.74929	1.0338
H	-0.84376	-3.80742	1.09576
C	1.64948	-3.77794	-1.1668
H	2.42372	-3.50152	-0.44737
H	1.82214	-3.19	-2.07109
C	1.58395	-5.28266	-1.48149
H	1.91506	-5.87886	-0.62594
H	2.24094	-5.54094	-2.31578
C	0.08822	-5.55151	-1.79599
H	-0.30274	-6.37344	-1.19076
H	-0.06004	-5.8362	-2.84139
C	-0.64746	-4.22052	-1.46977
H	-1.55978	-4.39176	-0.89017
C	-1.01532	-3.43726	-2.75105
H	-0.12078	-3.33873	-3.3734
C	-2.18371	-4.1136	-3.52322
H	-1.97429	-4.15316	-4.59525
H	-2.32386	-5.14719	-3.19445
C	-2.96044	-2.24059	-2.15808
H	-3.46624	-1.27306	-2.19559
H	-3.09646	-2.63987	-1.15027
C	-2.64314	-0.63678	1.54767
C	-3.43299	-3.24356	-3.22509
H	-4.27959	-3.83389	-2.86563
H	-3.77228	-2.72711	-4.1279
C	-3.44637	-0.04197	2.60719
H	-2.80731	0.15493	3.4744
H	-3.86923	0.90222	2.25006
H	-4.25697	-0.71752	2.8974
C	2.52405	0.10746	-1.84323
N	1.61614	-0.58559	-1.6387
C	3.65012	1.00015	-2.08121
H	4.23518	0.65702	-2.94006
H	3.27271	2.00941	-2.27644
H	4.28671	1.0202	-1.19114
C	-1.41176	0.33849	-2.95285
C	-1.07432	1.76295	-1.14955
C	-1.85893	1.39829	-3.7382
H	-0.76812	1.8617	-0.11287
H	-2.17536	1.22423	-4.76182
C	-1.88736	2.68097	-3.19601
H	-2.22307	3.52083	-3.79539
N	-1.03216	0.52892	-1.67253
N	-1.48853	-2.05893	-2.39293
C	-1.26727	-1.07389	-3.4838
H	-0.24498	-1.20652	-3.85822
H	-1.94351	-1.22927	-4.33343
C	-1.47856	4.24129	-1.23925
C	-2.53357	4.66282	-0.4068
C	-0.41453	5.13541	-1.47063
C	-2.53714	5.946	0.14699
C	-0.42517	6.41651	-0.91251
C	-1.48973	6.8248	-0.1137
H	-3.36365	6.25434	0.77643
H	0.40098	7.09062	-1.10579
H	-1.49972	7.82367	0.30984
C	2.5194	0.55242	3.88011
C	1.77748	1.13339	4.92759
C	3.78297	1.09627	3.57785
C	2.29853	2.20034	5.66448
C	4.29711	2.16319	4.31972
C	3.56031	2.70804	5.36744
H	1.71391	2.6297	6.46954

H	5.27618	2.55978	4.0777
H	3.96608	3.53016	5.94767
C	1.97659	-0.6169	3.11735
C	-1.48507	2.88268	-1.87004
C	0.77403	4.71834	-2.3094
C	-3.66769	3.72218	-0.06728
C	4.59632	0.55504	2.42372
C	0.39261	0.62505	5.26506
F	-3.20995	2.66428	0.6821
F	-4.62707	4.31395	0.65296
F	-4.24284	3.18564	-1.16151
F	1.3551	3.58277	-1.80763
F	1.72768	5.65644	-2.34389
F	0.43085	4.43615	-3.58437
F	-0.42713	0.66341	4.16723
F	0.40423	-0.65852	5.68428
F	-0.20103	1.35704	6.21511
F	4.76705	-0.78004	2.49107
F	5.80577	1.12	2.33872
F	3.96338	0.80055	1.22824

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4333.25037
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4335.11914
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4336.49746
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -4337.10786

Compound C cis-α Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.744543 (Hartree/Particle)
Thermal correction to Energy= 0.790190
Thermal correction to Enthalpy= 0.791134
Thermal correction to Gibbs Free Energy= 0.664036
Sum of electronic and zero-point Energies= -3342.199674
Sum of electronic and thermal Energies= -3342.154027
Sum of electronic and thermal Enthalpies= -3342.153083
Sum of electronic and thermal Free Energies= -3342.280181

Fe	-0.00445	0.03278	0.01548
N	-1.59912	-0.71795	0.9944
N	0.74154	-1.84805	0.42188
N	-0.45434	-0.74315	-1.84388
N	1.59823	0.72475	-0.99449
N	0.59461	0.76262	1.70309
N	-0.87368	1.72178	-0.35099
C	-2.86105	-0.23362	1.0145
H	-3.02359	0.63735	0.39113
C	-3.58997	-1.91284	2.52814
H	-4.34877	-2.39911	3.13604
C	-2.29869	-2.43448	2.51638
H	-2.04531	-3.31472	3.09972
C	-1.32363	-1.80653	1.74651
C	0.11209	-2.25469	1.71589
H	0.66969	-1.76694	2.52203
H	0.185	-3.33539	1.88061
C	2.2233	-2.08615	0.48582
H	2.62367	-1.68211	1.41864
H	2.68441	-1.54286	-0.34092
C	2.40963	-3.5984	0.31279
H	2.3249	-4.11822	1.2718
H	3.39664	-3.83715	-0.09078
C	1.26213	-4.00637	-0.64614
H	0.76848	-4.92367	-0.31665
H	1.64008	-4.20063	-1.6545
C	0.27839	-2.80097	-0.66238
H	-0.74129	-3.10964	-0.41554
C	0.2593	-2.07051	-2.0042
H	1.28914	-1.85693	-2.30336
C	-0.50561	-2.85747	-3.10767
H	0.10364	-2.98545	-4.00551
H	-0.75419	-3.86259	-2.75362
C	-1.87412	-1.06259	-2.21475
H	-2.41927	-0.13899	-2.42364
H	-2.34338	-1.54194	-1.35388
C	0.11477	0.22785	-2.82839
H	-0.58766	1.06362	-2.91164
H	0.21059	-0.21426	-3.8263
C	1.44549	0.72911	-2.33739
C	2.44103	1.19888	-3.18958
H	2.2897	1.17583	-4.26472
C	3.61994	1.69784	-2.64114
H	4.39468	2.06911	-3.30736
C	2.75271	1.20902	-0.48428
H	2.82033	1.18015	0.59659
C	0.88834	1.2569	2.70968
C	-1.34103	2.77012	-0.51322
C	-1.93984	4.08475	-0.71577
H	-1.78438	4.41719	-1.74722
H	-3.01567	4.04284	-0.5163
H	-1.4829	4.8141	-0.03924
C	-1.78672	-2.03412	-3.398
H	-2.67922	-2.6605	-3.46971
H	-1.70118	-1.49402	-4.34568
C	1.2689	1.88004	3.9725
H	1.25001	1.14156	4.78051
H	2.27928	2.29529	3.89749
H	0.57173	2.68746	4.21836
C	-3.90985	-0.7771	1.76294
Si	-5.68415	-0.03403	1.74533
C	-6.19744	0.25801	3.53462
H	-7.21474	0.66526	3.57333
H	-6.20086	-0.66839	4.12084
H	-5.53779	0.97206	4.04075
C	-5.62111	1.59397	0.78453
H	-4.93872	2.31926	1.24516
H	-5.32776	1.45146	-0.26294
H	-6.61646	2.05334	0.7745
C	-6.82261	-1.27281	0.89487
H	-6.84829	-2.23389	1.42141
H	-7.84956	-0.88902	0.87236
H	-6.52177	-1.46685	-0.14113
C	3.80833	1.71744	-1.24758
Si	5.42518	2.39079	-0.45228
C	5.69542	4.14074	-1.09706
H	6.61106	4.56347	-0.66666
H	5.81107	4.16827	-2.18682
H	4.86831	4.80885	-0.83105
C	6.83519	1.24378	-0.95178
H	7.78334	1.60784	-0.53847
H	6.68608	0.22275	-0.582
H	6.95587	1.1914	-2.04001
C	5.19231	2.39403	1.42467
H	4.35997	3.03738	1.73666
H	5.02938	1.3876	1.82977
H	6.09629	2.78648	1.90489

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.09659
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.34217
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.34172
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.76509

Compound C cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.741758
(Hartree/Particle)
Thermal correction to Energy= 0.788929
Thermal correction to Enthalpy= 0.789873
Thermal correction to Gibbs Free Energy=
0.655899
Sum of electronic and zero-point Energies= -
3342.182693
Sum of electronic and thermal Energies= -
3342.135522
Sum of electronic and thermal Enthalpies= -
3342.134577
Sum of electronic and thermal Free Energies= -
3342.268552

Fe	-0.05006	0.02544	-0.01947
N	-1.63954	-0.69955	1.01895
N	0.67398	-1.86561	0.34463
N	-0.43882	-0.83122	-2.08017
N	1.60181	0.71753	-1.07689
N	0.84791	0.834	2.07871
N	-0.82605	1.7552	-0.30837
C	-2.89489	-0.19931	1.0613
H	-3.04649	0.70205	0.47875
C	-3.62954	-1.93638	2.50234
H	-4.39102	-2.44134	3.09172
C	-2.34312	-2.47169	2.46698
H	-2.09871	-3.37721	3.01395
C	-1.36647	-1.82455	1.71695
C	0.0657	-2.27533	1.65097
H	0.63701	-1.78198	2.4441
H	0.14305	-3.35548	1.81382
C	2.15815	-2.10159	0.39788
H	2.5652	-1.68057	1.31993
H	2.60987	-1.56989	-0.44076
C	2.34418	-3.61782	0.24698
H	2.31492	-4.11781	1.21958
H	3.31198	-3.85588	-0.20096
C	1.15304	-4.06026	-0.64405
H	0.63761	-4.92604	-0.221
H	1.48941	-4.35735	-1.64137
C	0.21104	-2.82611	-0.73669
H	-0.82692	-3.08911	-0.51311
C	0.25659	-2.16119	-2.12066
H	1.30193	-1.98831	-2.39364
C	-0.47717	-3.01987	-3.19883
H	0.17702	-3.25074	-4.04293
H	-0.79174	-3.97903	-2.77523
C	-1.83523	-1.13306	-2.51649
H	-2.34237	-0.21254	-2.81673
H	-2.37631	-1.54733	-1.65961
C	0.2104	0.13433	-2.99605
H	-0.47896	0.97742	-3.12502
H	0.38798	-0.28557	-3.99505
C	1.51035	0.65136	-2.42279
C	2.54878	1.09026	-3.24192
H	2.454	1.01161	-4.32097
C	3.69312	1.63042	-2.66143
H	4.49756	1.97468	-3.30677
C	2.72089	1.24468	-0.53098
H	2.72644	1.2709	0.55263
C	1.05993	1.34343	3.09952
C	-1.24767	2.82373	-0.4655
C	-1.77978	4.16692	-0.66038
H	-2.86729	4.16378	-0.53354
H	-1.3405	4.85446	0.06975
H	-1.54256	4.52458	-1.66758
C	-1.7011	-2.17692	-3.63375
H	-2.60691	-2.77816	-3.74562
H	-1.51927	-1.68997	-4.59704
C	1.34039	1.98031	4.382
H	1.33629	1.23353	5.18221
H	2.32346	2.46091	4.35193
H	0.58127	2.73774	4.6006
C	-3.94622	-0.76724	1.78688
Si	-5.71782	-0.01442	1.80863
C	-6.19092	0.26872	3.61048
H	-7.2043	0.68279	3.6731
H	-6.18855	-0.66167	4.19041
H	-5.5159	0.9749	4.1073
C	-5.66468	1.61647	0.85457
H	-4.97524	2.33997	1.30715
H	-5.38678	1.4777	-0.19749
H	-6.65948	2.0772	0.86088
C	-6.87507	-1.24777	0.97664
H	-6.89056	-2.21216	1.49755
H	-7.90187	-0.86295	0.97956
H	-6.59762	-1.43532	-0.06698
C	3.80991	1.72728	-1.26333
Si	5.37455	2.46633	-0.42515
C	5.62079	4.20728	-1.10418
H	6.5098	4.66555	-0.65473
H	5.77152	4.21171	-2.19001
H	4.76744	4.85838	-0.88237
C	6.83482	1.34902	-0.8412
H	7.75477	1.74773	-0.39728
H	6.6976	0.33219	-0.45557
H	7.00303	1.27692	-1.922
C	5.06974	2.51049	1.4407
H	4.20916	3.13826	1.70343
H	4.91451	1.51034	1.86362
H	5.94459	2.93785	1.94453

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.05826
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.32790
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.31089
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.74523

Compound C cis-α Quintet

UB3LYP/6-31G(d)
Zero-point correction= 0.739569
(Hartree/Particle)
Thermal correction to Energy= 0.787806
Thermal correction to Enthalpy= 0.788751

Thermal correction to Gibbs Free Energy= 0.650563
Sum of electronic and zero-point Energies= -3342.201942
Sum of electronic and thermal Energies= -3342.153705
Sum of electronic and thermal Enthalpies= -3342.152760
Sum of electronic and thermal Free Energies= -3342.290948

Fe	-0.01183	0.11062	0.06508
N	-1.73271	-0.74668	1.11109
N	0.64898	-1.99396	0.46354
N	-0.34741	-0.77223	-1.96972
N	1.72501	0.8217	-1.06389
N	0.73484	0.9487	1.94432
N	-1.0503	1.99642	-0.32635
C	-2.9839	-0.23973	1.16291
H	-3.1149	0.6999	0.63611
C	-3.76514	-2.06082	2.4653
H	-4.54333	-2.60042	2.9999
C	-2.48227	-2.60208	2.42023
H	-2.25737	-3.5457	2.90853
C	-1.48043	-1.91425	1.73846
C	-0.05006	-2.40611	1.70883
H	0.49461	-1.96307	2.55115
H	-0.02915	-3.49351	1.85402
C	2.11726	-2.26062	0.57603
H	2.48582	-1.91823	1.54628
H	2.62411	-1.67626	-0.19712
C	2.28956	-3.76717	0.32683
H	2.19531	-4.32887	1.26105
H	3.27532	-3.99861	-0.08431
C	1.13877	-4.1202	-0.65144
H	0.59203	-5.0072	-0.3219
H	1.52088	-4.34515	-1.65139
C	0.21583	-2.8637	-0.68733
H	-0.83302	-3.13011	-0.52565
C	0.32962	-2.11619	-2.03009
H	1.38919	-1.94617	-2.24416
C	-0.36868	-2.9015	-3.18286
H	0.28786	-3.00375	-4.05048
H	-0.61791	-3.91684	-2.86117
C	-1.75329	-1.06479	-2.39023
H	-2.26152	-0.13692	-2.66447
H	-2.27928	-1.48958	-1.53071
C	0.29316	0.16868	-2.92578
H	-0.39304	1.01326	-3.06098
H	0.44004	-0.28242	-3.91515
C	1.61259	0.69101	-2.40204
C	2.64617	1.0695	-3.25654
H	2.53702	0.94463	-4.32983
C	3.81026	1.6089	-2.71391
H	4.61272	1.90499	-3.38536
C	2.86369	1.34228	-0.55638
H	2.88555	1.41632	0.526
C	1.00286	1.40282	2.97691
C	-1.48158	3.05317	-0.53019
C	-2.03155	4.37898	-0.78471
H	-1.81031	4.68659	-1.81171
H	-3.11742	4.36416	-0.64582
H	-1.59427	5.10661	-0.09374
C	-1.6448	-2.09027	-3.52903
H	-2.53641	-2.71894	-3.59321
H	-1.53947	-1.58883	-4.49584
C	1.34704	1.97581	4.27239
H	1.32465	1.20043	5.04475
H	2.35271	2.40669	4.23275
H	0.63323	2.76228	4.53705
C	-4.05726	-0.84146	1.82709
Si	-5.81975	-0.07346	1.86559
C	-6.29098	0.18627	3.67193
H	-7.30051	0.60849	3.74211
H	-6.29561	-0.75348	4.23653
H	-5.60882	0.87796	4.17934
C	-5.75604	1.57308	0.93858
H	-5.06492	2.28593	1.40525
H	-5.47273	1.44833	-0.11376
H	-6.74886	2.03799	0.9478
C	-6.9917	-1.2803	1.01497
H	-7.01359	-2.25484	1.51645
H	-8.01526	-0.88728	1.02953
H	-6.71958	-1.44963	-0.03318
C	3.95407	1.76492	-1.32302
Si	5.55019	2.50408	-0.54601
C	5.77774	4.23769	-1.24999
H	6.68745	4.69497	-0.8429
H	5.88192	4.23066	-2.34124
H	4.93798	4.89562	-0.99844
C	6.98886	1.37625	-1.00584
H	7.92596	1.77339	-0.59786
H	6.8602	0.36315	-0.60776
H	7.11881	1.29522	-2.09131
C	5.31293	2.5645	1.32878
H	4.47089	3.20456	1.62025
H	5.16275	1.56881	1.76383
H	6.21048	2.985	1.79728

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.05401
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.35192
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.32909
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.77090

Compound C cis-β singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.744200 (Hartree/Particle)
Thermal correction to Energy= 0.789958
Thermal correction to Enthalpy= 0.790903
Thermal correction to Gibbs Free Energy= 0.662366
Sum of electronic and zero-point Energies= -3342.194174
Sum of electronic and thermal Energies= -3342.148416
Sum of electronic and thermal Enthalpies= -3342.147472
Sum of electronic and thermal Free Energies= -3342.276008

Fe	-1.28095	-0.51897	-0.41367
N	-0.39922	-0.28342	1.37151
N	-0.37862	-2.35402	-0.312
N	-2.00166	-1.14723	-2.24608
N	0.20333	0.23857	-1.5211
N	-2.84514	-1.13526	0.57327
N	-2.11799	1.2181	-0.48152
C	-0.16386	0.85516	2.05842
H	-0.47018	1.76343	1.55065
C	0.79271	-0.33023	3.88057
H	1.26312	-0.3777	4.85956

C	0.56337	-1.51702	3.1868
H	0.84884	-2.47547	3.61018
C	-0.0479	-1.46323	1.93816
C	-0.41276	-2.69556	1.14338
H	0.25602	-3.52834	1.38509
H	-1.42715	-3.01348	1.40092
C	1.02646	-2.59593	-0.80903
H	1.74346	-2.23168	-0.07034
H	1.17832	-2.02357	-1.72233
C	1.11502	-4.11025	-1.08655
H	1.53318	-4.65038	-0.23257
H	1.77576	-4.30811	-1.93416
C	-0.34937	-4.55598	-1.35671
H	-0.66174	-5.3287	-0.64925
H	-0.47605	-4.97939	-2.35701
C	-1.19729	-3.27527	-1.17155
H	-2.14458	-3.47052	-0.6613
C	-1.4781	-2.5587	-2.50377
H	-0.5382	-2.45644	-3.05294
C	-2.54534	-3.28801	-3.36985
H	-2.11728	-3.69237	-4.29007
H	-2.96237	-4.13486	-2.8142
C	-3.48464	-1.27299	-2.46921
H	-3.92375	-0.28415	-2.61808
H	-3.92259	-1.70519	-1.56782
C	-1.43306	-0.19664	-3.25005
H	-2.08963	0.68024	-3.27354
H	-1.42905	-0.62095	-4.26038
C	-0.05071	0.2448	-2.85105
C	0.89064	0.69118	-3.77245
H	0.66294	0.66791	-4.83407
C	2.11643	1.17187	-3.31262
H	2.85001	1.52259	-4.03293
C	2.40205	1.19949	-1.93813
C	1.39552	0.70801	-1.09728
H	1.54313	0.67155	-0.02354
C	-3.79131	-1.34098	1.21139
C	0.42332	0.90862	3.32764
C	-2.60114	2.27157	-0.50716
C	-3.20268	3.60027	-0.53681
H	-4.29405	3.52288	-0.50101
H	-2.86211	4.18616	0.32322
H	-2.91558	4.12428	-1.45416
C	-3.64082	-2.23662	-3.64599
H	-4.64113	-2.67526	-3.68705
H	-3.4744	-1.72711	-4.60046
C	-4.98154	-1.60728	2.01161
H	-4.93393	-1.04874	2.95205
H	-5.8801	-1.30271	1.46518
H	-5.05398	-2.67565	2.24013
Si	0.69784	2.56138	4.27391
Si	4.06962	1.84569	-1.226
C	2.55287	2.79125	4.5189
H	3.00069	1.96339	5.08078
H	3.08684	2.87661	3.56529
H	2.74708	3.70901	5.08673
C	-0.02381	3.95859	3.22521
H	-1.09956	3.83213	3.05036
H	0.10356	4.91329	3.74879
H	0.47795	4.0584	2.25489
C	-0.20372	2.42096	5.92309
H	0.17916	1.59539	6.5342
H	-0.07318	3.34029	6.50631
H	-1.28061	2.2668	5.78942
C	4.83118	0.4451	-0.21242
H	4.18463	0.13088	0.61628
H	5.04276	-0.43549	-0.82986
H	5.78205	0.77002	0.22644
C	3.67866	3.32768	-0.12147
H	3.2001	4.13869	-0.68211
H	3.01801	3.05682	0.71174
H	4.60167	3.73027	0.31246
C	5.17824	2.33165	-2.66643
H	4.75234	3.142	-3.26953
H	6.14183	2.69017	-2.28552
H	5.39208	1.48674	-3.33137

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.09141
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.33769
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.33657
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.76073

Compound C cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.740972 (Hartree/Particle)
Thermal correction to Energy= 0.788760
Thermal correction to Enthalpy= 0.789704
Thermal correction to Gibbs Free Energy= 0.651761
Sum of electronic and zero-point Energies= -3342.181578
Sum of electronic and thermal Energies= -3342.133790
Sum of electronic and thermal Enthalpies= -3342.132846
Sum of electronic and thermal Free Energies= -3342.270788

Fe	-0.98872	-0.1782	-0.3846
N	-0.31383	0.02926	1.45658
N	-0.72799	-2.14614	0.00707
N	-1.86479	-0.79591	-2.1193
N	0.55717	0.36703	-1.72985
N	-4.53448	-2.01011	1.02735
N	-2.07785	1.48497	-0.30208
C	0.22127	1.12452	2.04287
C	0.47789	-0.00981	4.11216
H	0.78212	-0.0529	5.15501
C	-0.06463	-1.15129	3.52479
H	-0.18179	-2.0699	4.09156
C	-0.45554	-1.10317	2.19116
C	-1.08984	-2.26158	1.45647
H	-0.77269	-3.2207	1.8815
H	-2.18198	-2.20601	1.53594
C	0.65575	-2.69948	-0.22376
H	1.30835	-2.41416	0.6043
H	1.05733	-2.24881	-1.13348
C	0.46357	-4.21767	-0.38608
H	0.56451	-4.72934	0.57538
H	1.22435	-4.63908	-1.04765
C	-0.97485	-4.38188	-0.94831
H	-1.55755	-5.08075	-0.34318
H	-0.96965	-4.77924	-1.96746
C	-1.59856	-2.96308	-0.90941
H	-2.61177	-2.96165	-0.49985
C	-1.59918	-2.2815	-2.28986
H	-0.60903	-2.38803	-2.74337
C	-2.71964	-2.82028	-3.21914
H	-2.33841	-3.03168	-4.22123
H	-3.11662	-3.76325	-2.83228

C	-3.36863	-0.71926	-2.16229
H	-3.67861	0.31088	-2.3471
H	-3.74629	-1.01609	-1.1802
C	-1.27369	-0.02692	-3.25788
H	-1.8067	0.92924	-3.31493
H	-1.42855	-0.53725	-4.21505
C	0.19169	0.24971	-3.02418
C	1.10229	0.44333	-4.05882
H	0.78778	0.33533	-5.09262
C	2.41637	0.78577	-3.7419
H	3.12518	0.94183	-4.55145
C	2.82627	0.92873	-2.40362
C	1.83471	0.69703	-1.44402
H	2.06034	0.77362	-0.38399
C	-5.54768	-2.31846	1.50326
C	0.64157	1.17738	3.37436
C	-2.67491	2.46891	-0.16527
C	-3.43073	3.70269	-0.00105
H	-4.37514	3.63977	-0.55151
H	-3.64614	3.87354	1.05859
H	-2.85154	4.5475	-0.38839
C	-3.80639	-1.71294	-3.24762
H	-4.80639	-2.10404	-3.04548
H	-3.84552	-1.23011	-4.22866
C	-6.82163	-2.70658	2.10174
H	-7.21095	-1.89289	2.72141
H	-7.55189	-2.93482	1.31915
H	-6.68838	-3.59412	2.72814
Si	4.63447	1.393	-1.93612
C	5.11977	2.89866	-2.9596
C	4.67295	1.78659	-0.08839
C	5.72748	-0.09227	-2.33112
Si	1.40279	2.76046	4.16238
C	0.28952	3.26688	5.5967
C	3.13826	2.32402	4.75359
C	1.45916	4.10303	2.83514
H	0.30968	1.99103	1.39443
H	-0.72608	3.50853	5.2629
H	0.69335	4.1573	6.09312
H	0.21338	2.48078	6.35686
H	2.08732	3.82084	1.98138
H	1.8904	5.01785	3.25835
H	0.46346	4.3668	2.45826
H	3.78925	2.02124	3.92541
H	3.13341	1.51241	5.49042
H	3.60183	3.1934	5.23499
H	5.68608	-0.36127	-3.39294
H	5.44411	-0.97742	-1.74992
H	6.77398	0.13471	-2.09496
H	5.68831	2.08087	0.20206
H	4.40292	0.92315	0.53198
H	4.01017	2.6213	0.17109
H	5.06818	2.70405	-4.03722
H	6.1536	3.18785	-2.73609
H	4.4829	3.76427	-2.74456

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.05533
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.31730
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.29843
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.73883

Compound C cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.739561 (Hartree/Particle)
Thermal correction to Energy= 0.787769
Thermal correction to Enthalpy= 0.788713
Thermal correction to Gibbs Free Energy= 0.649831
Sum of electronic and zero-point Energies= -3342.196456
Sum of electronic and thermal Energies= -3342.148248
Sum of electronic and thermal Enthalpies= -3342.147304
Sum of electronic and thermal Free Energies= -3342.286186

Fe	-21.15486	25.00585	18.2149
N	-20.27313	25.2414	20.00008
N	-20.25253	23.1708	18.31656
N	-21.87557	24.37759	16.38248
N	-19.67058	25.76339	17.10746
N	-22.71905	24.38956	19.20184
N	-21.9919	26.74292	18.14705
C	-20.03777	26.37997	20.68698
H	-20.3441	27.28824	20.17921
C	-19.0812	25.19459	22.50913
H	-18.61079	25.14712	23.48812
C	-19.31054	24.0078	21.81537
H	-19.02507	23.04935	22.23874
C	-19.92181	24.06159	20.56673
C	-20.28668	22.82926	19.77195
H	-19.61789	21.99648	20.01365
H	-21.30106	22.51134	20.02948
C	-18.84745	22.92889	17.81954
H	-18.13046	23.29314	18.55822
H	-18.6956	23.50124	16.90623
C	-18.7589	21.41457	17.54201
H	-18.34073	20.87444	18.39599
H	-18.09815	21.21671	16.6944
C	-20.22328	20.96884	17.27185
H	-20.53565	20.19612	17.97931
H	-20.34997	20.54543	16.27156
C	-21.0712	22.24955	17.45701
H	-22.01849	22.0543	17.96726
C	-21.35201	22.96612	16.12479
H	-20.41212	23.06838	15.57562
C	-22.41925	22.23681	15.25871
H	-21.9912	21.83244	14.33849
H	-22.83628	21.38995	15.81436
C	-23.35855	24.25183	16.15935
H	-23.79766	25.24067	16.01048
H	-23.7965	23.81963	17.06075
C	-21.30697	25.32817	15.37852
H	-21.96354	26.20506	15.35503
H	-21.30296	24.90387	14.36818
C	-19.92462	25.76962	15.77752
C	-18.98328	26.216	14.85612
H	-19.21097	26.19273	13.7945
C	-17.75748	26.69669	15.31594
H	-17.0239	27.04741	14.59563
C	-17.47186	26.72431	16.69043
C	-18.4784	26.23283	17.53129
H	-18.33078	26.19637	18.60502
C	-23.66522	24.18383	19.83995
C	-19.45059	26.43344	21.95621
C	-22.47505	27.79639	18.12141
C	-23.07659	29.12509	18.09175
H	-24.16796	29.0477	18.12755
H	-22.73603	29.71098	18.95178

H	-22.78949	29.6491	17.1744
C	-23.51473	23.2882	14.98257
H	-24.51504	22.84955	14.94151
H	-23.34831	23.7977	14.0281
C	-24.85545	23.91754	20.64018
H	-24.80784	24.47608	21.58061
H	-25.75401	24.22211	20.09374
H	-24.92789	22.84917	20.86869
Si	-19.17607	28.0862	22.90247
Si	-15.80429	27.37051	17.40256
C	-17.32104	28.31607	23.14747
H	-16.87323	27.48821	23.70934
H	-16.78707	28.40143	22.19386
H	-17.12683	29.23383	23.71529
C	-19.89772	29.4834	21.85377
H	-20.97347	29.35694	21.67892
H	-19.77035	30.43811	22.37736
H	-19.39596	29.58322	20.88345
C	-20.07763	27.94578	24.55165
H	-19.69476	27.12021	25.16276
H	-19.94709	28.86511	25.13488
H	-21.15452	27.79162	24.41798
C	-15.04274	25.96992	18.41615
H	-15.68928	25.6557	19.24485
H	-14.83115	25.08933	17.79871
H	-14.09186	26.29484	18.855
C	-16.19525	28.8525	18.50709
H	-16.67381	29.66351	17.94645
H	-16.8559	28.58164	19.3403
H	-15.27224	29.25509	18.94103
C	-14.69568	27.85647	15.96214
H	-15.12157	28.66682	15.35904
H	-13.73209	28.21499	16.34305
H	-14.48183	27.01156	15.29719

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.05079
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.34799
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.32555
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.75515

Compound C trans Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.744310 (Hartree/Particle)
Thermal correction to Energy= 0.789799
Thermal correction to Enthalpy= 0.790743
Thermal correction to Gibbs Free Energy= 0.663497
Sum of electronic and zero-point Energies= -3342.182286
Sum of electronic and thermal Energies= -3342.136797
Sum of electronic and thermal Enthalpies= -3342.135852
Sum of electronic and thermal Free Energies= -3342.263099

Fe	-0.1066339	-0.5822087	0.3660914
N	0.9576591	-0.4732817	1.3436946
N	0.5606221	-2.5133417	-0.3029264
N	-1.6428629	-0.8382107	0.7835046
C	1.5049221	0.5891683	1.9619136
H	1.3820201	1.5470863	1.4660116
C	2.3690961	-0.7616277	3.7868706
C	1.8067961	-1.8596877	3.1128276
H	1.9101541	-2.8633847	3.5162296
C	1.1153421	-1.6933507	1.9161746
C	0.4943991	-2.8478627	1.1519486
H	1.0068011	-3.7866647	1.3881326
H	-0.5556829	-2.9723067	1.4301016
C	1.9305981	-2.8920927	-0.8080604
H	2.6886361	-2.6021347	-0.0774424
H	2.1240291	-2.3397847	-1.7274164
C	1.8565051	-4.3987647	-1.0914284
H	2.0877591	-4.9842967	-0.1967194
H	2.5815051	-4.6928687	-1.8545144
C	0.3909531	-4.6287207	-1.5413904
H	-0.0584669	-5.4784507	-1.0216884
H	0.3304501	-4.8486257	-2.6111524
C	-0.3523669	-3.3076267	-1.2044174
H	-1.2863599	-3.4894737	-0.6658364
C	-0.6541489	-2.4542907	-2.4652194
H	0.2769671	-2.2775727	-3.0108494
C	-1.7423099	-3.0951107	-3.3699594
H	-1.4314739	-3.1065327	-4.4174484
H	-1.9208939	-4.1358917	-3.0846194
C	-2.6787529	-1.3770487	-1.9289494
H	-3.2177569	-0.4292287	-1.8699744
H	-2.8816399	-1.9355297	-1.0152844
C	-2.5224509	-0.8029617	1.5379026
C	2.1977921	0.4861983	3.1624106
C	-3.0094049	-2.2280727	-3.1617054
H	-3.9082649	-2.8282077	-2.9994164
H	-3.2032669	-1.6012397	-4.0373614
C	-3.6357119	-0.7632247	2.4792166
H	-3.2635369	-0.5920637	3.4944966
H	-4.3227889	0.0469413	2.2140606
H	-4.1838829	-1.7108757	2.4597366
H	2.6070811	1.3926583	3.5995066
C	2.4507731	0.4548193	-1.7425904
N	1.4819441	-0.0182867	-1.3165374
C	3.6733941	1.0391553	-2.2818724
H	3.9589121	0.5329353	-3.2098584
H	3.5206471	2.1024803	-2.4930244
H	4.4893521	0.9366453	-1.5590724
C	-1.1839339	1.3053203	-2.1572024
C	-1.0282319	2.3284723	-0.0853994
C	-1.6980119	2.4696413	-2.7204914
C	-1.5280239	3.5218773	-0.5938864
H	-0.7711459	2.2294353	0.9646456
H	-1.9673219	2.4606933	-3.7732354
H	-1.6483119	4.3607333	0.0859006
C	-1.8784049	3.6322413	-1.9508364
N	-0.8424479	1.2343103	-0.8457254
N	-1.1944709	-1.1193417	-2.0119324
C	-0.9764089	0.0262803	-2.9465164
H	0.0468211	-0.0294237	-3.3276914
H	-1.6478029	-0.0058467	-3.8114594
Si	-2.5759809	5.2752153	-2.6857644
C	-3.1582609	4.9310043	-4.4443304
C	-1.1709309	6.5340643	-2.6585044
C	-4.0036569	5.8159363	-1.5787364
Si	3.3415151	-0.9356997	5.4453296
C	3.3056821	-2.7483867	5.9581746
C	2.4747101	0.1572533	6.7148666
C	5.1026981	-0.3439787	5.1196006
H	5.6070191	-0.9536087	4.3612446
H	5.6951871	-0.4106427	6.0398906
H	5.1348231	0.7008713	4.7894726
H	2.2866681	-3.1166477	6.1259546
H	3.8483081	-2.8731897	6.9027426

H	3.7913251	-3.4027027	5.2245466
H	-2.3400059	4.6251693	-5.1070324
H	-3.5877739	5.8442933	-4.8728534
H	-3.9388649	4.1621503	-4.4844694
H	-0.3264919	6.2190933	-3.2820934
H	-0.7946659	6.7113263	-1.6443354
H	-1.5239259	7.4967603	-3.0472484
H	1.4413011	-0.1612947	6.8928136
H	2.4562381	1.2112433	6.4141106
H	3.0028131	0.1045853	7.6744156
H	-4.8123869	5.0764903	-1.5618124
H	-4.4285729	6.7563473	-1.9494234
H	-3.6855279	5.9927733	-0.5446414

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.07758
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.32131
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.32013
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.74250

Compound C trans Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.741475
(Hartree/Particle)
Thermal correction to Energy= 0.788378
Thermal correction to Enthalpy= 0.789322
Thermal correction to Gibbs Free Energy=
0.653972
Sum of electronic and zero-point Energies= -
3342.169385
Sum of electronic and thermal Energies= -
3342.122482
Sum of electronic and thermal Enthalpies= -
3342.121537
Sum of electronic and thermal Free Energies= -
3342.256888

Fe	-0.04853	-0.20788	-0.1284
N	1.11013	-0.45984	1.61532
N	0.63572	-2.39098	-0.24094
N	-1.5763	-0.47666	0.99339
C	1.68257	0.51739	2.34425
H	1.57761	1.52999	1.9627
C	2.52511	-1.04984	3.99493
C	1.92977	-2.05014	3.20849
C	1.23196	-1.73465	2.04412
C	0.55574	-2.78725	1.18633
H	1.00524	-3.76936	1.3788
H	-0.50223	-2.86191	1.46106
C	1.99934	-2.71507	-0.77194
H	2.76153	-2.44882	-0.03593
H	2.17438	-2.10808	-1.663
C	1.96076	-4.20904	-1.13238
H	2.24201	-4.82816	-0.27513
H	2.66487	-4.44516	-1.93436
C	0.48676	-4.46178	-1.53902
H	0.07632	-5.33712	-1.02933
H	0.39588	-4.65421	-2.61178
C	-0.27878	-3.16608	-1.13768
H	-1.19353	-3.39273	-0.58149
C	-0.648	-2.30801	-2.37273
H	0.26307	-2.10614	-2.94412
C	-1.73776	-2.9904	-3.25047
H	-1.47385	-2.94698	-4.31022
H	-1.83927	-4.04953	-2.99775
C	-2.68369	-1.29518	-1.77881
H	-3.25323	-0.36373	-1.73874
H	-2.83368	-1.81635	-0.83088
C	-2.46738	-0.4948	1.73377
C	2.37947	0.26596	3.5192
C	-3.04517	-2.2095	-2.96125
H	-3.88215	-2.86764	-2.71423
H	-3.35309	-1.62455	-3.83298
C	-3.59428	-0.52217	2.65759
H	-3.23811	-0.41764	3.68755
H	-4.28135	0.30065	2.43478
H	-4.13578	-1.46936	2.5648
H	2.81366	1.10702	4.05245
C	2.48822	0.77198	-1.54469
N	1.52449	0.33088	-1.07651
C	3.70368	1.31713	-2.13601
H	3.97145	0.75378	-3.036
H	3.5508	2.36652	-2.40809
H	4.52994	1.25311	-1.42051
C	-1.30898	1.43316	-2.22744
C	-1.16725	2.68207	-0.28215
C	-1.86949	2.5147	-2.90464
C	-1.70767	3.79835	-0.90746
H	-2.14535	2.38442	-3.94764
C	-2.07919	3.74689	-2.26327
N	-0.96095	1.51684	-0.92542
N	-1.22167	-0.99961	-1.92504
C	-1.03511	0.10183	-2.90112
H	0.00299	0.07495	-3.25029
H	-1.67301	-0.00538	-3.78727
Si	-2.82667	5.28136	-3.16541
C	-3.30416	4.75932	-4.9117
C	-1.48827	6.61092	-3.18287
C	-4.33167	5.83555	-2.17306
Si	3.49729	-1.43405	5.61834
C	3.5423	-3.30406	5.84671
C	2.57286	-0.58708	7.02776
C	5.23154	-0.724	5.40725
H	5.767	-1.1922	4.57348
H	5.82042	-0.90222	6.31493
H	5.22142	0.35887	5.23674
H	2.54201	-3.74016	5.95396
H	4.09454	-3.54792	6.76202
H	4.05313	-3.81446	5.02161
H	-2.44432	4.41383	-5.49791
H	-3.72893	5.61674	-5.44705
H	-4.06499	3.96992	-4.91954
H	-0.59798	6.28931	-3.73521
H	-1.17401	6.89592	-2.17205
H	-1.86744	7.51626	-3.67176
H	1.5524	-0.9712	7.1382
H	2.5121	0.49868	6.89004
H	3.09388	-0.76479	7.97612
H	-5.09941	5.0552	-2.12121
H	-4.78847	6.71254	-2.64703
H	-4.07179	6.12264	-1.14748
H	2.00898	-3.09485	3.49667
H	-0.88931	2.71011	0.76854
H	-1.84109	4.70393	-0.32252

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.05095
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.31387
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas

HF = -3343.30102
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.72953

Compound C trans Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.739227 (Hartree/Particle)
Thermal correction to Energy= 0.787518
Thermal correction to Enthalpy= 0.788462
Thermal correction to Gibbs Free Energy= 0.649512
Sum of electronic and zero-point Energies= -3342.193191
Sum of electronic and thermal Energies= -3342.144900
Sum of electronic and thermal Enthalpies= -3342.143956
Sum of electronic and thermal Free Energies= -3342.282907

Fe	-0.0502	-0.26506	-0.16863
N	1.13293	-0.50014	1.64129
N	0.62494	-2.40643	-0.24956
N	-1.77132	-0.43111	1.23738
C	1.7053	0.46134	2.39131
H	1.59981	1.48151	2.03018
C	2.54629	-1.13888	4.00977
C	1.95028	-2.12393	3.20493
H	2.02748	-3.17365	3.47472
C	1.25458	-1.78302	2.04637
C	0.56505	-2.81869	1.17836
H	1.00866	-3.80729	1.34881
H	-0.49067	-2.88729	1.46535
C	1.984	-2.70983	-0.80791
H	2.75398	-2.44414	-0.08004
H	2.13684	-2.08401	-1.69004
C	1.95609	-4.2002	-1.18491
H	2.27645	-4.82397	-0.34494
H	2.63717	-4.41452	-2.01243
C	0.47392	-4.4777	-1.54598
H	0.09308	-5.35567	-1.01817
H	0.3525	-4.67905	-2.6141
C	-0.29999	-3.19276	-1.12976
H	-1.1988	-3.43067	-0.55259
C	-0.70778	-2.34332	-2.35689
H	0.18256	-2.15468	-2.96446
C	-1.83527	-3.02363	-3.18488
H	-1.61832	-2.97762	-4.25512
H	-1.92427	-4.0835	-2.93057
C	-2.71372	-1.30038	-1.69482
H	-3.27118	-0.36159	-1.66102
H	-2.82989	-1.78701	-0.72398
C	-2.60534	-0.31028	2.0341
C	2.40151	0.18713	3.561
C	-3.12918	-2.24241	-2.83799
H	-3.94712	-2.9	-2.53269
H	-3.48785	-1.67741	-3.70341
C	-3.65888	-0.16584	3.03142
H	-3.21976	0.0172	4.01721
H	-4.3076	0.67618	2.7697
H	-4.26274	-1.07796	3.07487
H	2.83623	1.01612	4.11242
C	2.72142	0.99668	-1.6141
N	1.76959	0.46018	-1.22534
C	3.91997	1.66338	-2.10853
H	4.25233	1.19598	-3.04102
H	3.71038	2.72126	-2.29589
H	4.72245	1.58605	-1.368
C	-1.33681	1.41	-2.27836
C	-1.12063	2.72646	-0.38642
C	-1.90191	2.47315	-2.98067
C	-1.66476	3.82657	-1.03557
H	-0.81036	2.78863	0.65385
H	-2.20781	2.31098	-4.01071
H	-1.76859	4.75581	-0.48244
C	-2.0783	3.7295	-2.37727
N	-0.94966	1.53453	-0.99033
N	-1.25432	-1.02209	-1.90453
C	-1.08825	0.05584	-2.91608
H	-0.05706	0.01451	-3.28583
H	-1.74654	-0.0788	-3.78302
Si	-2.83901	5.23811	-3.31068
C	-3.32739	4.67292	-5.04044
C	-1.50721	6.57313	-3.37043
C	-4.33902	5.80942	-2.31997
Si	3.51573	-1.55653	5.62632
C	3.57125	-3.43117	5.8102
C	2.58123	-0.74969	7.05284
C	5.2463	-0.83063	5.43982
H	5.78619	-1.27103	4.59386
H	5.8344	-1.03181	6.3432
H	5.22995	0.25666	5.30094
H	2.57315	-3.87496	5.90554
H	4.12376	-3.69394	6.72009
H	4.0855	-3.91879	4.97355
H	-2.47029	4.31615	-5.62385
H	-3.75902	5.51573	-5.5932
H	-4.08556	3.88109	-5.02385
H	-0.62125	6.24293	-3.92464
H	-1.18387	6.88231	-2.36959
H	-1.89541	7.4656	-3.87556
H	1.56305	-1.1432	7.15069
H	2.51366	0.33859	6.94058
H	3.10056	-0.94657	7.99833
H	-5.10414	5.02823	-2.2466
H	-4.80134	6.67527	-2.80881
H	-4.07214	6.11775	-1.30242

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3341.04763
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3342.33978
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.32120
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3343.74950

Compound D-Me cis-α Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.573504 (Hartree/Particle)
Thermal correction to Energy= 0.607142
Thermal correction to Enthalpy= 0.608086
Thermal correction to Gibbs Free Energy= 0.509060
Sum of electronic and zero-point Energies= -2753.594481
Sum of electronic and thermal Energies= -2753.560843
Sum of electronic and thermal Enthalpies= -2753.559898

Sum of electronic and thermal Free Energies= -2753.658924

Fe	-21.56948	24.83377	-18.03477
N	-20.60608	24.95547	-19.78225
N	-19.9697	25.31518	-16.93121
N	-22.11323	26.68422	-17.95564
C	-21.54256	24.99237	-15.08712
H	-21.98874	25.87334	-14.61151
H	-21.47656	24.22219	-14.31571
C	-20.1652	25.33499	-15.59501
C	-19.15164	25.67916	-14.70005
H	-19.35291	25.6768	-13.63312
C	-17.89545	26.02308	-15.1879
H	-17.09448	26.29613	-14.50812
C	-17.69106	26.00738	-16.56799
C	-18.74466	25.64679	-17.39551
H	-18.6143	25.61896	-18.46915
C	-22.44242	27.79524	-17.90352
C	-22.82642	29.20014	-17.81185
H	-23.68439	29.31446	-17.13888
H	-23.1303	29.55449	-18.8126
H	-22.00377	29.80947	-17.45605
N	-22.45805	24.52482	-16.18771
N	-21.08929	22.84264	-18.17304
C	-24.4542	20.87238	-15.261
C	-25.17062	22.05741	-15.42448
H	-22.51213	19.95217	-15.30843
C	-23.07047	20.87635	-15.42311
C	-24.49178	23.23453	-15.73666
C	-23.1035	23.24028	-15.89945
H	-25.04826	24.16587	-15.82592
C	-22.36244	22.04748	-15.74918
C	-18.70831	21.30176	-15.01092
C	-20.08815	21.44266	-14.86717
H	-17.02334	21.57381	-16.32963
C	-18.09623	21.6815	-16.20487
C	-20.87813	21.96348	-15.90317
C	-20.24307	22.32412	-17.10722
C	-18.86309	22.19188	-17.25416
H	-18.37505	22.47785	-18.18057
H	-16.73112	26.2667	-17.0011
H	-18.11759	20.89343	-14.19725
H	-20.56927	21.14563	-13.93975
H	-24.96716	19.94996	-15.00842
H	-26.2479	22.07418	-15.29243
C	-23.56278	25.49381	-16.2317
H	-24.25612	25.20983	-16.99557
H	-24.06161	25.50908	-15.28511
H	-23.17483	26.46759	-16.44611
C	-23.83881	23.1729	-18.7745
C	-23.78699	25.3205	-19.85096
C	-25.03015	22.90733	-19.47524
C	-24.97909	24.96292	-20.50744
H	-23.32563	26.29937	-20.0335
H	-25.55819	21.9459	-19.34947
H	-25.46671	25.6586	-21.21309
N	-23.21181	24.40424	-18.96817
C	-25.59887	23.77959	-20.33054
H	-26.50523	23.54232	-20.84749
C	-22.39265	22.19282	-17.97658
C	-20.67525	22.54033	-19.55179
H	-19.8785	23.19524	-19.83646
H	-20.34103	21.52555	-19.61003
H	-21.50555	22.68076	-20.21206
C	-19.89422	25.04687	-21.06413
C	-19.14773	25.14273	-22.40834
H	-19.65432	24.54973	-23.14082
H	-19.12261	26.1628	-22.73047
H	-18.14755	24.78227	-22.28721
H	-22.35896	21.21471	-18.4091
H	-22.5769	22.10003	-16.92666

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2752.67549
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2753.59902
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2754.56631
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2754.91363

Compound D-Me cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.569411 (Hartree/Particle)
Thermal correction to Energy= 0.605080
Thermal correction to Enthalpy= 0.606024
Thermal correction to Gibbs Free Energy= 0.497599
Sum of electronic and zero-point Energies= -2753.604279
Sum of electronic and thermal Energies= -2753.568610
Sum of electronic and thermal Enthalpies= -2753.567666
Sum of electronic and thermal Free Energies= -2753.676091

Fe	-0.44692	0.63853	-0.02893
N	2.52882	2.44235	-3.34096
N	1.23474	1.29471	0.79203
N	-0.51243	2.22552	-1.21921
C	0.26152	0.42139	2.8449
H	0.0102	0.87678	3.8102
H	0.6442	-0.57694	3.05562
C	1.3381	1.20233	2.13939
C	2.42063	1.73801	2.83474
H	2.45842	1.65664	3.91654
C	3.44423	2.36287	2.128
H	4.29763	2.78261	2.65147
C	3.34764	2.44129	0.73803
C	2.23074	1.9093	0.10992
H	2.1179	1.98208	-0.96673
C	-0.46189	3.12192	-1.95196
C	-0.37494	4.2436	-2.87185
H	-1.20249	4.2141	-3.58768
H	0.57818	4.17373	-3.4064
H	-0.41349	5.18635	-2.31614
N	-0.9765	0.30155	2.00243
N	0.18913	-1.28135	-0.74612
C	-2.97489	-3.43862	2.64373
C	-3.63291	-2.23789	2.88736
H	-1.14031	-4.3426	1.99379
C	-1.66174	-3.40849	2.18171
C	-2.97117	-1.02826	2.67606
C	-1.65342	-0.99035	2.20423
H	-3.50371	-0.11509	2.90617
C	-0.97291	-2.20581	1.93554
C	2.64242	-3.29235	2.13686
C	1.30187	-3.03201	2.4084
H	4.21569	-3.08131	0.67581
C	3.17635	-2.88417	0.91919
C	0.46304	-2.35622	1.50192
C	1.0182	-1.96476	0.25613
C	2.36625	-2.23444	-0.01178

H	2.80621	-1.95733	-0.96058
H	4.11831	2.91844	0.14274
H	3.25488	-3.81187	2.86684
H	0.87821	-3.34874	3.3571
H	-3.46975	-4.38903	2.8162
H	-4.65318	-2.22943	3.25776
C	-1.82563	1.49298	2.29706
H	-2.71369	1.49869	1.66585
H	-2.13567	1.51453	3.34801
H	-1.23597	2.39194	2.09839
C	-2.2135	-1.21307	-1.36875
C	-3.25115	0.82655	-0.97679
C	-3.33974	-1.6838	-2.04414
C	-4.41168	0.41861	-1.61633
H	-3.1665	1.82699	-0.56686
H	-3.33459	-2.68495	-2.46381
H	-5.25485	1.09674	-1.69049
N	-2.16574	0.03077	-0.83946
C	-4.4578	-0.86456	-2.16555
H	-5.34492	-1.21577	-2.68324
C	-1.00999	-2.08976	-1.14065
C	0.90938	-0.90657	-1.9969
H	1.73168	-0.22359	-1.7837
H	1.29985	-1.79037	-2.51459
H	0.20124	-0.40494	-2.66028
C	3.3275	2.56154	-4.17586
C	4.32956	2.71331	-5.22723
H	3.89042	2.48399	-6.20312
H	4.70699	3.74054	-5.24266
H	5.16848	2.03315	-5.04989
H	-0.78211	-2.68194	-2.03542
H	-1.24244	-2.79805	-0.34605

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2752.66173
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2753.60177
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.55059
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.91298

Compound D-Me cis-α Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.567503
(Hartree/Particle)
Thermal correction to Energy= 0.604164
Thermal correction to Enthalpy= 0.605109
Thermal correction to Gibbs Free Energy=
0.492688
Sum of electronic and zero-point Energies= -
2753.619279
Sum of electronic and thermal Energies= -
2753.582618
Sum of electronic and thermal Enthalpies= -
2753.581673
Sum of electronic and thermal Free Energies= -
2753.694094

Fe	-0.45282	0.5613	-0.02778
N	2.5224	2.51119	-3.30154
N	1.33128	1.37697	0.86447
N	-0.57093	2.35086	-1.20444
C	0.3695	0.42381	2.89765
H	0.13383	0.82464	3.89127
H	0.78595	-0.57332	3.04545
C	1.41304	1.27413	2.20839
C	2.45192	1.8594	2.93158
H	2.47634	1.77004	4.01326
C	3.4515	2.54718	2.24808
H	4.27109	3.00722	2.79164
C	3.37824	2.63621	0.8569
C	2.30278	2.04732	0.20528
H	2.20394	2.11557	-0.87411
C	-0.46401	3.25301	-1.92389
C	-0.31601	4.38238	-2.82601
H	-1.12386	4.38277	-3.56472
H	0.64874	4.28701	-3.33508
H	-0.34436	5.31957	-2.26075
N	-0.88325	0.30422	2.0889
N	0.08532	-1.40205	-0.78612
C	-2.95648	-3.38456	2.77536
C	-3.56386	-2.16901	3.07262
H	-1.18306	-4.3319	2.02337
C	-1.66736	-3.38614	2.24906
C	-2.87639	-0.97637	2.84984
C	-1.58261	-0.96964	2.31255
H	-3.36615	-0.05083	3.12253
C	-0.95569	-2.20012	1.98739
C	2.64538	-3.34891	2.04756
C	1.32885	-3.04068	2.38047
H	4.13545	-3.25528	0.49019
C	3.11738	-3.01714	0.78199
C	0.45591	-2.38766	1.48995
C	0.94796	-2.07134	0.19705
C	2.27125	-2.39175	-0.13305
H	2.6617	-2.1738	-1.1184
H	4.13528	3.15965	0.28326
H	3.28609	-3.84902	2.76677
H	0.95033	-3.30528	3.36373
H	-3.4714	-4.32244	2.9575
H	-4.56363	-2.13714	3.49416
C	-1.71042	1.51748	2.34075
H	-2.6102	1.4994	1.72385
H	-2.00002	1.60117	3.39464
H	-1.11577	2.39794	2.08266
C	-2.30689	-1.31446	-1.4816
C	-3.35964	0.73683	-1.21826
C	-3.38978	-1.80826	-2.21041
C	-4.48119	0.31194	-1.91582
H	-3.29738	1.74657	-0.82442
H	-3.36565	-2.82282	-2.59608
H	-5.31974	0.9844	-2.06068
N	-2.28803	-0.05498	-0.99821
C	-4.49388	-0.98825	-2.42667
H	-5.34869	-1.35457	-2.9869
C	-1.12997	-2.19949	-1.13629
C	0.76542	-1.02097	-2.05627
H	1.61201	-0.36119	-1.85967
H	1.11407	-1.90135	-2.60873
H	0.04437	-0.49017	-2.683
C	3.33729	2.60229	-4.12426
C	4.35972	2.71902	-5.16045
H	3.93137	2.48931	-6.14103
H	4.76116	3.73702	-5.18065
H	5.17968	2.02181	-4.96196
H	-0.90192	-2.88347	-1.96325
H	-1.40548	-2.81524	-0.27961

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2752.65368
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2753.62215

UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2754.56287
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.93241

Compound D-Me cis-β Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.572721
(Hartree/Particle)
Thermal correction to Energy= 0.606580
Thermal correction to Enthalpy= 0.607524
Thermal correction to Gibbs Free Energy=
0.509197
Sum of electronic and zero-point Energies= -
2753.592663
Sum of electronic and thermal Energies= -
2753.558803
Sum of electronic and thermal Enthalpies= -
2753.557859
Sum of electronic and thermal Free Energies= -
2753.656186

Fe	-0.35161	0.61069	-0.5817
N	0.92216	0.78324	-2.12932
N	1.12846	0.9482	0.77164
N	-1.84616	0.50512	-1.81631
N	-0.62771	2.53531	-0.55093
C	1.58973	1.89455	-2.50964
H	1.3923	2.79097	-1.93735
C	2.73987	0.72806	-4.25986
H	3.44265	0.70345	-5.08683
C	2.06779	-0.42609	-3.86556
H	2.23393	-1.37016	-4.3752
C	1.16788	-0.36206	-2.80254
C	-0.80108	1.33416	2.17605
H	-1.13762	2.34797	1.93793
H	-1.09682	1.13221	3.2103
C	0.68901	1.27101	2.01063
C	1.55557	1.59439	3.05119
H	1.15412	1.83488	4.03062
C	2.92835	1.60703	2.81506
H	3.62366	1.86139	3.609
C	3.38567	1.2754	1.54132
C	2.45951	0.94545	0.55859
H	2.78964	0.65402	-0.42862
C	-2.71585	0.55543	-2.58087
C	2.49382	1.91181	-3.56382
C	-0.79327	3.68082	-0.61902
C	-1.00124	5.12253	-0.69762
H	-0.20939	5.64765	-0.15353
H	-1.96788	5.38853	-0.25719
H	-0.9897	5.44858	-1.74283
C	-3.81326	0.60648	-3.54021
H	-3.48311	1.0913	-4.46467
H	-4.65214	1.1734	-3.1234
H	-4.15668	-0.40634	-3.77543
N	-1.50823	0.38914	1.23924
N	-0.06371	-1.50395	-0.94607
C	0.33592	-1.53779	-2.38678
H	-0.595	-1.50346	-2.9593
H	0.81482	-2.48868	-2.64118
C	-2.05141	-3.26867	3.49116
C	-3.05316	-2.31054	3.40954
H	-0.09346	-3.81063	2.84007
C	-0.86281	-3.04705	2.80826
C	-2.8382	-1.1601	2.65557
C	-1.64414	-0.92308	1.95324
H	-3.64151	-0.43878	2.63782
C	-0.6102	-1.89223	2.03143
C	3.10475	-2.49761	1.76099
C	1.82436	-2.21381	2.23085
H	4.30673	-2.76992	-0.01049
C	3.32855	-2.52246	0.39019
C	0.74356	-1.93508	1.3755
C	1.00112	-1.91396	-0.01678
C	2.28274	-2.2241	-0.48523
H	2.50014	-2.23829	-1.54459
H	4.44444	1.25882	1.30696
H	2.99721	2.83632	-3.82527
H	3.90552	-2.71485	2.46077
H	1.64028	-2.22027	3.30061
H	-2.18912	-4.17906	4.06568
H	-3.99909	-2.44201	3.92539
C	-1.23005	-2.45612	-0.8814
H	-0.93292	-3.4183	-1.31318
H	-1.55607	-2.61971	0.13693
H	-2.05808	-2.04227	-1.45717
C	-2.85596	0.9818	0.9585
H	-3.47801	0.24786	0.44713
H	-3.35979	1.30798	1.87234
H	-2.72983	1.85144	0.31935

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2752.67363
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2753.59904
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2754.56739
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.91371

Compound D-Me cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.569351
(Hartree/Particle)
Thermal correction to Energy= 0.605407
Thermal correction to Enthalpy= 0.606351
Thermal correction to Gibbs Free Energy=
0.496367
Sum of electronic and zero-point Energies= -
2753.593218
Sum of electronic and thermal Energies= -
2753.557162
Sum of electronic and thermal Enthalpies= -
2753.556218
Sum of electronic and thermal Free Energies= -
2753.666202

Fe	-0.12497	0.12971	-0.4169
N	0.82513	0.36289	-2.13831
N	1.33668	1.13089	0.61661
N	-1.85127	0.2038	-1.47312
N	-0.61254	3.92493	-0.69336
C	1.01148	1.5837	-2.69341
H	0.54832	2.41793	-2.1739
C	2.36472	0.65721	-4.44213
H	2.977	0.76803	-5.33176
C	2.15002	-0.60133	-3.88664
H	2.57487	-1.49079	-4.34189
C	1.3512	-0.71952	-2.74827
C	-0.04281	0.46172	2.49437
H	-0.53984	0.97167	3.32703
H	0.37957	-0.46111	2.89194

C	1.08762	1.27538	1.93981
C	1.8995	2.04119	2.77431
H	1.6478	2.14118	3.82534
C	3.03447	2.65035	2.24837
H	3.68476	3.24663	2.88104
C	3.3224	2.46767	0.89573
C	2.45218	1.71479	0.12164
H	2.64873	1.56955	-0.93075
C	-2.77643	0.29112	-2.16515
C	1.76237	1.76778	-3.84631
C	-0.81083	5.06858	-0.66211
C	-1.05983	6.50718	-0.62274
H	-2.03084	6.73513	-1.07309
H	-0.28087	7.03973	-1.17721
H	-1.05953	6.86193	0.41259
C	-3.94818	0.40343	-3.02298
H	-3.66333	0.27191	-4.07169
H	-4.4037	1.3915	-2.89913
H	-4.68329	-0.36183	-2.75286
N	-1.05491	0.1139	1.43583
N	0.1993	-2.03884	-0.93504
C	0.88634	-2.06686	-2.25667
H	0.14453	-2.40491	-2.98669
H	1.68171	-2.8179	-2.28923
C	-2.93869	-3.515	2.73118
C	-3.68154	-2.34434	2.61986
H	-1.01372	-4.42107	2.42727
C	-1.59412	-3.50531	2.36517
C	-3.06925	-1.17029	2.17696
C	-1.71865	-1.15318	1.81474
H	-3.66456	-0.2673	2.14422
C	-0.96085	-2.34914	1.87953
C	2.73797	-2.92326	2.41174
C	1.36088	-2.80471	2.57829
H	4.35566	-2.76214	0.99318
C	3.28401	-2.69504	1.15297
C	0.49515	-2.46857	1.5214
C	1.05595	-2.31609	0.22338
C	2.44978	-2.40304	0.07468
H	2.91483	-2.24659	-0.88995
H	4.204	2.90522	0.44027
H	1.88003	2.76373	-4.25941
H	3.37025	-3.1822	3.25488
H	0.92618	-2.96063	3.56182
H	-3.39656	-4.42944	3.09466
H	-4.73111	-2.32671	2.89611
C	-0.95333	-2.98912	-1.05788
H	-0.58795	-3.99716	-1.28805
H	-1.53914	-3.0271	-0.14854
H	-1.59758	-2.64352	-1.86809
C	-1.98627	1.28249	1.34884
H	-2.77855	1.08104	0.63216
H	-2.42845	1.50555	2.32507
H	-1.42192	2.15459	1.01029

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2752.65006
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2753.59051
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2754.53972
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.90248

Compound D-Me cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.568037 (Hartree/Particle)
Thermal correction to Energy= 0.604610
Thermal correction to Enthalpy= 0.605554
Thermal correction to Gibbs Free Energy= 0.494960
Sum of electronic and zero-point Energies= -2753.611469
Sum of electronic and thermal Energies= -2753.574896
Sum of electronic and thermal Enthalpies= -2753.573951
Sum of electronic and thermal Free Energies= -2753.684545

Fe	-0.18344	0.56551	-0.5261
N	1.03978	0.64236	-2.3422
N	1.4035	1.30875	0.81838
N	-2.16631	0.38908	-1.45544
N	-0.629	2.79288	-0.832
C	1.54957	1.76817	-2.88867
H	1.16781	2.70072	-2.4909
C	2.97522	0.52985	-4.35833
H	3.73263	0.4801	-5.13467
C	2.44392	-0.63565	-3.81381
H	2.76885	-1.6108	-4.16353
C	1.46582	-0.54365	-2.82074
C	-0.00482	0.52803	2.66043
H	-0.43672	1.00886	3.5475
H	0.38238	-0.43636	2.98778
C	1.16433	1.32742	2.14482
C	2.01355	1.97787	3.04355
H	1.77364	1.98256	4.10239
C	3.16495	2.59749	2.57011
H	3.84126	3.10191	3.25345
C	3.43197	2.55309	1.20065
C	2.52603	1.91129	0.36878
H	2.6982	1.87007	-0.69917
C	-3.18088	0.32941	-2.01215
C	2.50553	1.76046	-3.8955
C	-0.91693	3.91145	-0.93539
C	-1.27331	5.31973	-1.0655
H	-2.15889	5.54082	-0.46109
H	-1.49093	5.55584	-2.1121
H	-0.44537	5.94927	-0.72412
C	-4.45881	0.24876	-2.70794
H	-4.29585	0.27219	-3.79034
H	-5.09406	1.09465	-2.42646
H	-4.96966	-0.68312	-2.44475
N	-1.0717	0.3006	1.63963
N	0.0721	-1.70094	-1.0357
C	0.7244	-1.77755	-2.37136
H	-0.08025	-1.91369	-3.10057
H	1.35502	-2.67019	-2.45296
C	-2.95499	-3.43999	2.55909
C	-3.69629	-2.26305	2.56579
H	-1.03454	-4.30975	2.14397
C	-1.61418	-3.39224	2.18466
C	-3.08378	-1.05005	2.24491
C	-1.73136	-0.99053	1.88542
H	-3.68192	-0.1507	2.30631
C	-0.98559	-2.19329	1.80969
C	2.72249	-2.8387	2.15167
C	1.35717	-2.70491	2.38335
H	4.27842	-2.63373	0.67069
C	3.21733	-2.5496	0.88427
C	0.45332	-2.28837	1.38814
C	0.95903	-2.06119	0.0797
C	2.3433	-2.1755	-0.13473

H	2.76964	-1.98122	-1.11003
H	4.32132	3.01166	0.78202
H	2.87494	2.69587	-4.30182
H	3.38424	-3.16115	2.9491
H	0.95891	-2.919	3.37149
H	-3.41151	-4.38579	2.83295
H	-4.74527	-2.27189	2.84545
C	-1.12524	-2.59841	-1.13683
H	-0.80841	-3.63804	-1.28407
H	-1.74449	-2.53916	-0.25177
H	-1.72084	-2.28136	-1.99314
C	-1.99515	1.46292	1.71221
H	-2.75031	1.40193	0.9282
H	-2.48891	1.52632	2.68886
H	-1.41093	2.37165	1.56844

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2752.64767
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2753.62382
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2754.56622
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.92044

Compound D-Me trans Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.567484 (Hartree/Particle)
Thermal correction to Energy= 0.604330
Thermal correction to Enthalpy= 0.605274
Thermal correction to Gibbs Free Energy= 0.492889
Sum of electronic and zero-point Energies= -2753.595734
Sum of electronic and thermal Energies= -2753.558888
Sum of electronic and thermal Enthalpies= -2753.557944
Sum of electronic and thermal Free Energies= -2753.670328

Fe	0.03517	0.51009	-0.39858
N	1.22268	0.66438	-2.20261
N	-0.99314	2.40541	-0.21833
N	-2.01938	0.13946	-1.45822
N	2.12095	1.26862	0.36013
C	1.76813	1.80842	-2.66252
H	1.39157	2.72811	-2.22616
C	3.2506	0.62099	-4.11721
C	2.69836	-0.56507	-3.63896
C	1.67458	-0.50632	-2.69143
C	-0.92781	1.91528	2.16388
H	-1.61381	1.8894	3.01675
H	-0.08362	2.53308	2.4843
C	-1.5333	2.64702	0.99152
C	-2.49514	3.64045	1.18524
H	-2.91558	3.80447	2.17275
C	-2.88685	4.42718	0.10444
C	-2.3105	4.19154	-1.14541
C	-1.38289	3.16464	-1.26214
C	-3.07688	0.07999	-1.92915
C	2.76831	1.83571	-3.62564
C	3.20275	1.60347	0.60751
C	4.56188	2.02425	0.92627
H	4.54227	2.96788	1.48086
H	5.13687	2.16586	0.00579
H	5.05392	1.26227	1.53915
C	-4.40646	-0.00205	-2.52194
H	-4.3292	-0.266	-3.58154
H	-4.91726	0.96185	-2.43279
H	-4.99763	-0.76652	-2.00769
N	-0.35865	0.56488	1.8771
N	0.2584	-1.72099	-0.95596
C	0.90834	-1.74518	-2.29961
H	0.09189	-1.82147	-3.02409
H	1.51083	-2.64902	-2.43766
C	-3.06318	-2.69748	2.53698
C	-3.53214	-1.38763	2.55374
H	-1.36985	-3.95572	2.13762
C	-1.73418	-2.93392	2.19472
C	-2.65591	-0.33224	2.29962
C	-1.3044	-0.558	2.00115
H	-3.04852	0.67511	2.35447
C	-0.84074	-1.89639	1.87476
C	2.65203	-3.32178	2.2217
C	1.33658	-2.92742	2.45232
H	4.24569	-3.36931	0.76795
C	3.21572	-3.09197	0.97052
C	0.54859	-2.31193	1.46366
C	1.10295	-2.17725	0.16132
C	2.44233	-2.53627	-0.04881
H	2.90398	-2.40246	-1.01866
H	3.16144	2.78391	-3.97645
H	0.90071	-3.06739	3.43747
H	3.22795	-3.78979	3.0137
H	-3.72184	-3.5274	2.77217
H	-4.56921	-1.17386	2.79366
C	0.74203	0.39214	2.88839
H	0.31084	0.34062	3.89509
H	1.31194	-0.50845	2.69539
H	1.41552	1.24509	2.82877
C	-0.92438	-2.64137	-1.08827
H	-0.57519	-3.66926	-1.24203
H	-1.54994	-2.60378	-0.20489
H	-1.52029	-2.33216	-1.94497
H	4.04002	0.59847	-4.86237
H	3.04311	-1.52659	-4.00695
H	-0.93915	2.92315	-2.22281
H	-2.57704	4.78649	-2.01242
H	-3.62487	5.21277	0.23545

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2752.60075
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2753.53113
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2754.49995
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.86103

Compound D-Me trans Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.567489 (Hartree/Particle)
Thermal correction to Energy= 0.604330
Thermal correction to Enthalpy= 0.605274
Thermal correction to Gibbs Free Energy= 0.492977
Sum of electronic and zero-point Energies= -2753.595731

Sum of electronic and thermal Energies= -2753.558890
Sum of electronic and thermal Enthalpies= -2753.557946
Sum of electronic and thermal Free Energies= -2753.670243

Fe	0.03036	0.50904	-0.40077
N	1.21253	0.65984	-2.20906
N	-1.00964	2.39897	-0.23215
N	-2.02401	0.11862	-1.4559
N	2.11351	1.27704	0.34891
C	1.75124	1.80404	-2.67637
H	1.37112	2.72424	-2.24417
C	3.23623	0.61612	-4.12808
C	2.69102	-0.57007	-3.64212
C	1.66928	-0.51124	-2.69243
C	-0.9421	1.9242	2.1532
H	-1.62846	1.89823	3.00575
H	-0.10334	2.55103	2.47039
C	-1.55253	2.64368	0.97588
C	-2.52207	3.63087	1.16297
H	-2.94455	3.79752	2.14918
C	-2.91874	4.40838	0.07732
C	-2.33957	4.16982	-1.17065
C	-1.40427	3.14916	-1.28067
C	-3.08169	0.05024	-1.92522
C	2.74914	1.83108	-3.64189
C	3.19505	1.61524	0.59275
C	4.55391	2.04001	0.90724
H	4.53289	2.97793	1.47139
H	5.12239	2.19385	-0.01532
H	5.05365	1.2745	1.50938
C	-4.4114	-0.04293	-2.5161
H	-4.333	-0.29594	-3.57828
H	-4.93406	0.91359	-2.41688
H	-4.9919	-0.81956	-2.00796
N	-0.36148	0.57674	1.87559
N	0.26589	-1.72347	-0.94508
C	0.91053	-1.75169	-2.29118
H	0.09148	-1.8357	-3.01186
H	1.51687	-2.65334	-2.42683
C	-3.03395	-2.70588	2.56485
C	-3.51506	-1.40038	2.5739
H	-1.33003	-3.95092	2.1689
C	-1.70374	-2.93224	2.22039
C	-2.64947	-0.33861	2.31008
C	-1.29673	-0.55378	2.00939
H	-3.05145	0.66535	2.35917
C	-0.82098	-1.88863	1.89081
C	2.68523	-3.28211	2.23403
C	1.36782	-2.89603	2.46746
H	4.27245	-3.32999	0.77322
C	3.24146	-3.05838	0.9784
C	0.57063	-2.29449	1.47752
C	1.11834	-2.16556	0.17179
C	2.45934	-2.51651	-0.04168
H	2.9154	-2.38714	-1.01475
H	3.13684	2.7793	-3.99863
H	0.93733	-3.03206	3.45554
H	3.2682	-3.73947	3.02709
H	-3.6842	-3.54027	2.80751
H	-4.55345	-1.19465	2.81516
C	0.74157	0.4213	2.88717
H	0.31183	0.37668	3.89484
H	1.3171	-0.47739	2.70226
H	1.40924	1.27816	2.81846
C	-0.9108	-2.65303	-1.06657
H	-0.55491	-3.67952	-1.21415
H	-1.53363	-2.6135	-0.18136
H	-1.51182	-2.35417	-1.92338
H	4.02401	0.59349	-4.87498
H	3.03975	-1.53185	-4.00566
H	-0.9581	2.90536	-2.23962
H	-2.60975	4.75773	-2.04133
H	-3.66273	5.18918	0.20319

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2752.60637
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2753.55664
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2754.50827
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2754.86503

Compound D-Me trans Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.567486 (Hartree/Particle)
Thermal correction to Energy= 0.604331
Thermal correction to Enthalpy= 0.605275
Thermal correction to Gibbs Free Energy= 0.492898
Sum of electronic and zero-point Energies= -2753.595733
Sum of electronic and thermal Energies= -2753.558887
Sum of electronic and thermal Enthalpies= -2753.557943
Sum of electronic and thermal Free Energies= -2753.670321

Fe	0.03118	0.50928	-0.39947
N	1.21734	0.66826	-2.20343
N	-1.00575	2.4003	-0.22159
N	-2.02085	0.1266	-1.45774
N	2.11642	1.27984	0.35769
C	1.75587	1.81504	-2.66467
H	1.37347	2.73298	-2.22968
C	3.24606	0.63476	-4.11731
C	2.70099	-0.55405	-3.63766
C	1.67659	-0.50031	-2.69052
C	-0.93663	1.91373	2.16115
H	-1.62167	1.88575	3.01472
H	-0.09507	2.53597	2.47985
C	-1.54656	2.64087	0.98821
C	-2.51329	3.62971	1.18102
H	-2.93409	3.79301	2.1685
C	-2.9094	4.41299	0.0993
C	-2.33253	4.17847	-1.1505
C	-1.39989	3.15602	-1.26628
C	-3.07818	0.06085	-1.92821
C	2.75615	1.84717	-3.62753
C	3.19748	1.61859	0.60304
C	4.5558	2.04392	0.9193
H	4.53185	2.92672	1.56618
H	5.0952	2.29268	-0.00001
H	5.08718	1.23883	1.4368
C	-4.40745	-0.02912	-2.52054
H	-4.32801	-0.26901	-3.58569
H	-4.93298	0.92458	-2.40992
H	-4.98578	-0.81355	-2.02199
N	-0.36137	0.5656	1.87551
N	0.26728	-1.7207	-0.95368
C	0.91785	-1.74331	-2.29707

H	0.10222	-1.82578	-3.0218
H	1.52591	-2.64368	-2.43333
C	-3.05013	-2.70875	2.54174
C	-3.52506	-1.40105	2.55737
H	-1.3512	-3.95958	2.1429
C	-1.72027	-2.93943	2.19896
C	-2.65392	-0.34194	2.30134
C	-1.30158	-0.56173	2.00208
H	-3.05123	0.66361	2.35529
C	-0.83178	-1.89819	1.87726
C	2.66787	-3.30589	2.22652
C	1.35011	-2.91867	2.45609
H	4.2629	-3.34495	0.77401
C	3.23123	-3.0733	0.9757
C	0.55945	-2.30785	1.46664
C	1.11392	-2.17096	0.16453
C	2.45546	-2.52246	-0.04446
H	2.91699	-2.38655	-1.01408
H	3.14351	2.79729	-3.97957
H	0.91449	-3.06035	3.4411
H	3.24579	-3.77038	3.01912
H	-3.70482	-3.54142	2.77829
H	-4.56293	-1.19176	2.79779
C	0.74133	0.39946	2.88579
H	0.31141	0.34589	3.89293
H	1.31609	-0.49794	2.69249
H	1.41001	1.25609	2.82514
C	-0.91064	-2.64747	-1.08485
H	-0.55607	-3.67378	-1.23656
H	-1.53692	-2.61148	-0.20188
H	-1.50769	-2.34292	-1.94244
H	4.03584	0.61611	-4.86219
H	3.05177	-1.51391	-4.00424
H	-0.9555	2.91536	-2.22686
H	-2.6025	4.77083	-2.01821
H	-3.65125	5.19508	0.22959

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2752.63291
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2753.60935
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.55126
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.90420

Compound D-H cis-α Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.515836
(Hartree/Particle)
Thermal correction to Energy= 0.547557
Thermal correction to Enthalpy= 0.548501
Thermal correction to Gibbs Free Energy=
0.451560
Sum of electronic and zero-point Energies= -
2675.080272
Sum of electronic and thermal Energies= -
2675.048551
Sum of electronic and thermal Enthalpies= -
2675.047607
Sum of electronic and thermal Free Energies= -
2675.144547

Fe	0.10129	0.75541	-0.61221
N	0.88693	1.01129	-2.36161
N	1.73404	1.28039	0.4261
N	-0.42727	2.61632	-0.5765
C	0.27726	0.85781	2.34046
H	-0.13264	1.62013	3.01278
H	0.43468	-0.03738	2.94431
C	1.597	1.30989	1.76983
C	2.63347	1.71566	2.61133
H	2.48044	1.72826	3.68625
C	3.85357	2.0939	2.06075
H	4.67294	2.40957	2.69899
C	3.99917	2.05966	0.67285
C	2.92109	1.65467	-0.10049
H	2.99075	1.62932	-1.18098
C	-0.64508	3.75541	-0.54947
C	-0.91473	5.18853	-0.52529
H	-1.78369	5.40109	0.10599
H	-1.11844	5.54938	-1.53877
H	-0.04838	5.72612	-0.1262
N	-0.72617	0.54965	1.26081
N	0.66359	-1.22101	-0.71967
C	-3.23049	-2.7745	2.16341
C	-3.76989	-1.49838	2.0079
H	-1.43848	-3.96016	2.13134
C	-1.8584	-2.96541	2.01382
C	-2.92676	-0.42841	1.71299
C	-1.55233	-0.62199	1.55477
H	-3.34386	0.57303	1.62397
C	-0.9901	-1.9049	1.69815
C	2.46678	-3.17096	2.60915
C	1.11095	-2.85177	2.64874
H	4.27649	-3.08517	1.43348
C	3.22131	-2.83637	1.48558
C	0.47153	-2.18915	1.58554
C	1.24751	-1.87111	0.45432
C	2.60545	-2.19598	0.41158
H	3.18722	-1.96447	-0.4788
H	4.92938	2.34638	0.19437
H	2.92753	-3.68084	3.44921
H	0.52443	-3.10715	3.52648
H	-3.87105	-3.61676	2.4048
H	-4.83483	-1.32908	2.13142
C	-1.57373	-1.2234	-1.83247
C	-2.6095	0.8484	-1.90081
C	-2.6454	-1.81105	-2.50568
C	-3.71216	0.33358	-2.56664
H	-2.55256	1.90079	-1.65144
H	-2.62312	-2.87332	-2.72954
H	-4.53398	0.98799	-2.83646
N	-1.55098	0.09339	-1.53196
C	-3.73224	-1.02701	-2.87818
H	-4.57631	-1.46619	-3.40069
C	-0.39365	-2.05367	-1.39626
C	1.2608	1.18193	-3.44641
C	1.72782	1.4082	-4.80941
H	0.9079	1.24978	-5.51755
H	2.09278	2.43508	-4.91529
H	2.54228	0.7178	-5.05177
H	0.04748	-2.57052	-2.25632
H	-0.73069	-2.83004	-0.70737
H	1.43047	-1.15548	-1.38669
H	-1.37738	1.33281	1.25942

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2674.20418
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.06721
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2675.98157

UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2676.31227

Compound D-H cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.515836 (Hartree/Particle)
Thermal correction to Energy= 0.44658
Thermal correction to Enthalpy= 0.547134
Thermal correction to Gibbs Free Energy= 0.451560
Sum of electronic and zero-point Energies= -2675.080272
Sum of electronic and thermal Energies= -2675.048551
Sum of electronic and thermal Enthalpies= -2675.031149
Sum of electronic and thermal Free Energies= -2675.131702

Fe	0.1454571	0.6650281	-0.6196436
N	0.8797741	1.0584151	-2.4567176
N	1.7259281	1.2987851	0.4021634
N	-0.5820989	2.8696751	-0.4650286
C	0.3949541	0.7158091	2.3432274
H	0.0069791	1.3587431	3.1404064
H	0.6322501	-0.2431769	2.7969314
C	1.6496131	1.2829401	1.7555784
C	2.6935441	1.7350671	2.5627684
H	2.5863051	1.7105461	3.6426474
C	3.8618731	2.2062291	1.9711574
H	4.6879531	2.5556451	2.5822294
C	3.9452211	2.2231211	0.5788594
C	2.8630231	1.7700641	-0.1602146
H	2.8867161	1.7808691	-1.2435536
C	-0.6980159	4.0226331	-0.4195566
C	-0.8500619	5.4720141	-0.3590126
H	-1.6772079	5.7348431	0.3087584
H	-1.0660859	5.8675701	-1.3563926
H	0.0703171	5.9302561	0.0164774
N	-0.6544539	0.5103881	1.2887814
N	0.7218291	-1.4972359	-0.7280506
C	-3.2926369	-2.7297139	2.0741184
C	-3.7844809	-1.4331229	1.9220104
H	-1.5404169	-3.9746069	2.0873274
C	-1.9265989	-2.9672649	1.9601124
C	-2.9014869	-0.3879769	1.6673614
C	-1.5304589	-0.6289079	1.5398854
H	-3.2793769	0.6289441	1.5891164
C	-1.0157419	-1.9334469	1.6775734
C	2.3886131	-3.1533599	2.8105234
C	1.0351871	-2.8259959	2.7679304
H	4.2383311	-3.1841599	1.6992364
C	3.1843651	-2.9257759	1.6895124
C	0.4432851	-2.2579039	1.6268074
C	1.2573921	-2.0582959	0.4891764
C	2.6147641	-2.3910789	0.5350674
H	3.2329261	-2.2582009	-0.3508656
H	4.8319161	2.5843621	0.0698754
H	2.8143491	-3.5874859	3.7094034
H	0.4104321	-2.9993439	3.6392734
H	-3.9688529	-3.5508939	2.2894504
H	-4.8458509	-1.2303759	2.0242034
C	-1.5166209	-1.3738599	-1.8386486
C	-2.4846569	0.7346741	-1.9676016
C	-2.5923149	-1.9303149	-2.5353856
C	-3.5866119	0.2471191	-2.6535236
H	-2.3940949	1.7875951	-1.7286326
H	-2.5982219	-2.9953449	-2.7466496
H	-4.3794999	0.9239821	-2.9534596
N	-1.4626709	-0.0526339	-1.5592596
C	-3.6427919	-1.1173269	-2.9472866
H	-4.4865119	-1.5368609	-3.4864796
C	-0.3916779	-2.2621989	-1.3562856
C	1.1614491	1.2802901	-3.5583286
C	1.5182021	1.5635491	-4.9422126
H	0.6570011	1.3893951	-5.5951136
H	1.8330001	2.6080431	-5.0400876
H	2.3404111	0.9135441	-5.2581236
H	-0.0120379	-2.8634369	-2.1902946
H	-0.7916939	-2.9634959	-0.6251876
H	1.4835991	-1.4621319	-1.4036476
H	-1.2437279	1.3457911	1.2872934

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2674.18658
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.06056
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.94937
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2676.30536

Compound D-H cis-α Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.511047 (Hartree/Particle)
Thermal correction to Energy= 0.545259
Thermal correction to Enthalpy= 0.546203
Thermal correction to Gibbs Free Energy= 0.438938
Sum of electronic and zero-point Energies= -2675.085081
Sum of electronic and thermal Energies= -2675.050869
Sum of electronic and thermal Enthalpies= -2675.049924
Sum of electronic and thermal Free Energies= -2675.157189

Fe	0.0909288	0.7149765	-0.5781821
N	1.1170238	1.0397395	-2.5022721
N	1.8242938	1.4194645	0.5666279
N	-0.6447332	2.7954365	-0.5911121
C	0.5231498	0.7049725	2.5213469
H	0.1720968	1.2543725	3.4028879
H	0.8418818	-0.2790655	2.8711599
C	1.7203158	1.3988185	1.9111949
C	2.7083448	1.9445995	2.7340749
H	2.5868598	1.9192895	3.8127679
C	3.8430948	2.5064965	2.1577439
H	4.6243008	2.9303065	2.7814049
C	3.9568958	2.5171125	0.7656429
C	2.9263978	1.9717325	0.0142609
H	2.9643668	1.9701805	-1.0691521
C	-0.8750352	3.9307205	-0.5297121
C	-1.1678922	5.3567445	-0.4582041
H	-2.1295302	5.5197025	0.0390569
H	-1.2124502	5.7800565	-1.4668831
H	-0.3835552	5.8704185	0.1071109
N	-0.5895932	0.5174865	1.5462649
N	0.4801428	-1.4841955	-0.7652211
C	-3.2321142	-2.6966145	2.4400409
C	-3.6957692	-1.3824295	2.3983669

H	-1.5278002	-3.9838995	2.2012259
C	-1.8903072	-2.9602215	2.1727639
C	-2.8064602	-0.3500245	2.1076449
C	-1.4598902	-0.6131965	1.8348809
H	-3.1604922	0.6793955	2.1157249
C	-0.9783632	-1.9393655	1.8464569
C	2.4655878	-3.3995745	2.4756099
C	1.1425758	-2.9881085	2.6227449
H	4.1568538	-3.4834305	1.1349129
C	3.1284598	-3.1643385	1.2718389
C	0.4470308	-2.3257185	1.5944059
C	1.1250498	-2.1214335	0.3738919
C	2.4520548	-2.5383955	0.2267439
H	2.9570878	-2.3929975	-0.7266301
H	4.8235238	2.9437495	0.2723859
H	2.9708748	-3.9030555	3.2936149
H	0.6252428	-3.1669825	3.5610919
H	-3.9066202	-3.5114645	2.6829499
H	-4.7356202	-1.1555495	2.6114039
C	-1.6995822	-1.3213285	-1.9786971
C	-2.5800542	0.8067505	-2.2565891
C	-2.6847702	-1.8637715	-2.8071411
C	-3.5992622	0.3394335	-3.0731011
H	-2.4920552	1.8609465	-2.0196381
H	-2.6939432	-2.9309455	-3.0071611
H	-4.3308382	1.0293325	-3.4795661
N	-1.6426652	-0.0001975	-1.7132991
C	-3.6500322	-1.0270355	-3.3580771
H	-4.4272432	-1.4313935	-3.9994021
C	-0.6982102	-2.2270895	-1.2982501
C	1.4983708	1.1811295	-3.5886651
C	1.9816268	1.3632545	-4.9516141
H	1.2473958	0.9712115	-5.6628431
H	2.1372708	2.4278855	-5.1539121
H	2.9290088	0.8322145	-5.0896261
H	-0.3740982	-3.0203815	-1.9823041
H	-1.1988072	-2.7188635	-0.4617811
H	1.1746078	-1.4665135	-1.5113101
H	-1.1749312	1.3496525	1.6101029

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2674.18031
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.07979
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.96261
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2676.32114

Compound D-H cis-β Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.515889 (Hartree/Particle)
Thermal correction to Energy= 0.547550
Thermal correction to Enthalpy= 0.548494
Thermal correction to Gibbs Free Energy= 0.451659
Sum of electronic and zero-point Energies= -2675.081293
Sum of electronic and thermal Energies= -2675.049632
Sum of electronic and thermal Enthalpies= -2675.048688
Sum of electronic and thermal Free Energies= -2675.145523

Fe	-21.57586	24.8312	-18.0373
N	-20.60657	24.95556	-19.78215
N	-19.96978	25.31511	-16.93129
N	-23.21467	24.40373	-18.97053
N	-22.10809	26.68574	-17.95293
C	-20.29264	26.08466	-20.45333
H	-20.64047	27.01109	-20.01283
C	-19.11671	24.86478	-22.14786
H	-18.5326	24.82602	-23.06199
C	-19.44015	23.69457	-21.46469
H	-19.11855	22.72646	-21.83639
C	-20.19354	23.77186	-20.29437
C	-21.54246	24.99243	-15.08727
H	-21.98871	25.87339	-14.61148
H	-21.4766	24.22217	-14.31567
C	-20.16514	25.33489	-15.59489
C	-19.15165	25.67924	-14.70009
H	-19.35292	25.67679	-13.63309
C	-17.89549	26.02307	-15.18792
H	-17.09446	26.29614	-14.5081
C	-17.69108	26.00739	-16.56799
C	-18.74458	25.64682	-17.39539
H	-18.61434	25.61895	-18.46917
C	-24.20384	24.19118	-19.53659
C	-19.56025	26.08376	-21.63362
C	-22.43618	27.79627	-17.88584
C	-22.83945	29.19615	-17.81261
H	-23.68823	29.31103	-17.1306
H	-23.13507	29.55434	-18.8042
H	-22.00817	29.80815	-17.44766
C	-25.4478	23.9241	-20.24875
H	-25.23477	23.47616	-21.22481
H	-25.9993	24.85717	-20.40348
H	-26.0717	23.23487	-19.67058
N	-22.45816	24.52491	-16.18774
N	-21.08877	22.84173	-18.17373
C	-20.66854	22.53536	-19.57447
H	-21.54679	22.14549	-20.10196
H	-19.91593	21.74308	-19.59403
C	-24.45418	20.8724	-15.261
C	-25.17059	22.0574	-15.42451
H	-22.51211	19.95215	-15.30845
C	-23.07055	20.87638	-15.42315
C	-24.49176	23.23448	-15.73676
C	-23.10346	23.24025	-15.8994
H	-25.04828	24.1659	-15.82588
C	-22.3623	22.04743	-15.74925
C	-18.70833	21.30177	-15.01094
C	-20.08808	21.44269	-14.86721
H	-17.02332	21.5738	-16.32965
C	-18.09627	21.68152	-16.20485
C	-20.87827	21.96365	-15.90307
C	-20.24311	22.32393	-17.10724
C	-18.86311	22.19189	-17.25413
H	-18.37503	22.47785	-18.1806
H	-16.7311	26.2667	-17.00112
H	-19.33895	27.02157	-22.13161
H	-18.11758	20.89341	-14.19723
H	-20.56929	21.14562	-13.93973
H	-24.96717	19.94994	-15.00841
H	-26.24792	22.07419	-15.2924
H	-23.20963	25.18399	-16.21759
H	-21.97598	22.40028	-18.03965

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2674.20484
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.06936

UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2675.98318
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2676.31331

Compound D-H cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.512954
(Hartree/Particle)
Thermal correction to Energy= 0.546040
Thermal correction to Enthalpy= 0.546984
Thermal correction to Gibbs Free Energy=
0.444295
Sum of electronic and zero-point Energies= -
2675.066342
Sum of electronic and thermal Energies= -
2675.033255
Sum of electronic and thermal Enthalpies= -
2675.032311
Sum of electronic and thermal Free Energies= -
2675.135000

Fe	-0.35317	0.70846	-0.49477
N	0.67166	0.7072	-2.31613
N	1.23319	1.20701	0.60652
N	-1.9727	0.28315	-1.43428
N	-0.98278	2.84989	-0.36339
C	0.96113	1.82888	-3.01191
H	0.60009	2.75914	-2.58527
C	2.13788	0.59008	-4.68702
H	2.71613	0.53873	-5.60439
C	1.83686	-0.56835	-3.97649
H	2.17007	-1.53933	-4.33072
C	1.08907	-0.48125	-2.80018
C	-0.26172	0.74784	2.49616
H	-0.71186	1.57368	3.0595
H	-0.128	-0.07525	3.2009
C	1.07857	1.1711	1.95082
C	2.10857	1.51988	2.82443
H	1.94002	1.47345	3.89605
C	3.33813	1.92017	2.31337
H	4.15049	2.19479	2.97895
C	3.50115	1.95765	0.92829
C	2.43511	1.59371	0.11979
H	2.53415	1.60783	-0.95714
C	-2.96073	0.06972	-2.00167
C	1.68071	1.81604	-4.1986
C	-1.26496	3.97338	-0.30291
C	-1.61955	5.38563	-0.2283
H	-2.46029	5.52374	0.45927
H	-1.91001	5.75127	-1.21848
H	-0.76621	5.96873	0.13236
C	-4.20237	-0.20083	-2.71504
H	-3.98537	-0.6307	-3.69835
H	-4.76592	0.72768	-2.85341
H	-4.81555	-0.90719	-2.14603
N	-1.20776	0.32304	1.41137
N	0.18934	-1.50013	-0.69606
C	0.64557	-1.74101	-2.07854
H	-0.19741	-2.16248	-2.63933
H	1.43765	-2.49573	-2.10931
C	-3.22042	-3.35348	2.17889
C	-3.9327	-2.16085	2.05827
H	-1.27892	-4.27526	2.11366
C	-1.8351	-3.34642	2.02869
C	-3.24853	-0.97388	1.8008
C	-1.8585	-0.96625	1.65021
H	-3.80125	-0.03737	1.74789
C	-1.12006	-2.16647	1.75428
C	2.53248	-2.83633	2.57235
C	1.14798	-2.71319	2.68419
H	4.23435	-2.5851	1.2721
C	3.15711	-2.49524	1.37333
C	0.36747	-2.24992	1.61441
C	1.01235	-1.9446	0.39674
C	2.40084	-2.0515	0.28722
H	2.90223	-1.79872	-0.64179
H	4.43922	2.26086	0.4762
H	1.88302	2.74481	-4.72095
H	3.1156	-3.19818	3.41303
H	0.65408	-2.9778	3.61522
H	-3.73757	-4.28387	2.39071
H	-5.01087	-2.14609	2.18392
H	-1.9632	1.00778	1.39805
H	-0.72878	-1.92253	-0.57748

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2674.17189
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.05973
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2675.95888
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2676.29776

Compound D-H cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.511157
(Hartree/Particle)
Thermal correction to Energy= 0.545259
Thermal correction to Enthalpy= 0.546203
Thermal correction to Gibbs Free Energy=
0.439306
Sum of electronic and zero-point Energies= -
2675.086784
Sum of electronic and thermal Energies= -
2675.052683
Sum of electronic and thermal Enthalpies= -
2675.051738
Sum of electronic and thermal Free Energies= -
2675.158636

Fe	-0.28565	0.70535	-0.4995
N	0.80049	0.66152	-2.38071
N	1.30174	1.35454	0.84888
N	-2.28014	0.27842	-1.36552
N	-0.85418	2.80942	-0.62514
C	1.26716	1.75286	-3.02393
H	0.9812	2.71108	-2.60223
C	2.40102	0.41496	-4.65104
H	3.0292	0.31324	-5.53074
C	1.91694	-0.71534	-3.99639
H	2.15574	-1.71131	-4.35676
C	1.1108	-0.55866	-2.86817
C	-0.16669	0.58878	2.66293
H	-0.66238	1.20773	3.42014
H	0.11808	-0.34062	3.16027
C	1.09122	1.2747	2.17539
C	2.01315	1.77177	3.10079
H	1.80476	1.69748	4.16402
C	3.19289	2.34921	2.64493
H	3.92387	2.73647	3.34809
C	3.41844	2.4208	1.26778

C	2.44922	1.91876	0.41288
H	2.58249	1.96064	-0.6627
C	-3.30498	0.11595	-1.88273
C	2.06349	1.67742	-4.15887
C	-1.17128	3.92489	-0.6199
C	-1.56528	5.32815	-0.61865
H	-2.46942	5.46425	-0.01655
H	-1.76947	5.65786	-1.64257
H	-0.76235	5.9433	-0.2
C	-4.59471	-0.0951	-2.52748
H	-4.44923	-0.31553	-3.58996
H	-5.21262	0.80362	-2.43375
H	-5.11393	-0.93622	-2.05697
N	-1.12574	0.26196	1.56421
N	0.08219	-1.48709	-0.79197
C	0.46983	-1.7554	-2.19436
H	-0.44691	-1.99746	-2.74528
H	1.12082	-2.63304	-2.2653
C	-3.20285	-3.41044	2.14559
C	-3.88782	-2.19611	2.15851
H	-1.29031	-4.36593	1.90747
C	-1.82675	-3.42172	1.92387
C	-3.18732	-1.00643	1.96255
C	-1.8076	-1.01563	1.73786
H	-3.71689	-0.05672	2.01413
C	-1.09932	-2.2384	1.70641
C	2.5871	-2.97954	2.28853
C	1.21214	-2.8509	2.48381
H	4.21728	-2.68583	0.9074
C	3.14855	-2.59099	1.07288
C	0.37752	-2.33347	1.48185
C	0.95869	-1.97799	0.24725
C	2.33696	-2.09363	0.05184
H	2.78587	-1.81157	-0.89559
H	4.32496	2.85957	0.86517
H	2.41246	2.58404	-4.64119
H	3.2121	-3.38387	3.07826
H	0.768	-3.15507	3.42776
H	-3.73286	-4.34305	2.31076
H	-4.95738	-2.16809	2.34279
H	-1.85467	0.97512	1.5861
H	-0.83763	-1.89269	-0.62722

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2674.16861
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.08680
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2675.97697
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2676.32733

Compound D-H trans singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.516066 (Hartree/Particle)
Thermal correction to Energy= 0.547637
Thermal correction to Enthalpy= 0.548582
Thermal correction to Gibbs Free Energy= 0.452693
Sum of electronic and zero-point Energies= -2675.075953
Sum of electronic and thermal Energies= -2675.044381
Sum of electronic and thermal Enthalpies= -2675.043437
Sum of electronic and thermal Free Energies= -2675.139325

Fe	0.03557	0.52462	-0.41832
N	0.99891	0.59148	-2.19348
N	-0.7981	2.34433	-0.14813
N	-1.63914	0.04114	-1.24545
N	1.71562	1.08127	0.35053
C	1.45418	1.69492	-2.82331
H	1.18679	2.64567	-2.37905
C	2.60733	0.40464	-4.47886
H	3.22416	0.3272	-5.36872
C	2.18106	-0.7404	-3.8105
H	2.46577	-1.7275	-4.16187
C	1.38402	-0.61501	-2.67344
C	-0.89947	1.55116	2.15432
H	-1.70415	1.44861	2.88686
H	-0.01523	1.88762	2.70772
C	-1.24732	2.58034	1.10743
C	-1.97299	3.72587	1.4319
H	-2.31336	3.87651	2.45187
C	-2.25752	4.66107	0.44001
H	-2.81669	5.56153	0.67415
C	-1.82772	4.40281	-0.86137
C	-1.11756	3.23542	-1.11026
H	-0.8037	2.9882	-2.1169
C	-2.65855	-0.19294	-1.7445
C	2.24213	1.64918	-3.96626
C	2.74259	1.42685	0.76157
C	4.03657	1.85547	1.27764
H	3.91046	2.69831	1.96488
H	4.68378	2.16845	0.45187
H	4.51724	1.02925	1.81152
C	-3.94325	-0.487	-2.36703
H	-3.79325	-1.00888	-3.31766
H	-4.48809	0.44323	-2.55831
H	-4.54275	-1.11948	-1.70426
N	-0.56627	0.23166	1.53629
N	0.48056	-1.48943	-0.53297
C	0.88124	-1.82891	-1.93222
H	-0.00707	-2.21778	-2.44309
H	1.62297	-2.6316	-1.94338
C	-3.12198	-3.07912	2.27654
C	-3.6728	-1.80367	2.15442
H	-1.31362	-4.24822	2.22068
C	-1.74553	-3.25549	2.13417
C	-2.84948	-0.70318	1.90326
C	-1.47226	-0.88127	1.77931
H	-3.28714	0.28713	1.82015
C	-0.89556	-2.16889	1.87731
C	2.69378	-3.15041	2.69003
C	1.32015	-2.93437	2.80144
H	4.42479	-2.96674	1.41729
C	3.35642	-2.79914	1.51424
C	0.58341	-2.37485	1.7463
C	1.27125	-2.04607	0.5551
C	2.64702	-2.24428	0.44612
H	3.17108	-1.98395	-0.46863
H	-2.04434	5.08599	-1.6755
H	2.56774	2.57213	-4.43381
H	-0.45214	-1.88036	-0.40002
H	0.31925	-0.06181	1.94862
H	0.80148	-3.1995	3.71808
H	3.24113	-3.59148	3.51687
H	-3.75872	-3.93357	2.48217
H	-4.74272	-1.6568	2.26669

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas

HF = -2674.19799
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.05998
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.97410
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2676.30445

Compound D-H trans Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.513530 (Hartree/Particle)
Thermal correction to Energy= 0.546189
Thermal correction to Enthalpy= 0.547133
Thermal correction to Gibbs Free Energy= 0.446572
Sum of electronic and zero-point Energies= -2675.064752
Sum of electronic and thermal Energies= -2675.032094
Sum of electronic and thermal Enthalpies= -2675.031149
Sum of electronic and thermal Free Energies= -2675.131710

Fe	0.04577	0.69211	-0.55341
N	1.12771	0.45783	-2.35127
N	-0.92461	2.4834	0.00637
N	-1.59231	0.18599	-1.40559
N	1.68846	1.26552	0.24485
C	1.59145	1.50031	-3.0716
H	1.31668	2.49055	-2.71953
C	2.73649	0.04948	-4.58987
H	3.36384	-0.11566	-5.46037
C	2.27639	-1.02804	-3.83714
H	2.53815	-2.0468	-4.10677
C	1.46591	-0.79183	-2.7253
C	-0.92027	1.52288	2.25744
H	-1.68979	1.37516	3.0211
H	-0.02686	1.87878	2.78446
C	-1.34714	2.59997	1.28053
C	-2.09747	3.69819	1.70452
H	-2.43023	3.75767	2.73644
C	-2.40632	4.70771	0.79642
H	-2.98508	5.57112	1.10975
C	-1.9667	4.58477	-0.52311
C	-1.24166	3.45449	-0.87522
H	-0.90328	3.30818	-1.89709
C	-2.60919	-0.06643	-1.8997
C	2.38465	1.34322	-4.19999
C	2.71062	1.59943	0.67559
C	3.99657	2.01275	1.22092
H	3.86145	2.84361	1.92094
H	4.65937	2.33654	0.41177
H	4.46263	1.17346	1.74758
C	-3.88877	-0.38866	-2.51682
H	-3.73019	-0.90837	-3.46728
H	-4.45452	0.52949	-2.70606
H	-4.47051	-1.03321	-1.84966
N	-0.57457	0.24009	1.59996
N	0.47477	-1.55379	-0.55686
C	0.87825	-1.94021	-1.92964
H	-0.01872	-2.29125	-2.45367
H	1.57414	-2.78437	-1.90922
C	-3.12438	-3.09225	2.21238
C	-3.67434	-1.81493	2.10414
H	-1.3114	-4.25517	2.16537
C	-1.74512	-3.26208	2.09159
C	-2.84923	-0.70816	1.89188
C	-1.46611	-0.87759	1.79386
H	-3.28739	0.28332	1.82335
C	-0.89323	-2.16929	1.8718
C	2.71177	-3.07177	2.71015
C	1.33406	-2.88064	2.81624
H	4.4371	-2.88363	1.43051
C	3.36524	-2.73686	1.52422
C	0.58573	-2.36409	1.74786
C	1.26134	-2.05615	0.54318
C	2.64421	-2.22685	0.44221
H	3.16201	-1.98247	-0.48074
H	-2.18728	5.34274	-1.26686
H	2.72379	2.21331	-4.75158
H	-0.47699	-1.88247	-0.40482
H	0.3358	-0.05514	1.94771
H	0.82027	-3.13118	3.73983
H	3.26891	-3.47917	3.54762
H	-3.76322	-3.95159	2.3889
H	-4.74671	-1.67196	2.19776

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2674.17419
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.05481
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.95715
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2676.29436

Compound D-H trans Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.511267 (Hartree/Particle)
Thermal correction to Energy= 0.545276
Thermal correction to Enthalpy= 0.546220
Thermal correction to Gibbs Free Energy= 0.439947
Sum of electronic and zero-point Energies= -2675.087031
Sum of electronic and thermal Energies= -2675.053023
Sum of electronic and thermal Enthalpies= -2675.052078
Sum of electronic and thermal Free Energies= -2675.158352

Fe	0.03776	0.62572	-0.5013
N	1.20793	0.42261	-2.30718
N	-1.01875	2.43591	0.02821
N	-1.82773	0.07013	-1.56552
N	1.92469	1.37348	0.40302
C	1.74165	1.46299	-2.98017
H	1.49656	2.45368	-2.60743
C	2.87328	0.0037	-4.49999
H	3.52374	-0.165	-5.35279
C	2.33637	-1.07422	-3.79984
H	2.55968	-2.09512	-4.09444
C	1.49821	-0.83164	-2.71037
C	-0.84485	1.55486	2.3035
H	-1.54672	1.41633	3.13191
H	0.0797	1.95211	2.73823
C	-1.37722	2.5791	1.32071
C	-2.15189	3.65801	1.74974

H	-2.43305	3.74089	2.79521
C	-2.55141	4.62051	0.82546
H	-3.15081	5.46899	1.1411
C	-2.17562	4.47269	-0.51165
C	-1.41979	3.36354	-0.86557
H	-1.12444	3.19639	-1.89774
C	-2.84304	-0.11995	-2.09254
C	2.56765	1.30152	-4.08395
C	2.95462	1.75199	0.77808
C	4.24911	2.22535	1.25152
H	4.12209	3.14279	1.83518
H	4.90426	2.43563	0.40008
H	4.71786	1.463	1.88197
C	-4.11907	-0.36213	-2.75357
H	-3.95127	-0.80037	-3.74265
H	-4.66373	0.58006	-2.87204
H	-4.72442	-1.05119	-2.15598
N	-0.5107	0.25817	1.66585
N	0.41589	-1.60895	-0.59344
C	0.81858	-1.96958	-1.97443
H	-0.09469	-2.22843	-2.5227
H	1.45139	-2.86266	-1.97905
C	-3.137	-3.02165	2.25837
C	-3.65388	-1.72817	2.19798
H	-1.35642	-4.22988	2.1389
C	-1.76574	-3.22454	2.09883
C	-2.80425	-0.63803	1.99475
C	-1.4303	-0.84214	1.85443
H	-3.21828	0.36517	1.96245
C	-0.89104	-2.14923	1.88573
C	2.71593	-3.11359	2.64031
C	1.34558	-2.89157	2.78051
H	4.40738	-2.98467	1.30989
C	3.34182	-2.81442	1.43099
C	0.57946	-2.37839	1.72382
C	1.22671	-2.10654	0.49602
C	2.60114	-2.31077	0.35892
H	3.09988	-2.0954	-0.58123
H	-2.46716	5.19673	-1.26472
H	2.96591	2.16921	-4.59856
H	-0.53075	-1.95361	-0.43853
H	0.39323	-0.04851	2.0232
H	0.85168	-3.11624	3.72148
H	3.28765	-3.51787	3.46944
H	-3.79424	-3.86817	2.42934
H	-4.71917	-1.55862	2.3223

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2674.17035
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.05481
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.08402
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2675.97829

Compound E-Me cis-α Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.873693 (Hartree/Particle)
Thermal correction to Energy= 0.917512
Thermal correction to Enthalpy= 0.918456
Thermal correction to Gibbs Free Energy= 0.798561
Sum of electronic and zero-point Energies= -3071.438865
Sum of electronic and thermal Energies= -3071.395047
Sum of electronic and thermal Enthalpies= -3071.394103
Sum of electronic and thermal Free Energies= -3071.513998

Fe	-0.26626	0.41935	0.19213
N	-1.74137	-0.12494	1.46598
N	1.19797	0.90996	-1.11296
N	0.81016	0.81453	1.74892
N	-0.79264	2.27849	0.16806
C	-2.83413	0.58649	1.82796
H	-2.95188	1.55182	1.34752
C	-3.57849	-1.12244	3.34714
C	-2.45032	-1.85524	2.97884
H	-2.2658	-2.83542	3.40993
C	-1.55513	-1.329	2.05169
C	-0.70909	0.94086	-2.58284
H	-1.20767	1.90433	-2.43389
H	-0.94171	0.61693	-3.60408
C	0.77338	1.10215	-2.38119
C	1.63922	1.46844	-3.40985
H	1.25158	1.59455	-4.41752
C	2.99109	1.67209	-3.13962
C	3.43539	1.4931	-1.81085
C	2.50939	1.10946	-0.85007
H	2.82007	0.95649	0.17713
C	1.38978	1.1229	2.70446
C	-3.76898	0.14597	2.75322
C	-1.01641	3.41562	0.20022
C	-1.29781	4.84648	0.23978
H	-2.13	5.08892	-0.42908
H	-1.56368	5.15059	1.25733
H	-0.41508	5.41099	-0.07767
C	2.11998	1.50758	3.90736
H	2.86995	0.74934	4.1551
H	2.62608	2.46572	3.75123
H	1.42838	1.60708	4.75022
N	-1.26259	-0.01199	-1.57545
N	0.12991	-1.61575	0.28786
C	-1.35597	-3.50068	-3.37991
C	-1.32375	-4.36149	-2.11332
C	-0.37329	-3.74798	-1.07367
C	-0.77456	-2.30067	-0.72672
C	-0.8788	-1.42908	-1.98011
C	-1.796	-2.06757	-3.04236
H	-0.35519	-4.36356	-0.16675
H	-2.33655	-4.44812	-1.69629
H	-0.99403	-5.37907	-2.34652
H	-0.36232	-3.49149	-3.84875
H	-2.04531	-3.924	-4.1176
H	-1.76392	-2.33125	-0.25594
H	0.12491	-1.34268	-2.41203
H	-2.8262	-2.10834	-2.6703
H	-1.80961	-1.45185	-3.94925
H	0.64046	-3.7653	-1.49025
C	-0.28494	-2.0338	1.65916
H	0.51926	-1.75415	2.34737
H	-0.39513	-3.12248	1.7256
C	4.01613	2.05864	-4.18921
H	4.03625	1.29512	-4.97824
H	3.70355	2.99096	-4.67894
C	5.7824	1.01887	-2.62846
C	7.2699	1.02271	-2.24198
H	7.45825	0.30541	-1.4345
H	7.88009	0.71978	-3.10039
H	7.63392	1.99838	-1.91013

C	5.40531	-0.39799	-3.06914
H	6.00755	-0.69697	-3.93497
H	5.61552	-1.11616	-2.26696
H	4.35307	-0.51039	-3.34706
C	4.89339	1.74916	-1.53745
H	5.15651	1.61873	-0.48238
C	5.40622	2.23831	-3.54991
H	6.14271	2.55203	-4.29532
C	5.25273	3.08749	-2.25826
H	4.48885	3.87251	-2.2555
H	6.19379	3.51229	-1.90973
C	-4.63022	-1.58844	4.30976
H	-4.43093	-2.58907	4.70395
C	-4.9858	0.9609	3.16629
H	-4.66517	1.91638	3.60213
H	-5.58666	1.21119	2.28155
C	-4.97362	-0.42683	5.33672
C	-3.83252	0.41177	5.9186
H	-4.23912	1.26479	6.47468
H	-3.24261	-0.18393	6.62551
H	-3.14571	0.80501	5.16312
C	-5.84507	0.16453	4.16774
H	-6.74399	0.72403	4.4432
C	-6.01001	-1.28532	3.63897
H	-6.82719	-1.8267	4.1147
H	-6.0772	-1.42805	2.55523
C	1.56291	-1.96844	0.10441
H	1.87459	-1.76467	-0.91997
H	2.16114	-1.35135	0.77602
H	1.75404	-3.02075	0.33561
C	-2.73536	0.18179	-1.50862
H	-3.18503	-0.56632	-0.85589
H	-2.93842	1.17018	-1.09397
H	-3.19751	0.1187	-2.4985
C	-5.83384	-0.9438	6.50048
H	-6.67815	-1.5599	6.18165
H	-6.23939	-0.0986	7.06844
H	-5.22637	-1.5429	7.18848

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.41881
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.56879
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.74674
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.16454

Compound E-Me cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.870743 (Hartree/Particle)
Thermal correction to Energy= 0.916103
Thermal correction to Enthalpy= 0.917047
Thermal correction to Gibbs Free Energy= 0.790923
Sum of electronic and zero-point Energies= -3071.423291
Sum of electronic and thermal Energies= -3071.377931
Sum of electronic and thermal Enthalpies= -3071.376987
Sum of electronic and thermal Free Energies= -3071.503111

Fe	-0.18511	0.39908	0.23651
N	-1.68415	-0.17128	1.56982
N	1.23405	0.96242	-1.09927
N	0.83957	0.8884	1.78038
N	-1.02142	2.70276	0.16792
C	-2.73041	0.59152	1.96263
H	-2.77235	1.58796	1.53472
C	-3.60791	-1.15235	3.36296
C	-2.51808	-1.93017	2.97199
H	-2.40299	-2.94278	3.34896
C	-1.57144	-1.41303	2.09015
C	-0.70369	0.89295	-2.51748
H	-1.21628	1.84299	-2.33392
H	-0.96505	0.57623	-3.53313
C	0.77834	1.09319	-2.36512
C	1.61952	1.43389	-3.42073
H	1.21517	1.51877	-4.42589
C	2.9748	1.66057	-3.18031
C	3.45138	1.53323	-1.85544
C	2.54829	1.18033	-0.86244
H	2.87445	1.06509	0.1655
C	1.40307	1.2114	2.74096
C	-3.70514	0.16104	2.85056
C	-1.12481	3.85806	0.2067
C	-1.26493	5.30985	0.25065
H	-2.19395	5.61203	-0.24321
H	-1.28834	5.65432	1.28925
H	-0.42184	5.78411	-0.26141
C	2.10656	1.6186	3.95126
H	2.87579	0.88312	4.20864
H	2.58525	2.59162	3.80034
H	1.40152	1.69715	4.78522
N	-1.20253	-0.08247	-1.49893
N	0.13896	-1.83226	0.35808
C	-1.2809	-3.51276	-3.41637
C	-1.3008	-4.42867	-2.18919
C	-0.37694	-3.87169	-1.09774
C	-0.75244	-2.42987	-0.69647
C	-0.81481	-1.49903	-1.92157
C	-1.71167	-2.08974	-3.02917
H	-0.39916	-4.51656	-0.21101
H	-2.32773	-4.51758	-1.80855
H	-0.97853	-5.44025	-2.45693
H	-0.27294	-3.49793	-3.85378
H	-1.95269	-3.8915	-4.19359
H	-1.755	-2.46041	-0.25249
H	0.2017	-1.40507	-2.32178
H	-2.74993	-2.13515	-2.68047
H	-1.70234	-1.44114	-3.91285
H	0.65096	-3.89354	-1.47882
C	-0.33164	-2.1924	1.71145
H	0.47086	-1.94465	2.41682
H	-0.51209	-3.2714	1.81186
C	3.9734	2.01722	-4.2647
H	3.97917	1.22697	-5.02727
H	3.64162	2.92981	-4.77856
C	5.78159	1.04447	-2.70929
C	7.27729	1.07028	-2.35712
H	7.48797	0.38416	-1.52843
H	7.86957	0.73901	-3.2176
H	7.64289	2.05939	-2.06988
C	5.40328	-0.38926	-3.0904
H	5.98905	-0.71617	-3.95736
H	5.63406	-1.07666	-2.26729
H	4.34602	-0.51747	-3.34174
C	4.91289	1.8083	-1.62487
H	5.19999	1.71746	-0.57208
C	5.37663	2.22793	-3.66485
H	6.09338	2.5191	-4.43802
C	5.24659	3.12191	-2.40132

H	4.47825	3.90257	-2.40893
H	6.19251	3.56352	-2.08898
C	-4.71384	-1.61438	4.2651
H	-4.59013	-2.65112	4.59123
C	-4.87239	1.027	3.29903
H	-4.49671	1.92111	3.8141
H	-5.4312	1.38607	2.42435
C	-5.01353	-0.50809	5.36346
C	-3.83753	0.20603	6.03536
H	-4.20241	1.04393	6.64109
H	-3.31348	-0.47901	6.71246
H	-3.09985	0.6019	5.3305
C	-5.80973	0.22024	4.21893
H	-6.67896	0.81667	4.51175
C	-6.05147	-1.17548	3.58343
H	-6.91514	-1.69361	3.99915
H	-6.09579	-1.2374	2.49091
C	1.57019	-2.17782	0.20679
H	1.90774	-1.94987	-0.80614
H	2.15223	-1.56923	0.90378
H	1.77595	-3.23384	0.41743
C	-2.67769	0.0903	-1.38569
H	-3.09883	-0.68012	-0.74046
H	-2.87943	1.06603	-0.94174
H	-3.16365	0.04416	-2.36487
C	-5.9412	-1.04727	6.46366
H	-6.81736	-1.57499	6.07884
H	-6.30264	-0.21989	7.08509
H	-5.39791	-1.7389	7.11764

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.38218
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.55185
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.71262
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.14630

Compound E-Me cis-α Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.868610 (Hartree/Particle)
Thermal correction to Energy= 0.914987
Thermal correction to Enthalpy= 0.915931
Thermal correction to Gibbs Free Energy= 0.786131
Sum of electronic and zero-point Energies= -3071.443037
Sum of electronic and thermal Energies= -3071.396661
Sum of electronic and thermal Enthalpies= -3071.395716
Sum of electronic and thermal Free Energies= -3071.525517

Fe	-0.22596	0.57027	0.29227
N	-1.7814	-0.06451	1.68598
N	1.30424	1.0699	-1.18666
N	1.10633	1.04184	1.97086
N	-0.91497	2.65149	0.30927
C	-2.86167	0.64439	2.08652
H	-2.93133	1.65642	1.69778
C	-3.69793	-1.18626	3.3951
C	-2.57869	-1.9137	2.98743
H	-2.4398	-2.93835	3.32114
C	-1.63888	-1.32663	2.14357
C	-0.63387	0.93499	-2.65273
H	-1.12976	1.90498	-2.52607
H	-0.84714	0.60804	-3.67876
C	0.85564	1.11824	-2.45819
C	1.71028	1.37629	-3.52941
H	1.31327	1.39441	-4.54118
C	3.06589	1.60595	-3.29813
C	3.53422	1.56455	-1.96526
C	2.61836	1.28959	-0.9588
H	2.93571	1.24017	0.07847
C	1.66515	1.33391	2.94396
C	-3.83672	0.14427	2.93644
C	-1.10897	3.79456	0.29032
C	-1.35579	5.23106	0.2652
H	-2.28206	5.44551	-0.27738
H	-1.44481	5.61405	1.28682
H	-0.52595	5.7421	-0.23348
C	2.37083	1.6993	4.16613
H	3.13223	0.94871	4.4011
H	2.85675	2.67227	4.04144
H	1.66388	1.76069	4.99972
N	-1.21458	0.0094	-1.64951
N	0.07569	-1.6568	0.37696
C	-1.31279	-3.52131	-3.34599
C	-1.36733	-4.35783	-2.0648
C	-0.44997	-3.74869	-0.99586
C	-0.81033	-2.2816	-0.67747
C	-0.83723	-1.42224	-1.96162
C	-1.71998	-2.07135	-3.04927
H	-0.48719	-4.3475	-0.07816
H	-2.40118	-4.40491	-1.69537
H	-1.05875	-5.3898	-2.26192
H	-0.29825	-3.55192	-3.76718
H	-1.98024	-3.9357	-4.10875
H	-1.82029	-2.26972	-0.24979
H	0.18809	-1.37232	-2.34749
H	-2.76604	-2.07514	-2.72053
H	-1.68012	-1.47132	-3.96608
H	0.58098	-3.80237	-1.3654
C	-0.37354	-2.04875	1.73508
H	0.42764	-1.77887	2.43358
H	-0.5096	-3.13448	1.82169
C	4.07397	1.8773	-4.39849
H	4.07457	1.03833	-5.10716
H	3.75656	2.75778	-4.97385
C	5.86229	0.9905	-2.77027
C	7.35661	1.02116	-2.41283
H	7.5547	0.3905	-1.53816
H	7.94863	0.6244	-3.24542
H	7.73365	2.02293	-2.19197
C	5.46818	-0.46101	-3.0567
H	6.05414	-0.85181	-3.89672
H	5.68698	-1.09478	-2.18841
H	4.41061	-0.59319	-3.30431
C	4.99793	1.83661	-1.74513
H	5.27824	1.81344	-0.68681
C	5.47676	2.11122	-3.80597
H	6.20099	2.34073	-4.59295
C	5.35292	3.09028	-2.60626
H	4.59539	3.87887	-2.67046
H	6.30366	3.53916	-2.31954
C	-4.79569	-1.72332	4.26373
H	-4.63798	-2.76716	4.54997
C	-5.04237	0.94705	3.40186
H	-4.70757	1.83534	3.95382
H	-5.60452	1.31636	2.53361
C	-5.14641	-0.67306	5.4018
C	-4.00493	0.0564	6.11547

H	-4.40732	0.85758	6.74655
H	-3.46517	-0.63434	6.77412
H	-3.27248	0.50539	5.43738
C	-5.95815	0.07088	4.27877
H	-6.85147	0.62287	4.58564
C	-6.1417	-1.30567	3.58496
H	-6.98916	-1.87185	3.97013
H	-6.17284	-1.32471	2.49047
C	1.5115	-1.9956	0.21879
H	1.83967	-1.77456	-0.79807
H	2.09405	-1.37771	0.9064
H	1.72153	-3.0486	0.43758
C	-2.67938	0.22915	-1.56986
H	-3.12864	-0.4892	-0.88232
H	-2.86214	1.23411	-1.18146
H	-3.17136	0.14173	-2.54514
C	-6.06455	-1.28958	6.46883
H	-6.91733	-1.83231	6.05341
H	-6.46214	-0.50137	7.11838
H	-5.50333	-1.98707	7.10107

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.37887
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.58577
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.73651
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.16142

Compound E-Me cis-β Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.874132
(Hartree/Particle)
Thermal correction to Energy= 0.917864
Thermal correction to Enthalpy= 0.918808
Thermal correction to Gibbs Free Energy=
0.799814
Sum of electronic and zero-point Energies= -
3071.432836
Sum of electronic and thermal Energies= -
3071.389105
Sum of electronic and thermal Enthalpies= -
3071.388161
Sum of electronic and thermal Free Energies= -
3071.507154

C	-1.5595210	2.6266305	1.1142706
C	-2.8499610	3.4683005	1.1378806
C	-2.5447910	4.9647705	0.9681506
C	-1.5691010	5.4405605	2.0497006
C	-0.2735810	4.6126705	2.0156806
C	-0.5657810	3.1090705	2.1856806
C	-2.2881810	0.5040705	0.0221306
C	-1.9120910	-0.9579595	0.0171706
C	-2.6884410	-1.9414495	-0.5912494
C	-2.2511810	-3.2657395	-0.6003494
C	-1.0217010	-3.5649095	0.0271306
C	-0.3155610	-2.5289895	0.6260106
C	1.7763390	2.6404005	1.3458106
C	1.5251190	2.2399605	-0.0807394
C	2.0912490	2.9177705	-1.1570594
C	1.9380790	2.4178905	-2.4504294
C	0.6685390	0.6150705	-1.4894594
Fe	0.1218090	0.3294105	1.5098806
H	-1.0956410	2.7554705	0.1326606
H	-3.5308110	3.1258005	0.3491906
H	-3.3714310	3.3328805	2.0925806
H	-2.1167410	5.1512905	-0.0265594
H	-3.4794010	5.5328005	1.0167706
H	-2.0402210	5.3585505	3.0387906
H	-1.3235710	6.4981305	1.9086906
H	0.4144490	4.9564405	2.7965506
H	0.2160390	4.7900205	1.0499006
H	-1.0442210	2.9783805	3.1624306
H	-1.8345510	1.0098405	-0.8357194
H	-3.3735010	0.6290505	-0.0654994
H	-3.6339210	-1.6685095	-1.0528794
H	2.6753790	2.1164905	1.6883606
H	1.9878390	3.7089505	1.4386606
H	2.6574390	3.8286305	-0.9830194
N	-1.7625710	1.1375805	1.2686406
N	0.6703090	2.2053505	2.2495006
N	0.7931990	1.1141805	-0.2367094
N	-0.7341110	-1.2447895	0.6205106
N	1.8793290	-0.4534995	1.6803506
N	-0.2879110	-0.4380995	3.2364006
C	2.9290890	-0.9402995	1.7522706
C	-0.4450610	-0.9816995	4.2477306
C	4.2506590	-1.5525495	1.8368606
H	4.9994490	-0.8014695	2.1088706
H	4.5251090	-1.9887995	0.8709706
H	4.2540590	-2.3417995	2.5954206
C	-0.6589810	-1.6572195	5.5225906
H	-1.6847710	-1.4929295	5.8687406
H	0.0335290	-1.2705995	6.2773206
H	-0.4942610	-2.7337095	5.4112506
H	0.6269390	-2.7196695	1.1282506
C	-3.0307510	-4.4081095	-1.2243294
C	-0.5627810	-4.9977095	-0.0167794
C	-2.2575310	-5.7332695	-1.0842894
H	-3.2131910	-4.1891595	-2.2853094
H	-4.0215410	-4.4731395	-0.7550194
C	-1.7564110	-5.9583395	0.3905606
C	-1.2715510	-7.3979995	0.6227706
C	-2.6635310	-5.5636395	1.5589906
H	-0.6160310	-7.7719995	-0.1676694
H	-2.1301110	-8.0762595	0.6849206
H	-0.7247710	-7.4708095	1.5703006
H	-3.0436610	-4.5393495	1.5004106
H	-2.1252410	-5.6639895	2.5097306
H	-3.5296010	-6.2339695	1.6074406
C	-0.7765910	-5.4888695	-1.4842094
H	-2.7980010	-6.5546295	-1.5636494
H	-0.5797010	-4.7657795	-2.2830694
H	-0.2332610	-6.4082495	-1.7017394
H	0.4100190	-5.1458095	0.4637406
C	2.4751190	3.0654305	-3.6919594
C	3.2086290	1.9793005	-4.5893594
C	1.7583390	1.5699605	-5.0408094
C	4.0065590	2.6374105	-5.7258194
C	1.2155390	1.2145905	-2.6149094
H	0.1068590	-0.3085895	-1.5796994
C	1.0867790	0.6355505	-4.0158694
H	3.4458990	3.4002805	-6.2716394
H	4.3173590	1.8767805	-6.4511194
H	4.9141690	3.1097705	-5.3330394
H	0.0268590	0.5053005	-4.2726294
H	1.5369190	-0.3654295	-4.0470594
H	1.6378890	1.1855105	-6.0579494
C	1.3207890	3.0299805	-4.7461894
H	2.9918090	4.0081105	-3.4897294
H	0.3035790	3.1921905	-4.3740694
H	1.5018790	3.7093905	-5.5785694
C	4.1083990	0.9404805	-3.9141594

H	3.6382390	0.4262205	-3.0702894
H	5.0254890	1.4141805	-3.5439094
H	4.4097190	0.1767005	-4.6406594
C	-2.7196810	0.8104805	2.3645606
H	-3.7225410	1.1809505	2.1345206
H	-2.3861310	1.2436505	3.3074406
H	-2.7679710	-0.2726195	2.4765106
C	1.1999190	2.2276905	3.6420306
H	2.0388790	1.5339105	3.7214906
H	0.4199990	1.9123705	4.3352206
H	1.5425690	3.2298005	3.9247706

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.43006
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.56043
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.73017
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.17187

Compound E-Me cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.871106 (Hartree/Particle)
Thermal correction to Energy= 0.916326
Thermal correction to Enthalpy= 0.917270
Thermal correction to Gibbs Free Energy= 0.791976
Sum of electronic and zero-point Energies= -3071.416999
Sum of electronic and thermal Energies= -3071.371779
Sum of electronic and thermal Enthalpies= -3071.370834
Sum of electronic and thermal Free Energies= -3071.496129

C	-1.5865659	2.6163745	1.0696416
C	-2.8737349	3.4687045	1.0567636
C	-2.5800999	4.9627195	0.8631086
C	-1.6207359	5.4635905	1.9469496
C	-0.3237449	4.6391385	1.9410316
C	-0.6031629	3.1358775	2.1447426
C	-2.2958739	0.4840445	0.0115556
C	-1.9290369	-0.9877845	0.0206346
C	-2.7458009	-1.9598715	-0.5560174
C	-2.3381289	-3.2930775	-0.5768104
C	-1.0940699	-3.6203305	0.0077526
C	-0.3486869	-2.5968625	0.5785706
C	1.7774831	2.6982345	1.3804356
C	1.5635471	2.2579775	-0.0417974
C	2.0717091	2.9617575	-1.1295224
C	1.9461671	2.4392085	-2.4175184
C	0.8133581	0.5594635	-1.4331424
Fe	0.2764931	0.2661335	1.5222376
H	-1.1050119	2.7221985	0.0924306
H	-3.5417289	3.1047555	0.2665946
H	-3.4085629	3.3438305	2.0060886
H	-2.1403129	5.1345395	-0.1293084
H	-3.5188189	5.5257765	0.8894476
H	-2.1025229	5.3961765	2.9320226
H	-1.3769459	6.5195885	1.7908386
H	0.3578341	5.0044865	2.7181996
H	0.1724251	4.7969085	0.9748986
H	-1.0963999	3.0259185	3.1164836
H	-1.8155049	0.9684495	-0.8458624
H	-3.3798879	0.5954105	-0.1261984
H	-3.7010529	-1.6684885	-0.9853964
H	2.6748141	2.1931455	1.7570296
H	1.9778811	3.7712785	1.4446386
H	2.5692741	3.9140875	-0.9691254
N	-1.8232419	1.1491615	1.2448396
N	0.6565071	2.2758735	2.2694156
N	0.9188211	1.0759235	-0.1850034
N	-0.7424389	-1.3047185	0.5815196
N	2.2951701	-0.5662915	1.7596546
N	-0.1551909	-0.5095015	3.2217946
C	3.3481211	-1.0493615	1.8038446
C	-0.3608049	-1.0304195	4.2362766
C	4.6737511	-1.6539555	1.8606286
H	5.4159171	-0.8989545	2.1394596
H	4.9391731	-2.0656145	0.8817106
H	4.6902221	-2.4577815	2.6032756
C	-0.6258939	-1.6832565	5.5125076
H	-1.6528819	-1.4807325	5.8338346
H	0.0631641	-1.3110965	6.2776286
H	-0.4944819	-2.7657715	5.4155286
H	0.6084291	-2.8050265	1.0491076
C	-3.1633229	-4.4185795	-1.1723294
C	-0.6682659	-5.0624635	-0.0510604
C	-2.4141799	-5.7600745	-1.0597114
H	-3.3783189	-4.1946935	-2.2261454
H	-4.1381669	-4.4625205	-0.6684344
C	-1.8675039	-5.9973865	0.3967976
C	-1.4062369	-7.4474345	0.6118496
C	-2.7261979	-5.5852365	1.5956666
H	-0.7877929	-7.8353795	-0.2014074
H	-2.2767129	-8.1067525	0.7048336
H	-0.8277679	-7.5326315	1.5393416
H	-3.0846699	-4.5524515	1.5519516
H	-2.1592559	-5.7005305	2.5279016
H	-3.6050689	-6.2361025	1.6708256
C	-0.9429689	-5.5476245	-1.5104504
H	-2.9884209	-6.5692345	-1.5202464
H	-0.7579649	-4.8281895	-2.3154094
H	-0.4278479	-6.4785545	-1.7466884
H	0.3172331	-5.2320415	0.3953556
C	2.4253901	3.1132175	-3.6683354
C	3.2229721	2.0742405	-4.5670584
C	1.7997251	1.5630765	-5.0007954
C	3.9622081	2.7784335	-5.7156074
C	1.3073631	1.1875235	-2.5671214
H	0.3105241	-0.3984835	-1.5080874
C	1.2039701	0.5918265	-3.9631964
H	3.3456501	3.5010785	-6.2556464
H	4.3120371	2.0366795	-6.4426484
H	4.8423451	3.3100215	-5.3362144
H	0.1526751	0.3886735	-4.2076044
H	1.7201641	-0.3767345	-3.9933484
H	1.6953151	1.1645425	-6.0142854
C	1.2653411	2.9913885	-4.7101524
H	2.8780851	4.0904215	-3.4771664
H	0.2431501	3.0851685	-4.3282634
H	1.3909961	3.6765345	-5.5478964
C	4.1970811	1.1042725	-3.8928604
H	3.7642911	0.5578245	-3.0493964
H	5.0767251	1.6441525	-3.5223834
H	4.5537581	0.3642445	-4.6189364
C	-2.7526379	0.8219815	2.3494386
H	-3.7750919	1.1586135	2.1414146
H	-2.4152159	1.2769375	3.2824326
H	-2.7714739	-0.2611145	2.4851866
C	1.1379071	2.3314805	3.6760386
H	2.0012131	1.6720255	3.7918786

H 0.3476011 1.9902555 4.3458076
H 1.4324301 3.3477655 3.9647466
UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.39472
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.54873
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.70292
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.15418

Compound E-Me cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.868965 (Hartree/Particle)
Thermal correction to Energy= 0.915328
Thermal correction to Enthalpy= 0.916272
Thermal correction to Gibbs Free Energy= 0.786410
Sum of electronic and zero-point Energies= -3071.437019
Sum of electronic and thermal Energies= -3071.390657
Sum of electronic and thermal Enthalpies= -3071.389712
Sum of electronic and thermal Free Energies= -3071.519574

C	-1.58657	2.61637	1.06964
C	-2.87373	3.4687	1.05676
C	-2.5801	4.96272	0.86311
C	-1.62074	5.46359	1.94695
C	-0.32374	4.63914	1.94103
C	-0.60316	3.13588	2.14474
C	-2.29587	0.48404	0.01156
C	-1.92904	-0.98778	0.02063
C	-2.7458	-1.95987	-0.55602
C	-2.33813	-3.29308	-0.57681
C	-1.09407	-3.62033	0.00775
C	-0.34869	-2.59686	0.57857
C	1.77748	2.69823	1.38044
C	1.56355	2.25798	-0.0418
C	2.07171	2.96176	-1.12952
C	1.94617	2.43921	-2.41752
C	0.81336	0.55946	-1.43314
Fe	0.27649	0.26613	1.52224
H	-1.10501	2.7222	0.09243
H	-3.54173	3.10476	0.26659
H	-3.40856	3.34383	2.00609
H	-2.14031	5.13454	-0.12931
H	-3.51882	5.52578	0.88945
H	-2.10252	5.39618	2.93202
H	-1.37695	6.51959	1.79084
H	0.35783	5.00449	2.7182
H	0.17243	4.79691	0.9749
H	-1.0964	3.02592	3.11648
H	-1.8155	0.96845	-0.84586
H	-3.37989	0.59541	-0.1262
H	-3.70105	-1.66849	-0.9854
H	2.67481	2.19315	1.75703
H	1.97788	3.77128	1.44464
H	2.56927	3.91409	-0.96913
N	-1.82324	1.14916	1.24484
N	0.65651	2.27587	2.26942
N	0.91882	1.07592	-0.185
N	-0.74244	-1.30472	0.58152
N	2.29517	-0.56629	1.75965
N	-0.15519	-0.5095	3.22179
C	3.34812	-1.04936	1.80384
C	-0.3608	-1.03042	4.23628
C	4.67375	-1.65396	1.86063
H	5.41592	-0.89895	2.13946
H	4.93917	-2.06561	0.88171
H	4.69022	-2.45778	2.60328
C	-0.62589	-1.68326	5.51251
H	-1.65288	-1.48073	5.83383
H	0.06316	-1.3111	6.27763
H	-0.49448	-2.76577	5.41553
H	0.60843	-2.80503	1.04911
C	-3.16332	-4.41858	-1.17233
C	-0.66827	-5.06246	-0.05106
C	-2.41418	-5.76007	-1.05971
H	-3.37832	-4.19469	-2.22615
H	-4.13817	-4.46252	-0.66843
C	-1.8675	-5.99739	0.3968
C	-1.40624	-7.44743	0.61185
C	-2.7262	-5.58524	1.59567
H	-0.78779	-7.83538	-0.20141
H	-2.27671	-8.10675	0.70483
H	-0.82777	-7.53263	1.53934
H	-3.08467	-4.55245	1.55195
H	-2.15926	-5.70053	2.5279
H	-3.60507	-6.2361	1.67083
C	-0.94297	-5.54762	-1.51045
H	-2.98842	-6.56923	-1.52025
H	-0.75796	-4.82819	-2.31541
H	-0.42785	-6.47855	-1.74669
H	0.31723	-5.23204	0.39536
C	2.42539	3.11322	-3.66834
C	3.22297	2.07424	-4.56706
C	1.79973	1.56308	-5.0008
C	3.96221	2.77843	-5.71561
C	1.30736	1.18752	-2.56712
H	0.31052	-0.39848	-1.50809
C	1.20397	0.59183	-3.9632
H	3.34565	3.50108	-6.25565
H	4.31204	2.03668	-6.44265
H	4.84235	3.31002	-5.33621
H	0.15268	0.38867	-4.2076
H	1.72016	-0.37673	-3.99335
H	1.69532	1.16454	-6.01429
C	1.26534	2.99139	-4.71015
H	2.87809	4.09042	-3.47717
H	0.24315	3.08517	-4.32826
H	1.391	3.67653	-5.5479
C	4.19708	1.10427	-3.89286
H	3.76429	0.55782	-3.0494
H	5.07673	1.64415	-3.52238
H	4.55376	0.36424	-4.61894
C	-2.75264	0.82198	2.34944
H	-3.77509	1.15861	2.14141
H	-2.41522	1.27694	3.28243
H	-2.77147	-0.26111	2.48519
C	1.13791	2.33148	3.67604
H	2.00121	1.67203	3.79188
H	0.3476	1.99026	4.34581
H	1.43243	3.34777	3.96475

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.39095
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.57437

UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.72003
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.16909

Compound E-Me trans Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.872767
(Hartree/Particle)
Thermal correction to Energy= 0.916789
Thermal correction to Enthalpy= 0.917733
Thermal correction to Gibbs Free Energy=
0.797118
Sum of electronic and zero-point Energies= -
3071.392212
Sum of electronic and thermal Energies= -
3071.348190
Sum of electronic and thermal Enthalpies= -
3071.347246
Sum of electronic and thermal Free Energies= -
3071.467861

Fe	-0.08975	-0.82314	-0.61084
N	1.42586	-1.02335	0.72988
N	-1.41118	0.68354	-0.25919
N	-1.31808	-1.77985	0.55261
N	1.18289	0.40102	-1.42392
C	1.62975	-0.46268	1.93768
H	0.78748	0.08478	2.35316
C	3.88063	-1.29719	2.04885
C	3.66444	-1.88544	0.79896
H	4.44633	-2.47642	0.32982
C	2.43769	-1.7325	0.16354
C	-2.56685	0.43145	-0.92795
C	-3.70407	1.20891	-0.73446
H	-4.60604	0.99237	-1.30137
C	-3.67742	2.2712	0.17191
C	-2.47302	2.53516	0.85859
C	-1.37731	1.71609	0.60422
H	-0.42891	1.8883	1.106
C	-2.00564	-2.20682	1.38216
C	2.82681	-0.56367	2.63662
C	1.93729	1.22745	-1.72565
C	2.87683	2.27148	-2.1182
H	3.41044	1.97981	-3.02876
H	2.3413	3.20742	-2.308
H	3.60748	2.43836	-1.32023
C	-2.86141	-2.76252	2.42404
H	-2.72073	-2.21292	3.36041
H	-3.91311	-2.69165	2.12826
H	-2.61327	-3.8155	2.59336
C	-0.89851	-3.49355	-5.21115
C	-0.27206	-4.63649	-4.40262
C	0.65544	-4.10758	-3.29422
C	-0.09129	-3.11174	-2.38639
C	-0.60166	-1.93561	-3.23454
C	-1.58327	-2.46138	-4.29776
H	1.03891	-4.94655	-2.70402
H	-1.06565	-5.24463	-3.94705
H	0.29049	-5.30536	-5.06203
H	-0.12194	-2.99017	-5.80344
H	-1.62647	-3.88861	-5.9272
H	-0.9762	-3.62335	-1.99093
H	0.26831	-1.52517	-3.7597
H	-2.44698	-2.92401	-3.80023
H	-1.96877	-1.63357	-4.90229
H	1.52499	-3.60948	-3.74532
C	-4.86149	3.18351	0.43413
H	-5.1784	3.65007	-0.50814
H	-5.71621	2.58423	0.77677
C	-3.13876	4.9557	1.16117
C	-2.92414	6.21985	2.00862
H	-1.8881	6.56785	1.92229
H	-3.57335	7.02588	1.64826
H	-3.13822	6.07765	3.07097
C	-2.80042	5.29173	-0.2937
H	-3.45817	6.08889	-0.65931
H	-1.77104	5.66316	-0.36962
H	-2.89757	4.44496	-0.9796
C	-2.47552	3.68199	1.83303
H	-1.51535	3.80534	2.34475
C	-4.50427	4.24651	1.49121
H	-5.36453	4.88597	1.70943
C	-3.78343	3.54665	2.67574
H	-4.10337	2.53154	2.93515
H	-3.76318	4.15066	3.58268
C	5.14481	-1.42855	2.84794
H	5.90322	-2.0351	2.34456
C	3.06083	0.07783	3.99554
H	2.93347	1.16615	3.92217
H	2.30393	-0.27313	4.70981
C	5.57128	-0.01318	3.42515
C	5.4623	1.22057	2.52453
H	5.6384	2.13068	3.10997
H	6.2278	1.18711	1.73992
H	4.4886	1.3253	2.03545
C	4.46805	-0.27501	4.51504
H	4.63469	0.14592	5.51101
C	4.70946	-1.79406	4.30508
H	5.53693	-2.18418	4.89679
H	3.85166	-2.46611	4.41279
N	-1.10404	-0.75725	-2.42443
C	-2.50878	-0.71937	-1.93006
H	-3.2316	-0.55472	-2.73916
H	-2.75346	-1.67422	-1.45689
C	-0.94291	0.45685	-3.28981
N	0.65282	-2.69569	-1.13267
C	0.50496	-3.82327	-0.15475
C	2.10986	-2.38733	-1.17702
H	2.72317	-3.28594	-1.32001
H	2.31334	-1.71115	-2.01172
H	-1.64477	0.41295	-4.1295
H	0.06956	0.50634	-3.68428
H	-1.14224	1.36132	-2.71767
H	1.06702	-4.69601	-0.50416
H	-0.54234	-4.10093	-0.05556
H	0.88688	-3.53254	0.8224
C	6.98985	-0.05146	4.01556
H	7.73772	-0.08951	3.21523
H	7.16714	-0.90467	4.67498
H	7.17522	0.85811	4.59836

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.37297
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.52126
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.69844
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.11499

Compound E-Me trans triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.869955
(Hartree/Particle)
Thermal correction to Energy= 0.916062
Thermal correction to Enthalpy= 0.917007
Thermal correction to Gibbs Free Energy=
0.786594
Sum of electronic and zero-point Energies= -
3071.415621
Sum of electronic and thermal Energies= -
3071.369513
Sum of electronic and thermal Enthalpies= -
3071.368569
Sum of electronic and thermal Free Energies= -
3071.498982

Fe	-0.66959	-1.14425	-0.13116
N	1.11758	-0.79007	0.87528
N	-1.88446	0.40255	0.09896
N	-1.87855	-2.2249	1.06171
N	3.23422	-0.90459	-3.6334
C	1.34483	0.02976	1.92767
H	0.50282	0.6367	2.24835
C	3.62805	-0.68782	2.11349
C	3.39606	-1.5274	1.02281
H	4.1906	-2.16152	0.63987
C	2.13953	-1.55267	0.42543
C	-2.49333	0.72784	-1.06666
C	-3.4431	1.74214	-1.14129
H	-3.89893	1.98206	-2.09818
C	-3.80111	2.44288	0.0104
C	-3.17684	2.0931	1.22986
C	-2.23114	1.07685	1.21812
H	-1.73255	0.77431	2.13423
C	-2.63484	-2.71503	1.79121
C	2.56578	0.12374	2.57645
C	4.12547	-0.70956	-4.35074
C	5.2476	-0.46269	-5.25164
H	5.10866	-1.01339	-6.18712
H	5.32072	0.60533	-5.47902
H	6.18312	-0.7892	-4.787
C	-3.57608	-3.34759	2.70497
H	-3.12683	-3.43212	3.70007
H	-4.49217	-2.7527	2.77611
H	-3.82857	-4.35071	2.34569
C	-0.24028	-2.88029	-5.1831
C	-0.189	-4.21121	-4.42289
C	0.50597	-4.06214	-3.0572
C	-0.17411	-2.96629	-2.21626
C	-0.17446	-1.63771	-2.99305
C	-0.90814	-1.78197	-4.33692
H	0.48277	-5.02087	-2.52997
H	-1.20972	-4.59004	-4.27299
H	0.337	-4.96755	-5.01454
H	0.77787	-2.56511	-5.44756
H	-0.78801	-2.99949	-6.12361
H	-1.21633	-3.26797	-2.03613
H	0.86167	-1.38743	-3.23405
H	-1.96244	-2.04338	-4.17815
H	-0.88757	-0.82783	-4.8766
H	1.56093	-3.80017	-3.21209
C	-4.81296	3.5727	0.02694
H	-4.48076	4.36802	-0.65366
H	-5.76919	3.21082	-0.37504
C	-3.63075	4.40118	2.15989
C	-3.80149	5.22202	3.44791
H	-2.87133	5.22337	4.02812
H	-4.0355	6.26312	3.19845
H	-4.59829	4.85475	4.09977
C	-2.49049	5.01875	1.34616
H	-2.73001	6.05743	1.09025
H	-1.56643	5.0371	1.93683
H	-2.27302	4.49281	0.4118
C	-3.6092	2.84441	2.45979
H	-3.10459	2.4974	3.36748
C	-5.00835	4.10676	1.4584
H	-5.76491	4.89633	1.48169
C	-5.17017	2.89878	2.42116
H	-5.68907	2.01253	2.03988
H	-5.60271	3.17205	3.38336
C	4.92595	-0.59484	2.85851
H	5.6897	-1.27207	2.46545
C	2.82631	1.05845	3.7479
H	2.64446	2.0975	3.44301
H	2.1185	0.84609	4.56038
C	5.31064	0.93044	3.08078
C	5.10193	1.92482	1.93554
H	5.26274	2.94859	2.29345
H	5.83004	1.74378	1.13578
H	4.10447	1.88352	1.48841
C	4.26932	0.88106	4.25874
H	4.45876	1.52123	5.12553
C	4.56991	-0.63685	4.38082
H	5.43938	-0.85504	5.00033
H	3.74896	-1.29667	4.68061
N	-0.64933	-0.51157	-2.09183
C	-2.0838	-0.11779	-2.25309
H	-2.2513	0.41997	-3.19359
H	-2.69241	-1.02925	-2.28816
C	0.20349	0.69581	-2.31386
N	0.39125	-2.75817	-0.825
C	0.23885	-3.99455	-0.00872
C	1.83916	-2.37191	-0.80686
H	2.47762	-3.26138	-0.84764
H	2.08103	-1.782	-1.69527
H	0.13109	1.02517	-3.3574
H	1.24479	0.45836	-2.09516
H	-0.123	1.50803	-1.66285
H	0.87904	-4.79893	-0.38348
H	-0.79956	-4.32693	-0.03106
H	0.52138	-3.77733	1.02347
C	6.75448	1.07437	3.58659
H	7.46501	0.88125	2.7747
H	7.00047	0.39899	4.40968
H	6.9258	2.09802	3.93888

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.37265
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.53988
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.69817
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.13130

Compound E-Me trans Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.867780
(Hartree/Particle)
Thermal correction to Energy= 0.914091
Thermal correction to Enthalpy= 0.915036
Thermal correction to Gibbs Free Energy=
0.781563
Sum of electronic and zero-point Energies= -
3071.431714

Sum of electronic and thermal Energies= -3071.385403
Sum of electronic and thermal Enthalpies= -3071.384459
Sum of electronic and thermal Free Energies= -3071.517931

Fe	-0.54775	-0.92379	0.05063
N	1.35634	-0.89047	0.89133
N	-2.10764	0.53046	0.07013
N	-1.49229	-1.77075	1.80612
N	3.29918	-0.72371	-3.3642
C	1.75214	-0.12075	1.93557
H	1.02895	0.61057	2.2895
C	3.88498	-1.21391	2.03938
C	3.47602	-1.9994	0.96159
H	4.13821	-2.75781	0.55376
C	2.21392	-1.81285	0.40212
C	-2.67389	0.76641	-1.13019
C	-3.69532	1.70024	-1.28978
H	-4.12288	1.86675	-2.27498
C	-4.15576	2.41871	-0.18657
C	-3.55892	2.17328	1.07198
C	-2.54683	1.2272	1.14269
H	-2.06515	1.00419	2.09093
C	-2.03567	-2.24691	2.71231
C	2.99384	-0.23104	2.53585
C	4.18581	-0.46648	-4.06754
C	5.30237	-0.14151	-4.95051
H	5.19393	-0.66618	-5.9048
H	5.33086	0.93564	-5.14191
H	6.248	-0.44275	-4.4893
C	-2.72122	-2.84706	3.84872
H	-2.22976	-2.55127	4.78115
H	-3.76386	-2.51412	3.87268
H	-2.6982	-3.93845	3.76475
C	-0.11896	-2.58176	-5.25127
C	-0.2353	-3.9489	-4.57023
C	0.37245	-3.91569	-3.15872
C	-0.26548	-2.81581	-2.28432
C	-0.16395	-1.44473	-2.98384
C	-0.78249	-1.4922	-4.39513
H	0.25013	-4.89357	-2.68133
H	-1.29225	-4.24426	-4.51155
H	0.26908	-4.71932	-5.16277
H	0.93937	-2.33323	-5.40836
H	-0.58806	-2.60397	-6.24051
H	-1.32884	-3.06049	-2.14692
H	0.89649	-1.21202	-3.11393
H	-1.85809	-1.70194	-4.33553
H	-0.67227	-0.51438	-4.87868
H	1.45116	-3.73071	-3.24195
C	-5.24764	3.46885	-0.26249
H	-4.95157	4.24961	-0.97577
H	-6.15995	3.0148	-0.67306
C	-4.20386	4.48754	1.86078
C	-4.47635	5.36019	3.09583
H	-3.57041	5.45398	3.70606
H	-4.76869	6.36916	2.7836
H	-5.2709	4.9737	3.7392
C	-3.07985	5.14045	1.05174
H	-3.38493	6.1408	0.72308
H	-2.18443	5.26424	1.67303
H	-2.78606	4.57759	0.16074
C	-4.08788	2.95335	2.24455
H	-3.59397	2.68964	3.18567
C	-5.53191	4.06086	1.13107
H	-6.34128	4.79525	1.08644
C	-5.64601	2.89555	2.15141
H	-6.0885	1.95655	1.80159
H	-6.13155	3.1872	3.08238
C	5.20265	-1.34771	2.74187
H	5.82369	-2.14757	2.32861
C	3.45363	0.64768	3.68896
H	3.44807	1.7008	3.3792
H	2.74665	0.5681	4.52562
C	5.85435	0.08714	2.9435
C	5.78684	1.10116	1.79843
H	6.13687	2.08114	2.14344
H	6.44524	0.79271	0.97758
H	4.78393	1.23642	1.38286
C	4.85877	0.2207	4.15408
H	5.18556	0.81759	5.0107
C	4.89351	-1.32642	4.27501
H	5.73086	-1.69379	4.86768
H	3.98	-1.83296	4.6042
N	-0.69502	-0.33904	-2.09852
C	-2.14875	-0.0733	-2.27478
H	-2.354	0.42367	-3.23046
H	-2.67802	-1.03413	-2.29248
C	0.07193	0.91473	-2.34327
N	0.28871	-2.73657	-0.88213
C	-0.0883	-3.93529	-0.09107
C	1.77083	-2.56712	-0.83413
H	2.27775	-3.53837	-0.88068
H	2.10514	-1.9965	-1.70615
H	-0.03605	1.24828	-3.38328
H	1.13077	0.74065	-2.14185
H	-0.29277	1.70676	-1.68582
H	0.36134	-4.84919	-0.49516
H	-1.17524	-4.04765	-0.08581
H	0.2572	-3.81048	0.93791
C	7.31632	-0.02394	3.40374
H	7.95687	-0.33769	2.57155
H	7.46625	-0.73195	4.22265
H	7.67414	0.95405	3.74555

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3070.36939
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3071.56529
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3072.71802
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -3073.14541

Compound E-H cis-α Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.817139 (Hartree/Particle)
Thermal correction to Energy= 0.858441
Thermal correction to Enthalpy= 0.859385
Thermal correction to Gibbs Free Energy= 0.743328
Sum of electronic and zero-point Energies= -2992.893472
Sum of electronic and thermal Energies= -2992.852170
Sum of electronic and thermal Enthalpies= -2992.851226
Sum of electronic and thermal Free Energies= -2992.967283

Fe	-0.23875	0.3804	0.25078
N	-1.69227	-0.23866	1.50069
N	1.18126	0.87677	-1.08826

N	0.87927	0.75789	1.77986
N	-0.80484	2.22659	0.28897
C	-2.84119	0.40003	1.81892
H	-3.00688	1.35147	1.32331
C	-3.50295	-1.33552	3.34615
C	-2.32138	-1.99893	3.01172
H	-2.08795	-2.96326	3.45466
C	-1.44457	-1.42944	2.09425
C	-0.78795	0.98495	-2.47546
H	-1.31534	1.91799	-2.25502
H	-1.04731	0.69669	-3.50004
C	0.70386	1.15939	-2.32227
C	1.53437	1.56539	-3.36347
H	1.10726	1.77202	-4.34151
C	2.90583	1.69452	-3.14762
C	3.40875	1.38758	-1.8639
C	2.51245	0.98502	-0.88179
H	2.86171	0.7475	0.11757
C	1.50455	1.06156	2.70759
C	-3.76928	-0.09468	2.72449
C	-1.0692	3.3524	0.3703
C	-1.40079	4.76922	0.47224
H	-2.26635	5.00324	-0.15601
H	-1.63837	5.02684	1.50945
H	-0.55203	5.37757	0.14329
C	2.29113	1.44219	3.87554
H	3.0365	0.672	4.09894
H	2.80806	2.38912	3.6892
H	1.63722	1.56224	4.74538
N	-1.22851	-0.03639	-1.48315
N	0.15641	-1.62015	0.28672
H	1.13086	-1.8481	0.07882
H	-2.24577	0.01261	-1.39665
C	-1.39186	-3.43996	-3.36869
C	-1.1601	-4.35238	-2.15506
C	-0.20411	-3.71077	-1.13219
C	-0.70992	-2.32086	-0.72286
C	-0.86732	-1.42117	-1.94416
C	-1.85533	-2.03344	-2.94649
H	-0.104	-4.35769	-0.25287
H	-2.1204	-4.56639	-1.6663
H	-0.75563	-5.31675	-2.47861
H	-0.46292	-3.35453	-3.94903
H	-2.13532	-3.88359	-4.03861
H	-1.69387	-2.42792	-0.24919
H	0.11377	-1.32768	-2.42614
H	-2.84986	-2.09504	-2.47968
H	-1.95681	-1.39055	-3.82859
H	0.79923	-3.61275	-1.57317
C	-0.15486	-2.08751	1.66733
H	0.67054	-1.78614	2.31931
H	-0.23258	-3.17893	1.72066
C	3.89384	2.11532	-4.21934
H	3.82655	1.42398	-5.07001
H	3.60982	3.10236	-4.6094
C	5.67545	0.854	-2.85168
C	7.17942	0.74361	-2.55476
H	7.36763	-0.04374	-1.81542
H	7.72126	0.47346	-3.46826
H	7.62092	1.66824	-2.17457
C	5.19259	-0.49906	-3.38104
H	5.72278	-0.75204	-4.30656
H	5.41234	-1.29299	-2.65665
H	4.1205	-0.53546	-3.59627
C	4.89156	1.5395	-1.65581
H	5.20183	1.30813	-0.63139
C	5.32424	2.16443	-3.64962
H	6.03712	2.49813	-4.40919
C	5.29142	2.91068	-2.28779
H	4.5779	3.73445	-2.17774
H	6.27399	3.25137	-1.96188
C	-4.54455	-1.86312	4.28726
H	-4.28292	-2.8395	4.70507
C	-5.05534	0.63299	3.08736
H	-4.82014	1.61739	3.51331
H	-5.64603	0.82212	2.1809
C	-5.00561	-0.71494	5.28256
C	-3.9492	0.21592	5.88374
H	-4.43507	1.04462	6.41226
H	-3.3396	-0.32299	6.61893
H	-3.26896	0.64865	5.14369
C	-5.88252	-0.20938	4.07836
H	-6.82879	0.28524	4.31673
C	-5.92245	-1.67592	3.57133
H	-6.71069	-2.26962	4.03332
H	-5.94582	-1.8405	2.48887
C	-5.86019	-1.2781	6.42885
H	-6.64238	-1.96509	6.09644
H	-6.34973	-0.45844	6.9672
H	-5.23003	-1.81505	7.14706

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2991.91757
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2993.00598
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.13058
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.53140

Compound E-H cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.814271 (Hartree/Particle)
Thermal correction to Energy= 0.857090
Thermal correction to Enthalpy= 0.858034
Thermal correction to Gibbs Free Energy= 0.735468
Sum of electronic and zero-point Energies= -2992.876695
Sum of electronic and thermal Energies= -2992.833876
Sum of electronic and thermal Enthalpies= -2992.832931
Sum of electronic and thermal Free Energies= -2992.955497

Fe	-0.11971	0.24879	0.25807
N	-1.67878	-0.28864	1.53729
N	1.26299	0.84384	-1.1019
N	0.92035	0.7	1.79685
N	-0.94236	2.57008	0.21287
C	-2.74857	0.48119	1.84338
H	-2.7766	1.45613	1.36766
C	-3.66724	-1.19746	3.29729
C	-2.56082	-1.98743	2.98339
H	-2.45878	-2.98243	3.4081
C	-1.58671	-1.50902	2.11074
C	-0.72199	0.79536	-2.46547
H	-1.26638	1.7176	-2.23855
H	-0.99589	0.49103	-3.48037
C	0.76192	1.03004	-2.34515
C	1.56425	1.42935	-3.40964
H	1.12596	1.55861	-4.39572
C	2.92583	1.65406	-3.2045

C	3.44971	1.46323	-1.90538
C	2.58334	1.05684	-0.89983
H	2.94373	0.89655	0.11091
C	1.51084	0.99601	2.7498
C	-3.75694	0.08459	2.71001
C	-1.04572	3.72438	0.27225
C	-1.18601	5.17511	0.34338
H	-2.11682	5.48613	-0.14149
H	-1.20582	5.50021	1.38829
H	-0.3449	5.65921	-0.16267
C	2.24853	1.37006	3.95019
H	3.02553	0.62886	4.16413
H	2.72177	2.34774	3.81264
H	1.56791	1.42447	4.80609
N	-1.12123	-0.21994	-1.44795
N	0.07927	-1.98082	0.38584
H	1.03029	-2.32567	0.25076
H	-2.135	-0.16286	-1.3269
C	-1.38195	-3.59111	-3.38762
C	-1.33883	-4.53222	-2.17665
C	-0.40754	-3.98788	-1.08142
C	-0.79505	-2.55737	-0.67543
C	-0.80009	-1.62427	-1.89292
C	-1.75323	-2.15547	-2.97558
H	-0.42833	-4.6426	-0.20201
H	-2.35102	-4.65371	-1.76683
H	-1.00573	-5.52951	-2.4816
H	-0.4024	-3.58415	-3.88532
H	-2.10272	-3.95401	-4.12744
H	-1.81241	-2.57231	-0.26207
H	0.21985	-1.58036	-2.29648
H	-2.78069	-2.14175	-2.58113
H	-1.74371	-1.50273	-3.85564
H	0.62979	-3.98296	-1.44956
C	-0.36367	-2.32759	1.75211
H	0.45884	-2.09382	2.43838
H	-0.58192	-3.39709	1.86529
C	3.88417	2.06999	-4.30406
H	3.86898	1.3163	-5.10266
H	3.52894	3.00291	-4.76279
C	5.75183	1.03625	-2.86286
C	7.25864	1.05685	-2.56128
H	7.50238	0.33069	-1.77701
H	7.82289	0.77528	-3.45754
H	7.62763	2.03277	-2.23564
C	5.36979	-0.37971	-3.30208
H	5.92481	-0.65674	-4.2059
H	5.63631	-1.10573	-2.5243
H	4.30483	-0.50536	-3.51956
C	4.91646	1.73756	-1.71194
H	5.2404	1.59645	-0.67559
C	5.30604	2.26268	-3.74299
H	5.99306	2.59871	-4.52497
C	5.21403	3.09117	-2.43258
H	4.44076	3.86484	-2.37459
H	6.16732	3.52455	-2.13153
C	-4.80259	-1.62166	4.18167
H	-4.68141	-2.63693	4.57022
C	-4.94961	0.95944	3.06288
H	-4.60347	1.88534	3.54115
H	-5.47676	1.2621	2.14819
C	-5.15556	-0.45919	5.20348
C	-4.01411	0.30589	5.879
H	-4.41177	1.16999	6.42427
H	-3.508	-0.33409	6.61156
H	-3.25479	0.67385	5.18203
C	-5.91395	0.19423	3.98998
H	-6.79967	0.79578	4.21516
C	-6.11706	-1.23759	3.42574
H	-6.99095	-1.7421	3.83689
H	-6.11832	-1.36133	2.33758
C	-6.12066	-0.94677	6.29571
H	-6.97523	-1.50659	5.90765
H	-6.51533	-0.08992	6.85374
H	-5.59685	-1.59298	7.0093

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =--2991.87939
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =--2992.98714
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.09493
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.51236

Compound E-H cis-α Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.812284 (Hartree/Particle)
Thermal correction to Energy= 0.856029
Thermal correction to Enthalpy= 0.856973
Thermal correction to Gibbs Free Energy= 0.730889
Sum of electronic and zero-point Energies= -2992.895788
Sum of electronic and thermal Energies= -2992.852042
Sum of electronic and thermal Enthalpies= -2992.851098
Sum of electronic and thermal Free Energies= -2992.977183

Fe	-0.25107	0.43118	0.24151
N	-1.81981	-0.22706	1.62019
N	1.28422	0.95491	-1.23276
N	1.09073	0.8398	1.91388
N	-0.9491	2.49777	0.28929
C	-2.89782	0.48254	2.0256
H	-2.97829	1.48804	1.62222
C	-3.70246	-1.32966	3.37916
C	-2.58614	-2.05821	2.96547
H	-2.43816	-3.07759	3.31141
C	-1.66514	-1.48164	2.09474
C	-0.65046	0.86308	-2.71006
H	-1.187	1.80732	-2.55844
H	-0.84018	0.55141	-3.74403
C	0.83442	1.07875	-2.49886
C	1.68568	1.40956	-3.55215
H	1.28807	1.48636	-4.561
C	3.04034	1.6318	-3.30811
C	3.51091	1.50761	-1.98135
C	2.59773	1.16533	-0.99307
H	2.91596	1.05502	0.03922
C	1.67977	1.08352	2.88231
C	-3.85703	-0.00879	2.89863
C	-1.1738	3.6352	0.28158
C	-1.45814	5.06483	0.27275
H	-2.41106	5.25713	-0.23053
H	-1.51454	5.44205	1.29884
H	-0.66278	5.59863	-0.25732
C	2.42282	1.39045	4.09823
H	3.28014	0.71687	4.19645
H	2.78312	2.42364	4.06661
H	1.77393	1.26817	4.97141
N	-1.17413	-0.10841	-1.72211

N	-0.0327	-1.78967	0.28225
H	0.93166	-2.08372	0.11936
H	-2.19177	-0.02465	-1.70354
C	-1.36739	-3.57643	-3.47402
C	-1.39504	-4.44453	-2.21024
C	-0.50411	-3.84924	-1.10859
C	-0.88631	-2.39407	-0.7874
C	-0.83417	-1.52693	-2.05684
C	-1.73539	-2.11844	-3.15466
H	-0.56421	-4.46371	-0.2029
H	-2.42653	-4.52687	-1.84073
H	-1.06491	-5.46319	-2.4385
H	-0.36554	-3.61015	-3.92404
H	-2.05838	-3.97223	-4.22546
H	-1.91552	-2.37001	-0.4045
H	0.20443	-1.51384	-2.41364
H	-2.78078	-2.07224	-2.81264
H	-1.67397	-1.50736	-4.06248
H	0.54654	-3.87164	-1.43659
C	-0.42164	-2.22103	1.645
H	0.41223	-1.98243	2.31584
H	-0.58484	-3.30317	1.71108
C	4.04588	1.97528	-4.39085
H	4.0494	1.18094	-5.14913
H	3.72367	2.88779	-4.91085
C	5.84074	0.99693	-2.82317
C	7.33534	1.0135	-2.46587
H	7.53771	0.33099	-1.63207
H	7.9283	0.67215	-3.32198
H	7.70753	2.00162	-2.18356
C	5.45325	-0.4359	-3.19848
H	6.03906	-0.771	-4.06234
H	5.67675	-1.12094	-2.37139
H	4.39575	-0.55759	-3.45114
C	4.97345	1.77267	-1.74631
H	5.25561	1.68487	-0.69188
C	5.44823	2.17848	-3.78634
H	6.17046	2.4603	-4.558
C	5.32028	3.07987	-2.52776
H	4.55773	3.86608	-2.54231
H	6.26842	3.51621	-2.21448
C	-4.78547	-1.85963	4.27037
H	-4.61654	-2.89727	4.57239
C	-5.06179	0.79376	3.36652
H	-4.72569	1.69198	3.90132
H	-5.63632	1.14672	2.49963
C	-5.13163	-0.79301	5.39434
C	-3.9872	-0.04321	6.08179
H	-4.38785	0.76551	6.70431
H	-3.43417	-0.71884	6.74512
H	-3.26684	0.39933	5.38675
C	-5.96143	-0.07415	4.26788
H	-6.85543	0.47636	4.57537
C	-6.14223	-1.46363	3.59965
H	-6.9809	-2.02949	4.00401
H	-6.18541	-1.50172	2.5061
C	-6.0328	-1.39805	6.48217
H	-6.88578	-1.95431	6.08558
H	-6.42933	-0.60184	7.12256
H	-5.45901	-2.08018	7.1199

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2991.86057
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2993.02135
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.12050
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.52764

Compound E-H cis-β Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.817483
(Hartree/Particle)
Thermal correction to Energy= 0.858853
Thermal correction to Enthalpy= 0.859798
Thermal correction to Gibbs Free Energy=
0.743444
Sum of electronic and zero-point Energies= -
2992.891290
Sum of electronic and thermal Energies= -
2992.849919
Sum of electronic and thermal Enthalpies= -
2992.848975
Sum of electronic and thermal Free Energies= -
2992.965328

C	-1.61301	2.73197	1.30456
C	-2.96911	3.43304	1.48287
C	-2.80638	4.95703	1.61473
C	-1.82592	5.32289	2.73739
C	-0.46178	4.64007	2.52729
C	-0.6384	3.11908	2.42861
C	-2.32223	0.58938	0.14414
C	-1.92946	-0.87092	0.15928
C	-2.7074	-1.86909	-0.42216
C	-2.26366	-3.19128	-0.41228
C	-1.02553	-3.4738	0.20579
C	-0.31737	-2.42416	0.77742
C	1.699	2.84096	1.42233
C	1.50285	2.3627	0.00766
C	2.05216	3.02956	-1.0841
C	1.93788	2.48232	-2.36197
C	0.73312	0.65832	-1.35919
Fe	0.12314	0.44627	1.61558
H	-1.18175	3.01153	0.33679
H	-3.62866	3.1927	0.64096
H	-3.45366	3.03936	2.38966
H	-2.44701	5.37067	0.66248
H	-3.7848	5.41185	1.79961
H	-2.24254	5.02314	3.70881
H	-1.68582	6.40763	2.7809
H	0.22343	4.8857	3.34815
H	-0.01581	5.03173	1.6042
H	-1.08432	2.77384	3.37201
H	-1.93055	1.08084	-0.75345
H	-3.41085	0.70763	0.13291
H	-3.65926	-1.60977	-0.87865
H	2.64769	2.44091	1.799
H	1.77635	3.93003	1.47124
H	2.57334	3.97117	-0.9345
N	-1.69833	1.24218	1.32356
N	0.63324	2.30314	2.31367
N	0.82742	1.19821	-0.12066
N	-0.74239	-1.14216	0.75505
N	1.8603	-0.33006	1.91243
N	-0.44701	-0.16409	3.35102
C	2.90991	-0.79461	2.07614
C	-0.76969	-0.56374	4.39101
C	4.22984	-1.38167	2.27863
H	4.89853	-0.65617	2.75322
H	4.65973	-1.68059	1.31718
H	4.15588	-2.26391	2.92258
C	-1.1669	-1.07678	5.69737
H	-1.65199	-0.28996	6.28403

H	-0.28702	-1.43126	6.24404
H	-1.86675	-1.90998	5.57668
H	0.63198	-2.6006	1.27209
C	-3.04414	-4.34804	-1.00795
C	-0.55949	-4.90468	0.18154
C	-2.26212	-5.66654	-0.85458
H	-3.23976	-4.14785	-2.07028
H	-4.02909	-4.41044	-0.52617
C	-1.7436	-5.86429	0.61801
C	-1.24871	-7.29742	0.86878
C	-2.64007	-5.45497	1.78978
H	-0.59904	-7.68083	0.07802
H	-2.10316	-7.97883	0.9503
H	-0.69233	-7.35205	1.81191
H	-3.02469	-4.43307	1.71926
H	-2.09142	-5.53858	2.73614
H	-3.50289	-6.12787	1.85711
C	-0.78702	-5.42134	-1.27505
H	-2.80353	-6.49853	-1.31414
H	-0.60263	-4.71072	-2.08794
H	-0.24125	-6.34143	-1.48327
H	0.41919	-5.03938	0.6537
C	2.46175	3.11388	-3.6173
C	3.24725	2.03251	-4.47527
C	1.81914	1.55193	-4.92753
C	4.02996	2.68875	-5.62329
C	1.26671	1.24584	-2.49705
H	0.20865	-0.28899	-1.42441
C	1.17539	0.62145	-3.88128
H	3.44637	3.41615	-6.19294
H	4.37362	1.921	-6.32589
H	4.91687	3.20376	-5.2369
H	0.12417	0.44089	-4.14326
H	1.66575	-0.36096	-3.87879
H	1.72425	1.13347	-5.93391
C	1.32022	3.00111	-4.68013
H	2.93831	4.08207	-3.43847
H	0.29356	3.13277	-4.32204
H	1.48233	3.66264	-5.53059
C	4.18031	1.05149	-3.76011
H	3.7187	0.53763	-2.91142
H	5.06908	1.5745	-3.38721
H	4.52774	0.28417	-4.46192
H	-2.2658	0.98898	2.13624
H	1.031	2.2706	3.25223

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2991.91598
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2993.00193
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.12889
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.54204

Compound E-H cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.814303 (Hartree/Particle)
Thermal correction to Energy= 0.857285
Thermal correction to Enthalpy= 0.858230
Thermal correction to Gibbs Free Energy= 0.734840
Sum of electronic and zero-point Energies= -2992.873533
Sum of electronic and thermal Energies= -2992.830550
Sum of electronic and thermal Enthalpies= -2992.829606
Sum of electronic and thermal Free Energies= -2992.952995

C	-1.59916	2.62464	1.24018
C	-2.95951	3.31801	1.41426
C	-2.81141	4.84853	1.46327
C	-1.81127	5.28267	2.54292
C	-0.44584	4.60107	2.34073
C	-0.60724	3.07476	2.3256
C	-2.33474	0.45674	0.16543
C	-1.98097	-1.01255	0.20625
C	-2.7878	-1.99957	-0.35302
C	-2.37229	-3.33122	-0.32801
C	-1.13176	-3.63704	0.27737
C	-0.39286	-2.59719	0.82414
C	1.75098	2.79624	1.34789
C	1.57169	2.38923	-0.09909
C	2.11884	3.13596	-1.14172
C	2.02903	2.66199	-2.45111
C	0.84476	0.76466	-1.57489
Fe	0.13123	0.33139	1.58104
H	-1.18948	2.86419	0.25286
H	-3.63594	3.03032	0.6011
H	-3.41869	2.96665	2.35104
H	-2.47736	5.215	0.48292
H	-3.79101	5.3019	1.64566
H	-2.2044	5.03171	3.53768
H	-1.68137	6.36947	2.52521
H	0.25242	4.89474	3.13428
H	-0.01935	4.94519	1.38964
H	-1.03324	2.77367	3.29262
H	-1.9401	0.91236	-0.74991
H	-3.41966	0.60408	0.165
H	-3.73766	-1.72661	-0.80535
H	2.68393	2.35547	1.71902
H	1.85952	3.88048	1.43757
H	2.61916	4.07798	-0.9328
N	-1.67649	1.13147	1.31573
N	0.67012	2.27053	2.2285
N	0.92938	1.22628	-0.30903
N	-0.79507	-1.30688	0.79293
N	1.82846	-0.475	1.91655
N	-0.54263	-0.11143	3.81902
C	2.86581	-0.95782	2.10679
C	-0.78616	-0.52986	4.87369
C	4.17165	-1.56358	2.33805
H	4.84209	-0.84381	2.81897
H	4.61446	-1.87575	1.38656
H	4.07332	-2.43962	2.98731
C	-1.0958	-1.0502	6.20071
H	-1.56154	-0.2696	6.81063
H	-0.17925	-1.38661	6.69544
H	-1.78649	-1.89542	6.11921
H	0.56153	-2.7857	1.30477
C	-3.1853	-4.4757	-0.90184
C	-0.6978	-5.07773	0.25826
C	-2.42986	-5.80971	-0.75014
H	-3.39301	-4.27761	-1.96232
H	-4.16395	-4.51151	-0.4046
C	-1.89624	-6.00851	0.71679
C	-1.4283	-7.45007	0.97085
C	-2.76869	-5.57256	1.89718
H	-0.79869	-7.85291	0.17356
H	-2.29587	-8.11229	1.06985
H	-0.85953	-7.50965	1.90619
H	-3.13093	-4.54243	1.82689

H	-2.21072	-5.66348	2.83727
H	-3.64562	-6.22536	1.97804
C	-0.95577	-5.59881	-1.19192
H	-2.99551	-6.63244	-1.1969
H	-0.76681	-4.89781	-2.01205
H	-0.43251	-6.53167	-1.40065
H	0.28408	-5.22984	0.71811
C	2.56171	3.37505	-3.65962
C	3.37648	2.35812	-4.56649
C	1.96282	1.88735	-5.07184
C	4.16821	3.09141	-5.66049
C	1.37816	1.42661	-2.67311
H	0.32889	-0.18523	-1.69976
C	1.31423	0.88833	-4.09426
H	3.58185	3.83948	-6.19977
H	4.53896	2.37054	-6.39818
H	5.03834	3.59924	-5.22884
H	0.26913	0.71296	-4.38332
H	1.81539	-0.08739	-4.14427
H	1.89072	1.52908	-6.10314
C	1.43947	3.31239	-4.74607
H	3.02183	4.3371	-3.4157
H	0.40558	3.40721	-4.39729
H	1.60441	4.02647	-5.55241
C	4.31143	1.34798	-3.89555
H	3.84488	0.78334	-3.08289
H	5.18941	1.8585	-3.48188
H	4.67636	0.62488	-4.63453
H	-2.21858	0.90073	2.15324
H	1.05946	2.23411	3.16999

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2991.89294
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2992.98866
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.09881
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.52301

Compound E-H cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.815038 (Hartree/Particle)
Thermal correction to Energy= 0.857946
Thermal correction to Enthalpy= 0.858890
Thermal correction to Gibbs Free Energy= 0.735136
Sum of electronic and zero-point Energies= -2992.887814
Sum of electronic and thermal Energies= -2992.844905
Sum of electronic and thermal Enthalpies= -2992.843961
Sum of electronic and thermal Free Energies= -2992.967715

C	-1.63062	2.64306	1.25727
C	-3.00879	3.31609	1.40052
C	-2.91751	4.84814	1.46126
C	-1.96479	5.30002	2.57408
C	-0.5759	4.66779	2.3889
C	-0.66348	3.13249	2.35553
C	-2.29407	0.48619	0.1523
C	-1.96353	-0.99353	0.18433
C	-2.81154	-1.95005	-0.37151
C	-2.44256	-3.29491	-0.36692
C	-1.20376	-3.64927	0.21498
C	-0.42493	-2.63795	0.75987
C	1.70451	2.98508	1.37372
C	1.58484	2.45867	-0.04063
C	2.03623	3.19724	-1.13351
C	2.00563	2.63528	-2.40999
C	1.06868	0.66296	-1.40867
Fe	0.30728	0.29636	1.66086
H	-1.20673	2.88814	0.27594
H	-3.65734	3.00819	0.57214
H	-3.4801	2.94646	2.32454
H	-2.5653	5.2353	0.49514
H	-3.91703	5.26713	1.61696
H	-2.37431	5.01759	3.55383
H	-1.87048	6.39076	2.57897
H	0.10197	4.97971	3.19348
H	-0.15116	5.0406	1.44788
H	-1.08114	2.80138	3.31675
H	-1.84833	0.94013	-0.74148
H	-3.37837	0.62836	0.07692
H	-3.75927	-1.64036	-0.8046
H	2.6722	2.66421	1.78008
H	1.71639	4.07841	1.37768
H	2.41354	4.20587	-0.98723
N	-1.70637	1.15809	1.32952
N	0.66683	2.42216	2.27888
N	1.09402	1.21108	-0.17261
N	-0.78391	-1.33453	0.7476
N	2.1946	-0.67074	1.99224
N	-0.24656	-0.18555	3.74037
C	3.25202	-1.13043	2.11309
C	-0.51789	-0.54955	4.80756
C	4.58061	-1.7096	2.26444
H	5.14084	-1.61588	1.32876
H	4.49732	-2.76957	2.52537
H	5.12548	-1.19242	3.0608
C	-0.85886	-1.005	6.14967
H	-1.28742	-0.18082	6.72885
H	0.03715	-1.37091	6.661
H	-1.59177	-1.81617	6.09221
H	0.53076	-2.86432	1.22506
C	-3.30448	-4.4059	-0.93599
C	-0.82057	-5.10373	0.17711
C	-2.59361	-5.76661	-0.80709
H	-3.52265	-4.19253	-1.99135
H	-4.27544	-4.41235	-0.42275
C	-2.04247	-5.99601	0.64902
C	-1.62036	-7.45477	0.88443
C	-2.87996	-5.54044	1.84737
H	-1.01774	-7.87231	0.07393
H	-2.50804	-8.08826	0.99303
H	-1.03875	-7.54085	1.80982
H	-3.21011	-4.49889	1.78964
H	-2.30905	-5.65539	2.77706
H	-3.77579	-6.16552	1.93931
C	-1.12043	-5.60412	-1.27224
H	-3.19489	-6.5658	-1.2502
H	-0.92076	-4.90342	-2.09008
H	-0.63446	-6.55332	-1.49686
H	0.16301	-5.294	0.61912
C	2.4381	3.33453	-3.66506
C	3.36859	2.37517	-4.52218
C	2.02235	1.70074	-4.97889
C	4.05519	3.13635	-5.66716
C	1.51391	1.31634	-2.54904
H	0.67244	-0.34793	-1.46882
C	1.51215	0.68872	-3.93475
H	3.37665	3.77391	-6.23936

H	4.50759	2.42545	-6.36813
H	4.8584	3.77188	-5.27699
H	0.49621	0.3653	-4.19884
H	2.13286	-0.21693	-3.93409
H	1.9892	1.27456	-5.98606
C	1.32596	3.06561	-4.73067
H	2.77464	4.35957	-3.48461
H	0.29028	3.05179	-4.37461
H	1.39583	3.74538	-5.57933
C	4.42561	1.53051	-3.80581
H	4.03457	0.95944	-2.95846
H	5.2339	2.169	-3.42965
H	4.87555	0.81787	-4.50712
H	-2.2757	0.91692	2.14342
H	1.05518	2.44861	3.22072

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF =-2991.87241

UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF =-2993.01385

UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2994.10758

UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2994.53757

Compound E-H Trans Singlet

UB3LYP/6-31G(d)-gas

Zero-point correction= 0.816974 (Hartree/Particle)

Thermal correction to Energy= 0.858394

Thermal correction to Enthalpy= 0.859338

Thermal correction to Gibbs Free Energy= 0.743780

Sum of electronic and zero-point Energies= -2992.862124

Sum of electronic and thermal Energies= -2992.820705

Sum of electronic and thermal Enthalpies= -2992.819760

Sum of electronic and thermal Free Energies= -2992.935318

Fe	-0.10761	-0.94655	-0.74774
N	1.45192	-1.10726	0.55942
N	-1.45939	0.53045	-0.34729
N	-1.21088	-2.04862	0.39087
N	1.01989	0.30043	-1.69683
C	1.63367	-0.55751	1.77766
H	0.7887	-0.00154	2.17525
C	3.86619	-1.43078	1.94869
C	3.67472	-2.01016	0.69198
H	4.45963	-2.61104	0.24078
C	2.46936	-1.83114	0.02139
C	-2.62484	0.31953	-1.01408
C	-3.73256	1.14216	-0.82947
H	-4.64206	0.95247	-1.39391
C	-3.66748	2.20862	0.06793
C	-2.4547	2.43029	0.75589
C	-1.39023	1.57068	0.50762
H	-0.43631	1.71476	1.00722
C	-1.81181	-2.65452	1.17636
C	2.80857	-0.67988	2.50819
C	1.65974	1.13879	-2.17947
C	2.46982	2.19575	-2.77391
H	2.73783	1.93702	-3.80342
H	1.91294	3.13838	-2.77993
H	3.38844	2.33213	-2.19404
C	-2.5699	-3.40435	2.17132
H	-1.92779	-3.65769	3.02118
H	-3.41052	-2.80234	2.53144
H	-2.96017	-4.32961	1.73516
C	-0.97067	-3.5984	-5.3052
C	-0.2891	-4.72777	-4.51745
C	0.6715	-4.18414	-3.44245
C	-0.06747	-3.20438	-2.52361
C	-0.68595	-2.05369	-3.33465
C	-1.67387	-2.59001	-4.37623
H	1.0873	-5.00994	-2.8528
H	-1.05299	-5.35242	-4.0342
H	0.26061	-5.38432	-5.19939
H	-0.22306	-3.06837	-5.91142
H	-1.69861	-4.01572	-6.00822
H	-0.89611	-3.7463	-2.04839
H	0.13424	-1.55708	-3.87002
H	-2.51633	-3.07951	-3.86817
H	-2.08886	-1.76115	-4.96234
H	1.51735	-3.67352	-3.9237
C	-4.81764	3.16438	0.32441
H	-5.11507	3.63969	-0.61984
H	-5.69421	2.59747	0.66667
C	-3.03364	4.8749	1.0507
C	-2.77495	6.13237	1.89571
H	-1.72655	6.44176	1.8115
H	-3.39308	6.96084	1.53164
H	-2.99694	6.00067	2.95776
C	-2.68108	5.19513	-0.40443
H	-3.3086	6.01508	-0.77284
H	-1.63864	5.52853	-0.47951
H	-2.80837	4.35082	-1.08851
C	-2.41754	3.57992	1.72655
H	-1.45456	3.6701	2.2398
C	-4.42433	4.21596	1.37981
H	-5.26134	4.88651	1.59513
C	-3.73111	3.49315	2.56707
H	-4.08735	2.4908	2.82819
H	-3.69036	4.09803	3.47269
C	5.10545	-1.58388	2.78154
H	5.86725	-2.20226	2.29809
C	3.01575	-0.04433	3.87416
H	2.90776	1.04586	3.79871
H	2.23408	-0.38397	4.56695
C	5.53864	-0.17512	3.37059
C	5.47137	1.06038	2.46865
H	5.64787	1.96702	3.05933
H	6.25481	1.01549	1.70266
H	4.5125	1.18137	1.95536
C	4.40288	-0.42015	4.43088
H	4.54954	-0.00241	5.43132
C	4.62537	-1.94274	4.22609
H	5.43039	-2.34611	4.83964
H	3.75436	-2.60112	4.31036
N	-1.20854	-0.97731	-2.41702
C	-2.62339	-0.84956	-1.99203
H	-3.30488	-0.65995	-2.82885
H	-2.94002	-1.77765	-1.50677
H	-1.004	-0.09814	-2.89177
N	0.71496	-2.66836	-1.34966
H	0.54486	-3.3294	-0.59178
C	2.18345	-2.46053	-1.33772
H	2.74792	-3.39129	-1.46285
H	2.4598	-1.78897	-2.15587
C	6.94065	-0.23614	3.99725
H	7.70793	-0.28205	3.21592
H	7.08902	-1.0942	4.65749
H	7.12421	0.66873	4.58788

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2991.88685
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2992.97465
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.09782
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.49815

Compound E-H trans Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.814627
(Hartree/Particle)
Thermal correction to Energy= 0.857088
Thermal correction to Enthalpy= 0.858033
Thermal correction to Gibbs Free Energy=
0.737928
Sum of electronic and zero-point Energies= -
2992.853453
Sum of electronic and thermal Energies= -
2992.810992
Sum of electronic and thermal Enthalpies= -
2992.810048
Sum of electronic and thermal Free Energies= -
2992.930153

Fe	-0.04211	-0.63121	-0.33641
N	1.71888	-1.13287	0.68778
N	-1.66201	0.71013	-0.26825
N	-1.09257	-1.717	0.84977
N	1.04242	0.65324	-1.26404
C	2.10783	-0.59359	1.86452
H	1.39472	0.07294	2.34515
C	4.21708	-1.73906	1.796
C	3.81032	-2.29451	0.58193
H	4.45754	-2.98803	0.05205
C	2.5644	-1.97151	0.04937
C	-2.70624	0.41656	-1.07246
C	-3.88753	1.15607	-1.03289
H	-4.69995	0.90146	-1.70876
C	-4.01728	2.21737	-0.13869
C	-2.9238	2.52036	0.70391
C	-1.77835	1.74267	0.59534
H	-0.91272	1.95039	1.22
C	-1.70431	-2.30057	1.64235
C	3.33384	-0.85543	2.45837
C	1.6976	1.48534	-1.73448
C	2.52081	2.5333	-2.32466
H	2.91814	2.20273	-3.28993
H	1.92362	3.43789	-2.47866
H	3.3582	2.76958	-1.66017
C	-2.47219	-3.0337	2.64091
H	-1.8372	-3.27364	3.49996
H	-3.31719	-2.42739	2.98277
H	-2.85554	-3.96597	2.21339
C	-0.83224	-3.43759	-5.22248
C	-0.46961	-4.64616	-4.34959
C	0.44683	-4.23703	-3.18462
C	-0.18864	-3.11635	-2.34248
C	-0.55813	-1.90564	-3.21662
C	-1.47039	-2.31756	-4.38405
H	0.66382	-5.10139	-2.54449
H	-1.38646	-5.10386	-3.95272
H	0.02514	-5.41589	-4.95089
H	0.07156	-3.05581	-5.71754
H	-1.52026	-3.73572	-6.0203
H	-1.12116	-3.50697	-1.91171
H	0.37408	-1.50777	-3.64107
H	-2.43302	-2.67078	-3.98955
H	-1.68459	-1.44298	-5.01118
H	1.40781	-3.89122	-3.59005
C	-5.25745	3.08511	-0.03519
H	-5.46189	3.54615	-1.01068
H	-6.12727	2.45217	0.18786
C	-3.71508	4.91367	0.91968
C	-3.66265	6.17808	1.79162
H	-2.63693	6.56025	1.8521
H	-4.2817	6.96525	1.34642
H	-4.01849	6.02072	2.81292
C	-3.19926	5.27243	-0.47661
H	-3.83336	6.04584	-0.92544
H	-2.18421	5.6838	-0.41441
H	-3.17037	4.42743	-1.17101
C	-3.09935	3.66028	1.6707
H	-2.22177	3.81522	2.3069
C	-5.08513	4.15165	1.0625
H	-5.9901	4.75738	1.16558
C	-4.50239	3.47047	2.33101
H	-4.81605	2.4428	2.5443
H	-4.62349	4.06896	3.23351
C	5.51676	-2.03944	2.48229
H	6.13349	-2.75301	1.92842
C	3.77784	-0.23911	3.77602
H	3.79629	0.85534	3.68889
H	3.04865	-0.47366	4.56306
C	6.18747	-0.69007	2.98251
C	6.16506	0.53504	2.06438
H	6.52171	1.41837	2.60713
H	6.8388	0.38458	1.21232
H	5.17333	0.76941	1.66527
C	5.16456	-0.78104	4.1744
H	5.47981	-0.37541	5.14031
C	5.17107	-2.32129	3.98148
H	5.98746	-2.81744	4.5053
H	4.2416	-2.8642	4.18286
N	-1.07858	-0.7989	-2.3659
C	-2.51073	-0.75013	-2.0229
H	-3.16497	-0.63409	-2.89541
H	-2.78866	-1.69257	-1.53501
H	-0.86187	0.07659	-2.8398
N	0.60452	-2.67282	-1.16229
H	0.42069	-3.33039	-0.40618
C	2.0686	-2.54445	-1.26563
H	2.57692	-3.49334	-1.47535
H	2.30588	-1.86261	-2.09175
C	7.63576	-0.91967	3.44218
H	8.29227	-1.07203	2.5779
H	7.75468	-1.78079	4.10436
H	7.99932	-0.03777	3.98202

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2991.86557
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2992.97152
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.08576
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.49170

Compound E-H trans Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.811680
(Hartree/Particle)
Thermal correction to Energy= 0.855927
Thermal correction to Enthalpy= 0.856872
Thermal correction to Gibbs Free Energy=
0.728511
Sum of electronic and zero-point Energies= -
2992.879808
Sum of electronic and thermal Energies= -
2992.835560
Sum of electronic and thermal Enthalpies= -
2992.834616
Sum of electronic and thermal Free Energies= -
2992.962977

Fe	-0.07491	-0.67923	-0.33985
N	1.71756	-1.13875	0.79452
N	-1.7468	0.70852	-0.30584
N	-1.31251	-1.78897	1.16935
N	1.23977	0.94857	-1.2032
C	2.12212	-0.55886	1.94651
H	1.43748	0.16579	2.38279
C	4.17699	-1.79969	1.95672
C	3.75479	-2.40087	0.76997
H	4.37592	-3.14767	0.28305
C	2.52625	-2.05103	0.21419
C	-2.67381	0.49426	-1.26269
C	-3.83125	1.26704	-1.34834
H	-4.54862	1.07433	-2.14197
C	-4.05602	2.28585	-0.42377
C	-3.08638	2.50687	0.58131
C	-1.95887	1.69719	0.59017
H	-1.18601	1.8401	1.3421
C	-1.94637	-2.24709	2.02561
C	3.32842	-0.84597	2.56694
C	1.92001	1.83677	-1.50879
C	2.77569	2.95272	-1.89392
H	3.29496	2.72221	-2.82963
H	2.1725	3.85504	-2.03575
H	3.51896	3.14106	-1.11279
C	-2.74356	-2.82249	3.1021
H	-2.08729	-3.20492	3.8903
H	-3.40304	-2.05957	3.52772
H	-3.35428	-3.64593	2.71826
C	-0.58296	-3.46094	-5.19224
C	-0.41111	-4.6731	-4.26715
C	0.42261	-4.30954	-3.02842
C	-0.1919	-3.12123	-2.26813
C	-0.38951	-1.90532	-3.19219
C	-1.20856	-2.27479	-4.4399
H	0.5082	-5.17132	-2.35464
H	-1.39766	-5.04189	-3.95348
H	0.0715	-5.49693	-4.80295
H	0.39374	-3.16572	-5.60028
H	-1.21138	-3.72105	-6.05028
H	-1.18213	-3.42816	-1.9044
H	0.60397	-1.57493	-3.52481
H	-2.23036	-2.54495	-4.14132
H	-1.28919	-1.40081	-5.09837
H	1.44123	-4.05309	-3.34956
C	-5.27228	3.19201	-0.45103
H	-5.32249	3.70426	-1.42116
H	-6.18314	2.58132	-0.385
C	-3.82723	4.91482	0.80637
C	-3.86085	6.13508	1.74035
H	-2.84277	6.47986	1.95639
H	-4.39274	6.96205	1.25622
H	-4.35502	5.94292	2.69605
C	-3.10369	5.31607	-0.48151
H	-3.63444	6.14071	-0.97145
H	-2.09145	5.67305	-0.25463
H	-3.01307	4.50474	-1.20951
C	-3.36663	3.60495	1.57226
H	-2.58592	3.69677	2.33452
C	-5.22669	4.20017	0.71293
H	-6.11785	4.83452	0.71688
C	-4.85516	3.43788	2.01405
H	-5.22774	2.41372	2.12516
H	-5.089	3.99618	2.92023
C	5.45996	-2.11731	2.66552
H	6.05104	-2.88043	2.15116
C	3.78845	-0.18933	3.85966
H	3.84886	0.89887	3.7264
H	3.04582	-0.36175	4.65025
C	6.18133	-0.77223	3.1052
C	6.20924	0.40938	2.13192
H	6.59733	1.30198	2.63674
H	6.87923	0.19564	1.29049
H	5.22828	0.6623	1.71819
C	5.15022	-0.76599	4.29323
H	5.47678	-0.32769	5.24099
C	5.09584	-2.31256	4.17418
H	5.88887	-2.81525	4.72693
H	4.14425	-2.80753	4.39468
N	-0.92388	-0.75138	-2.40439
C	-2.3897	-0.6388	-2.23075
H	-2.91892	-0.4663	-3.17468
H	-2.76444	-1.58527	-1.82133
H	-0.61216	0.10541	-2.86124
N	0.54504	-2.70733	-1.03557
H	0.28761	-3.35439	-0.29035
C	2.02375	-2.66382	-1.07998
H	2.47584	-3.65116	-1.22777
H	2.32689	-2.04135	-1.93102
C	7.6177	-1.03627	3.58306
H	8.27232	-1.24799	2.72993
H	7.70102	-1.87352	4.28035
H	8.01115	-0.1471	4.08905

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2991.86340
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2993.00698
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.10951
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2994.51365

Compound F cis-α Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.606445
(Hartree/Particle)
Thermal correction to Energy= 0.641301
Thermal correction to Enthalpy= 0.642245
Thermal correction to Gibbs Free Energy=
0.539399
Sum of electronic and zero-point Energies= -
2754.037565
Sum of electronic and thermal Energies= -
2754.002709
Sum of electronic and thermal Enthalpies= -
2754.001765
Sum of electronic and thermal Free Energies= -
2754.104611

Fe	-0.05137	0.49956	0.272
N	-1.57384	-0.28127	1.33842
N	0.75885	-1.35953	0.65476
N	-0.58144	-0.30514	-1.5537
N	1.47607	1.21596	-0.83305
N	0.62266	1.26032	1.91714
N	-0.97903	2.16481	-0.0581
C	-2.84491	0.1563	1.42949
H	-3.09403	1.02386	0.82976
C	-3.46555	-1.56735	2.98303
C	-2.1396	-2.03419	2.89005
H	-1.84646	-2.90874	3.46124
C	-1.23897	-1.36905	2.0812
C	0.20815	-1.77122	1.98305
H	0.78654	-1.25368	2.75477
H	0.3249	-2.84645	2.15547
C	2.24726	-1.56147	0.64476
H	2.68449	-1.14057	1.55334
H	2.65222	-1.01402	-0.20831
C	2.46171	-3.07018	0.47317
H	2.43881	-3.58378	1.43902
H	3.43254	-3.28851	0.02162
C	1.27753	-3.51343	-0.42316
H	0.82431	-4.44022	-0.06346
H	1.60873	-3.70589	-1.44821
C	0.26416	-2.33299	-0.3968
H	-0.73293	-2.66531	-0.09461
C	0.15741	-1.61483	-1.74097
H	1.16472	-1.37731	-2.09391
C	-0.64223	-2.42983	-2.7982
H	-0.08028	-2.54056	-3.72863
H	-0.83725	-3.44152	-2.42978
C	-2.01041	-0.66654	-1.84145
H	-2.59156	0.23967	-2.02873
H	-2.4169	-1.14875	-0.95079
C	-0.09574	0.66936	-2.57825
H	-0.81821	1.49057	-2.62157
H	-0.05246	0.22194	-3.57709
C	1.25288	1.20267	-2.17374
C	2.17035	1.6712	-3.09377
H	1.96976	1.63565	-4.15937
C	3.3904	2.21324	-2.64372
C	2.64704	1.7319	-0.41092
H	2.8081	1.73428	0.66079
C	0.94839	1.76885	2.9069
C	-1.46655	3.20674	-0.20294
C	-2.07914	4.51819	-0.38534
H	-1.3266	5.2407	-0.71754
H	-2.87315	4.46612	-1.13734
H	-2.51012	4.86736	0.55858
C	-1.96384	-1.64955	-3.01795
H	-2.83893	-2.30394	-3.02792
H	-1.95398	-1.11954	-3.97498
C	1.35791	2.4074	4.1531
H	2.21765	1.88409	4.58405
H	1.63623	3.45009	3.96884
H	0.53446	2.38482	4.87428
C	-3.81486	-0.43556	2.22466
C	3.62224	2.23891	-1.2568
H	4.53755	2.63472	-0.83525
H	-4.81489	-0.02073	2.23985
O	4.22532	2.65244	-3.5816
O	-4.279	-2.24936	3.78472
C	5.49564	3.21362	-3.20402
H	6.10566	2.47043	-2.68063
H	5.97597	3.49147	-4.14091
H	5.3553	4.10285	-2.58118
C	-5.65168	-1.84142	3.92681
H	-6.17187	-1.89638	2.96517
H	-6.09108	-2.55195	4.6252
H	-5.713	-0.82933	4.33946

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2753.18437
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.13508
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.04288
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.39452

Compound F cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.603569 (Hartree/Particle)
Thermal correction to Energy= 0.639951
Thermal correction to Enthalpy= 0.640896
Thermal correction to Gibbs Free Energy= 0.531795
Sum of electronic and zero-point Energies= -2754.021915
Sum of electronic and thermal Energies= -2753.985533
Sum of electronic and thermal Enthalpies= -2753.984589
Sum of electronic and thermal Free Energies= -2754.093689

Fe	0.01733	0.50675	0.29838
N	-1.53437	-0.32057	1.41157
N	0.81196	-1.57166	0.71632
N	-0.51509	-0.33895	-1.50001
N	1.49279	1.29743	-0.84167
N	0.61613	1.32811	1.92284
N	-1.30373	2.4943	-0.16106
C	-2.78273	0.17263	1.53207
H	-2.98539	1.08584	0.98396
C	-3.48267	-1.6085	2.98017
C	-2.17952	-2.12837	2.85669
H	-1.92744	-3.04672	3.37653
C	-1.24332	-1.46212	2.08797
C	0.18774	-1.94613	2.0061
H	0.76754	-1.46418	2.80205
H	0.22499	-3.02705	2.19376
C	2.2862	-1.8116	0.74129
H	2.70698	-1.47327	1.69166
H	2.73977	-1.21419	-0.05638
C	2.46398	-3.31141	0.46693
H	2.36498	-3.88706	1.3926
H	3.44892	-3.53997	0.05198
C	1.31341	-3.63903	-0.51572
H	0.83438	-4.59148	-0.27673
H	1.68684	-3.72494	-1.54112
C	0.31354	-2.44562	-0.39809
H	-0.69011	-2.7924	-0.13399
C	0.23289	-1.64334	-1.70572
H	1.24961	-1.38807	-2.01803
C	-0.53955	-2.40632	-2.81891
H	0.00523	-2.3888	-3.76611
H	-0.65702	-3.45965	-2.54934
C	-1.94606	-0.72277	-1.75428
H	-2.54571	0.17587	-1.91619
H	-2.32028	-1.21785	-0.85744
C	-0.07883	0.6433	-2.54306
H	-0.82008	1.44873	-2.55985

H	-0.05615	0.19477	-3.54157
C	1.26416	1.21525	-2.18034
C	2.1704	1.65989	-3.12052
H	1.97066	1.57766	-4.18352
C	3.38472	2.23732	-2.69377
C	2.65716	1.84633	-0.43952
H	2.81517	1.89785	0.63172
C	0.91586	1.83523	2.92173
C	-1.68385	3.58344	-0.28828
C	-2.17002	4.94939	-0.45305
H	-1.35415	5.6012	-0.78091
H	-2.96728	4.97634	-1.20264
H	-2.56427	5.32517	0.49636
C	-1.91378	-1.69453	-2.94301
H	-2.75171	-2.39478	-2.90421
H	-1.99438	-1.15903	-3.89339
C	1.28728	2.47307	4.17913
H	2.19366	2.01246	4.58561
H	1.47441	3.54007	4.02025
H	0.47821	2.36185	4.90838
C	-3.77981	-0.41771	2.29354
C	3.62298	2.32613	-1.30895
H	4.53522	2.75147	-0.9103
H	-4.75894	0.04254	2.3372
O	4.20982	2.64656	-3.6502
O	-4.32688	-2.30018	3.74101
C	5.47693	3.2387	-3.30511
H	6.09752	2.52526	-2.754
H	5.94767	3.48038	-4.25667
H	5.32853	4.15238	-2.72116
C	-5.67851	-1.83763	3.91233
H	-6.20173	-1.81034	2.95115
H	-6.15032	-2.5672	4.56873
H	-5.69187	-0.85022	4.38482

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2753.14793
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.12221
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.01359
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.37596

Compound F cis-α Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.601482 (Hartree/Particle)
Thermal correction to Energy= 0.638867
Thermal correction to Enthalpy= 0.639811
Thermal correction to Gibbs Free Energy= 0.527124
Sum of electronic and zero-point Energies= -2754.041669
Sum of electronic and thermal Energies= -2754.004284
Sum of electronic and thermal Enthalpies= -2754.003340
Sum of electronic and thermal Free Energies= -2754.116027

Fe	-0.06723	0.62111	0.33873
N	-1.66061	-0.27851	1.51711
N	0.70662	-1.45524	0.70758
N	-0.52186	-0.3068	-1.65387
N	1.53878	1.38085	-0.92176
N	0.80433	1.51962	2.14175
N	-1.21939	2.46233	0.01925
C	-2.92501	0.16436	1.66244
H	-3.16117	1.09836	1.16289
C	-3.55641	-1.711	3.01698
C	-2.23624	-2.18152	2.86546
H	-1.95409	-3.11705	3.33682
C	-1.32876	-1.4449	2.12831
C	0.11777	-1.87179	2.0072
H	0.69626	-1.38074	2.79846
H	0.20127	-2.9528	2.17403
C	2.18815	-1.66408	0.71479
H	2.61219	-1.30025	1.65412
H	2.61444	-1.06628	-0.09578
C	2.40209	-3.16491	0.46226
H	2.40568	-3.72127	1.40431
H	3.36138	-3.35958	-0.02381
C	1.1944	-3.57477	-0.42023
H	0.70936	-4.47686	-0.0391
H	1.50712	-3.79996	-1.44394
C	0.223	-2.35553	-0.39835
H	-0.79934	-2.6608	-0.1555
C	0.20554	-1.6207	-1.75318
H	1.23776	-1.40839	-2.04696
C	-0.54175	-2.44712	-2.84443
H	0.04874	-2.52115	-3.76107
H	-0.71319	-3.47194	-2.50277
C	-1.94222	-0.6642	-1.95892
H	-2.50973	0.23737	-2.20302
H	-2.37959	-1.0985	-1.05555
C	-0.00012	0.64962	-2.66488
H	-0.72227	1.47125	-2.73866
H	0.07564	0.19985	-3.66255
C	1.34179	1.217	-2.2554
C	2.28282	1.58908	-3.19638
H	2.11101	1.43951	-4.25708
C	3.49189	2.18027	-2.77702
C	2.69815	1.94259	-0.52676
H	2.82779	2.05936	0.54435
C	1.10624	1.98702	3.15914
C	-1.67326	3.51253	-0.16987
C	-2.24554	4.83213	-0.40756
H	-1.48172	5.50004	-0.81864
H	-3.0751	4.76178	-1.11833
H	-2.61628	5.25458	0.53182
C	-1.88015	-1.70215	-3.09057
H	-2.74268	-2.37298	-3.07042
H	-1.88205	-1.21285	-4.06911
C	1.48817	2.57452	4.43757
H	2.40147	2.10174	4.81267
H	1.66582	3.64815	4.3188
H	0.68661	2.42748	5.16859
C	-3.8997	-0.49741	2.39232
C	3.69429	2.35893	-1.39577
H	4.59991	2.80134	-1.00043
H	-4.89498	-0.07678	2.46176
O	4.34838	2.51567	-3.73672
O	-4.37282	-2.46893	3.74225
C	5.61007	3.11862	-3.3948
H	6.20588	2.44125	-2.77484
H	6.11328	3.28799	-4.34545
H	5.45486	4.07295	-2.88173
C	-5.74002	-2.06505	3.94112
H	-6.26798	-2.00779	2.98398
H	-6.18157	-2.84417	4.5605
H	-5.7861	-1.10447	4.46384

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2753.14493

UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.14970
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.02649
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.39121

Compound F cis-β Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.606276 (Hartree/Particle)
Thermal correction to Energy= 0.641093
Thermal correction to Enthalpy= 0.642037
Thermal correction to Gibbs Free Energy= 0.539441
Sum of electronic and zero-point Energies= -2754.030865
Sum of electronic and thermal Energies= -2753.996047
Sum of electronic and thermal Enthalpies= -2753.995103
Sum of electronic and thermal Free Energies= -2754.097699

Fe	-0.61466	0.43761	0.13873
N	0.18724	0.72779	1.95466
N	0.11416	-1.453	0.43489
N	-1.26296	-0.26511	-1.6944
N	0.99523	0.98194	-0.91657
N	-2.28667	0.0337	1.05375
N	-1.28593	2.23178	-0.0958
C	0.50961	1.8862	2.5765
H	0.32796	2.79507	2.01359
C	1.27319	0.74344	4.54904
C	0.94258	-0.4658	3.91041
H	1.10065	-1.42218	4.39427
C	0.39938	-0.42583	2.63211
C	-0.04028	-1.67822	1.90493
H	0.52672	-2.5502	2.24768
H	-1.09477	-1.87561	2.11625
C	1.51978	-1.85095	0.05411
H	2.21785	-1.4997	0.81688
H	1.78293	-1.35862	-0.88017
C	1.48752	-3.38392	-0.11819
H	1.81367	-3.89662	0.79093
H	2.16984	-3.69616	-0.91262
C	0.0049	-3.72317	-0.43993
H	-0.41458	-4.40064	0.30869
H	-0.10708	-4.22003	-1.40758
C	-0.72951	-2.36249	-0.41195
H	-1.72327	-2.42939	0.03938
C	-0.85071	-1.73141	-1.81022
H	0.13118	-1.75284	-2.2902
C	-1.91483	-2.43288	-2.70291
H	-1.46079	-2.93573	-3.56002
H	-2.44037	-3.20191	-2.12632
C	-2.73301	-0.28609	-2.01412
H	-3.075	0.72137	-2.26098
H	-3.26317	-0.61415	-1.11843
C	-0.548	0.55192	-2.72183
H	-1.12071	1.47606	-2.85694
H	-0.51529	0.04911	-3.69492
C	0.83994	0.91168	-2.25687
C	1.85569	1.20915	-3.15925
H	1.66873	1.1196	-4.22267
C	3.10162	1.63471	-2.66603
C	3.25747	1.72594	-1.26819
C	2.20007	1.39121	-0.45024
C	-3.28952	-0.03207	1.63259
C	1.04218	1.94349	3.84741
C	-1.66922	3.31961	-0.2136
C	-2.14695	4.69032	-0.35977
H	-3.05237	4.71282	-0.97491
H	-2.37911	5.1152	0.62224
H	-1.37966	5.30757	-0.83814
C	-2.89554	-1.31992	-3.12897
H	-3.92518	-1.67778	-3.20929
H	-2.62536	-0.89925	-4.10283
C	-4.55202	-0.11762	2.35835
H	-4.55812	0.59994	3.18527
H	-5.38857	0.10841	1.68907
H	-4.68932	-1.12478	2.76528
H	1.28994	2.89138	4.31144
H	4.20576	2.05032	-0.85495
O	1.79559	0.85813	5.76739
C	2.06378	-0.3188	6.54877
H	2.47766	0.04769	7.48692
H	2.79662	-0.95825	6.04589
H	1.13967	-0.87294	6.74305
O	4.15874	1.95914	-3.40531
C	4.07993	1.89678	-4.83986
H	5.05967	2.21238	-5.19513
H	3.31185	2.58092	-5.21506
H	3.87806	0.87315	-5.17203
H	2.30516	1.43852	0.62671

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2753.17893
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.12977
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.03707
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.38907

Compound F cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.602900 (Hartree/Particle)
Thermal correction to Energy= 0.639815
Thermal correction to Enthalpy= 0.640759
Thermal correction to Gibbs Free Energy= 0.527799
Sum of electronic and zero-point Energies= -2754.019092
Sum of electronic and thermal Energies= -2753.982177
Sum of electronic and thermal Enthalpies= -2753.981233
Sum of electronic and thermal Free Energies= -2754.094193

Fe	-0.02769	0.67801	0.05149
N	0.58774	0.93148	1.9066
N	0.23899	-1.27846	0.50541
N	-0.84734	0.00814	-1.69169
N	1.54664	1.19	-1.26168
N	-3.59868	-1.16305	1.40796
N	-1.12142	2.33971	0.06003
C	1.0916	2.04482	2.49488
H	1.19588	2.91619	1.85662
C	1.31374	0.94066	4.61777
C	0.79785	-0.22105	4.01343

H	0.67071	-1.14027	4.57224
C	0.44709	-0.18127	2.67104
C	-0.15959	-1.36328	1.94641
H	0.15172	-2.31051	2.40138
H	-1.25352	-1.31069	1.99702
C	1.633	-1.824	0.32481
H	2.26134	-1.51319	1.16236
H	2.05434	-1.39076	-0.58421
C	1.45917	-3.34744	0.19338
H	1.54109	-3.83615	1.16853
H	2.24031	-3.77643	-0.43897
C	0.0369	-3.53897	-0.40023
H	-0.55563	-4.22619	0.20876
H	0.0707	-3.96369	-1.40768
C	-0.59884	-2.12479	-0.41468
H	-1.62346	-2.12221	-0.03474
C	-0.565	-1.47902	-1.81254
H	0.43898	-1.58909	-2.23352
C	-1.65423	-2.05244	-2.75868
H	-1.24295	-2.28691	-3.74365
H	-2.0543	-2.98836	-2.35821
C	-2.34957	0.07075	-1.77877
H	-2.6623	1.09286	-2.00008
H	-2.75172	-0.20171	-0.79943
C	-0.23094	0.75173	-2.83289
H	-0.76876	1.7018	-2.92892
H	-0.3552	0.21468	-3.77985
C	1.22639	1.05091	-2.56582
C	2.13893	1.23567	-3.59743
H	1.82487	1.10309	-4.62585
C	3.45826	1.60628	-3.275
C	3.7916	1.75987	-1.91285
C	2.8204	1.54017	-0.96054
H	3.05225	1.64016	0.09559
C	-4.6385	-1.45159	1.83647
C	1.46	2.09535	3.82035
C	-1.7094	3.33283	0.1684
C	-2.45169	4.57882	0.29943
H	-3.40639	4.50434	-0.23143
H	-2.64614	4.7911	1.35569
H	-1.87207	5.40341	-0.12874
C	-2.74963	-0.95628	-2.84716
H	-3.75119	-1.35128	-2.66103
H	-2.76672	-0.50124	-3.84205
C	-5.94601	-1.8148	2.3753
H	-6.07968	-1.3755	3.36873
H	-6.74027	-1.44785	1.71782
H	-6.03092	-2.90293	2.45651
H	1.86401	3.00062	4.25886
H	4.80146	2.04213	-1.6378
O	1.68898	1.04886	5.88797
C	1.58004	-0.08107	6.77178
H	1.94505	0.27244	7.73481
H	2.20517	-0.90783	6.41938
H	0.53667	-0.39931	6.86453
O	4.43445	1.82308	-4.15068
C	4.18056	1.69639	-5.56085
H	5.1285	1.92693	-6.04449
H	3.41702	2.41246	-5.88131
H	3.87737	0.6739	-5.8083

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2753.14434
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.09984
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.99373
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.36935

Compound F cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.601265
(Hartree/Particle)
Thermal correction to Energy= 0.639113
Thermal correction to Enthalpy= 0.640057
Thermal correction to Gibbs Free Energy=
0.522527
Sum of electronic and zero-point Energies= -
2754.031811
Sum of electronic and thermal Energies= -
2753.993963
Sum of electronic and thermal Enthalpies= -
2753.993019
Sum of electronic and thermal Free Energies= -
2754.110549

Fe	0.11934	0.8798	0.01055
N	0.56865	0.97388	2.09322
N	0.30378	-1.22881	0.53813
N	-0.82734	-0.00994	-1.78042
N	1.56692	1.32658	-1.42137
N	-3.55132	-1.01616	1.40815
N	-1.08019	2.6161	0.11162
C	1.00114	2.0589	2.78178
H	1.08332	2.98401	2.21841
C	1.20655	0.81031	4.82104
C	0.75763	-0.32008	4.1143
H	0.64686	-1.28252	4.59916
C	0.44882	-0.19177	2.76543
C	-0.1128	-1.34791	1.96294
H	0.19607	-2.30539	2.39917
H	-1.20772	-1.30464	1.99724
C	1.69636	-1.76283	0.35261
H	2.32133	-1.46645	1.19845
H	2.12093	-1.30816	-0.54647
C	1.5432	-3.28835	0.18563
H	1.69324	-3.80429	1.13811
H	2.29268	-3.68223	-0.50534
C	0.09223	-3.49201	-0.32925
H	-0.47557	-4.13718	0.34628
H	0.06975	-3.97256	-1.31134
C	-0.53292	-2.07276	-0.37951
H	-1.55945	-2.05885	-0.0049
C	-0.51149	-1.48363	-1.80666
H	0.49257	-1.60152	-2.22658
C	-1.5952	-2.13805	-2.71388
H	-1.18083	-2.42497	-3.68376
H	-1.97722	-3.055	-2.25617
C	-2.32442	0.0259	-1.86279
H	-2.65634	1.02878	-2.14237
H	-2.72222	-0.19488	-0.86839
C	-0.21612	0.67979	-2.94953
H	-0.78116	1.60445	-3.11881
H	-0.30057	0.08664	-3.86814
C	1.23245	1.05322	-2.70323
C	2.13272	1.17228	-3.75441
H	1.81442	0.93104	-4.76152
C	3.44152	1.61735	-3.48694
C	3.78471	1.91043	-2.14926
C	2.83302	1.7489	-1.16935
H	3.07135	1.95679	-0.13043
C	-4.59109	-1.30973	1.83341
C	1.3256	2.02851	4.11931
C	-1.72056	3.57382	0.23745

C	-2.52942	4.77377	0.39611
H	-3.46666	4.66947	-0.16
H	-2.75812	4.92995	1.45535
H	-1.98364	5.64387	0.01676
C	-2.71153	-1.07086	-2.86718
H	-3.70566	-1.47313	-2.65742
H	-2.73613	-0.67625	-3.88761
C	-5.89868	-1.67876	2.36844
H	-6.0531	-1.20909	3.34481
H	-6.69116	-1.34907	1.68944
H	-5.9651	-2.76492	2.48538
H	1.67363	2.91429	4.63824
H	4.78669	2.25122	-1.91512
O	1.53833	0.83574	6.1081
C	1.44822	-0.36186	6.89947
H	1.76659	-0.06951	7.89891
H	2.11822	-1.13431	6.50839
H	0.41672	-0.72731	6.93074
O	4.39844	1.78413	-4.39112
C	4.13616	1.52019	-5.78191
H	5.07032	1.74116	-6.29566
H	3.34293	2.1757	-6.15489
H	3.87034	0.46881	-5.93075

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2753.13895
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.13030
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.00725
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.38800

Compound F trans Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.605893 (Hartree/Particle)
Thermal correction to Energy= 0.639786
Thermal correction to Enthalpy= 0.640731
Thermal correction to Gibbs Free Energy= 0.540910
Sum of electronic and zero-point Energies= -2754.018884
Sum of electronic and thermal Energies= -2753.984990
Sum of electronic and thermal Enthalpies= -2753.984045
Sum of electronic and thermal Free Energies= -2754.083866

Fe	-0.00413	-0.04229	0.05454
N	1.17925	0.0855	1.69129
N	0.65278	-1.9788	0.10999
N	-1.45828	-0.2609	1.3158
C	1.77946	1.14251	2.264
H	1.64265	2.09775	1.76678
C	2.71643	-0.18685	4.02943
C	2.11028	-1.305	3.41966
H	2.25223	-2.28576	3.86127
C	1.35793	-1.13434	2.27502
C	0.67326	-2.2903	1.57025
H	1.18422	-3.23369	1.78985
H	-0.35853	-2.39044	1.91711
C	1.98671	-2.37666	-0.47162
H	2.79048	-2.07973	0.20533
H	2.12663	-1.84229	-1.41101
C	1.88522	-3.88709	-0.72232
H	2.16135	-4.45821	0.16904
H	2.56377	-4.20201	-1.51905
C	0.39497	-4.11068	-1.08583
H	-0.0299	-4.95365	-0.53548
H	0.27348	-4.33776	-2.14889
C	-0.3201	-2.78158	-0.71847
H	-1.21712	-2.95305	-0.11699
C	-0.70108	-1.94409	-1.96898
H	0.19416	-1.77838	-2.57485
C	-1.84715	-2.5912	-2.79268
H	-1.61525	-2.5904	-3.86059
H	-1.99218	-3.63642	-2.50511
C	-2.68095	-0.86042	-1.29922
H	-3.21733	0.08724	-1.21788
H	-2.80994	-1.39886	-0.36084
C	-2.28427	-0.20311	2.12735
C	2.54511	1.06788	3.41997
C	-3.1043	-1.73828	-2.48458
H	-3.97503	-2.34877	-2.23246
H	-3.38692	-1.13121	-3.34981
C	-3.33039	-0.13658	3.14147
H	-2.887	-0.16262	4.14213
H	-3.90095	0.79151	3.03246
H	-4.01469	-0.98502	3.03721
H	2.99472	1.96752	3.82092
C	2.45584	0.94533	-1.51987
N	1.51541	0.48964	-1.01761
C	3.64339	1.5072	-2.15347
H	3.83893	1.00566	-3.10699
H	3.50035	2.57639	-2.34045
H	4.5139	1.37649	-1.50239
C	-1.20499	1.82108	-1.69126
C	-0.88387	2.88917	0.3385
C	-1.7481	2.96771	-2.25792
C	-1.40003	4.07499	-0.14223
H	-0.55019	2.81131	1.36801
H	-2.09502	2.94459	-3.28406
H	-1.4772	4.95351	0.4882
C	-1.84206	4.13586	-1.47844
N	-0.76575	1.77068	-0.41015
N	-1.20798	-0.6017	-1.49962
C	-1.06311	0.52485	-2.46931
H	-0.07159	0.46283	-2.92602
H	-1.79944	0.47642	-3.27888
O	3.41747	-0.42675	5.13484
C	4.0807	0.65682	5.81054
H	4.57242	0.2015	6.66879
H	3.35445	1.40183	6.15104
H	4.82758	1.11959	5.15752
O	-2.33034	5.30363	-1.89017
C	-2.80999	5.44816	-3.23784
H	-3.13959	6.48308	-3.3158
H	-3.65467	4.77631	-3.42204
H	-2.00612	5.26035	-3.95713

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =--2753.16618
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.11566
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.02335
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.37517

Compound F trans Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.602613 (Hartree/Particle)
Thermal correction to Energy= 0.639795
Thermal correction to Enthalpy= 0.640740
Thermal correction to Gibbs Free Energy= 0.527276
Sum of electronic and zero-point Energies= -2754.014175
Sum of electronic and thermal Energies= -2753.976993
Sum of electronic and thermal Enthalpies= -2753.976048
Sum of electronic and thermal Free Energies= -2754.089512

Fe	0.40303	0.22327	-0.23177
N	1.4236	0.45986	1.48084
N	0.64588	-1.72967	0.15344
N	-2.92441	-2.20292	2.06373
C	2.18089	1.47361	1.94669
H	2.26213	2.34505	1.30574
C	2.74309	0.28892	3.95711
C	1.9803	-0.78949	3.46202
H	1.90882	-1.69788	4.05025
C	1.34644	-0.67205	2.24285
C	0.49856	-1.77315	1.64824
H	0.77842	-2.74971	2.05754
H	-0.55895	-1.61742	1.89188
C	1.93565	-2.3955	-0.25556
H	2.73047	-2.12759	0.44444
H	2.2106	-2.01654	-1.2425
C	1.60855	-3.8887	-0.31671
H	1.6357	-4.33848	0.68106
H	2.32639	-4.43625	-0.93283
C	0.17879	-3.91913	-0.89926
H	-0.41828	-4.73005	-0.47586
H	0.20813	-4.07687	-1.98288
C	-0.43002	-2.52749	-0.57313
H	-1.28342	-2.61594	0.10285
C	-0.85849	-1.75213	-1.83828
H	-0.05351	-1.78353	-2.57967
C	-2.21219	-2.2348	-2.39518
H	-2.26102	-2.06077	-3.47396
H	-2.35219	-3.30844	-2.24307
C	-2.46736	-0.33743	-0.83284
H	-2.88906	0.6688	-0.86105
H	-2.38574	-0.63841	0.21326
C	-3.76182	-2.5822	2.77245
C	2.84921	1.44399	3.15934
C	-3.27175	-1.3823	-1.64257
H	-3.87894	-1.98625	-0.96422
H	-3.95791	-0.90354	-2.34605
C	-4.81428	-3.05969	3.66438
H	-4.59546	-2.76608	4.69573
H	-5.77832	-2.63124	3.37321
H	-4.88368	-4.1508	3.61521
H	3.43903	2.29934	3.46357
C	3.05613	0.80045	-2.2871
N	2.10758	0.49679	-1.69167
C	4.24826	1.17332	-3.03967
H	4.23667	0.69315	-4.02341
H	4.28453	2.25901	-3.17391
H	5.14517	0.85209	-2.50041
C	-0.89944	2.04548	-1.91906
C	-0.15933	3.24304	-0.07687
C	-1.41575	3.18912	-2.51114
C	-0.63772	4.42819	-0.59057
H	0.31302	3.22032	0.89813
H	-1.92856	3.11408	-3.46251
H	-0.54326	5.35807	-0.04158
C	-1.27456	4.42332	-1.84825
N	-0.25598	2.05574	-0.7222
N	-1.08246	-0.31938	-1.44404
C	-1.0306	0.67407	-2.55615
H	-0.15279	0.45167	-3.17224
H	-1.91433	0.62409	-3.20274
O	3.31654	0.10946	5.14133
C	4.12094	1.15615	5.71756
H	4.46153	0.76138	6.67339
H	3.52095	2.05699	5.87972
H	4.98174	1.3759	5.07831
O	-1.71169	5.59502	-2.29672
C	-2.38512	5.67756	-3.56555
H	-2.62045	6.73256	-3.69664
H	-3.30954	5.0913	-3.55039
H	-1.72837	5.34063	-4.37405

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =--2753.13704
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.09880
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.99152
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.36367

Compound F trans Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.601428 (Hartree/Particle)
Thermal correction to Energy= 0.638791
Thermal correction to Enthalpy= 0.639735
Thermal correction to Gibbs Free Energy= 0.525433
Sum of electronic and zero-point Energies= -2754.030955
Sum of electronic and thermal Energies= -2753.993592
Sum of electronic and thermal Enthalpies= -2753.992648
Sum of electronic and thermal Free Energies= -2754.106950

Fe	0.03974	0.19631	0.18215
N	1.31591	-0.01727	1.92465
N	0.7034	-1.9519	0.0935
N	-1.61406	0.05895	1.67371
C	1.94188	0.94106	2.63199
H	1.8274	1.95971	2.27026
C	2.84487	-0.63537	4.19689
C	2.2016	-1.64521	3.45201
H	2.31005	-2.67849	3.76436
C	1.45248	-1.3029	2.34298
C	0.70535	-2.34159	1.52864
H	1.14036	-3.33453	1.69452
H	-0.33588	-2.38544	1.86794
C	2.03384	-2.27269	-0.52121
H	2.83833	-1.99877	0.16507
H	2.14781	-1.66336	-1.42061
C	1.98073	-3.76897	-0.86919
H	2.32779	-4.37975	-0.03027
H	2.62814	-4.00462	-1.71767
C	0.48374	-4.03969	-1.1685
H	0.11885	-4.91273	-0.62165

H	0.31878	-4.24535	-2.23005
C	-0.26526	-2.74699	-0.72977
H	-1.13425	-2.97553	-0.10517
C	-0.73226	-1.91336	-1.94634
H	0.12721	-1.73576	-2.6001
C	-1.90133	-2.60301	-2.70682
H	-1.73644	-2.57821	-3.78703
H	-1.98235	-3.65748	-2.42851
C	-2.70057	-0.8552	-1.20168
H	-3.25357	0.08552	-1.15169
H	-2.77049	-1.32943	-0.22033
C	-2.41123	0.18757	2.5062
C	2.70582	0.69601	3.76313
C	-3.17365	-1.80921	-2.31192
H	-3.98112	-2.45729	-1.9618
H	-3.56743	-1.2527	-3.16772
C	-3.41845	0.34207	3.54896
H	-2.9343	0.4889	4.51961
H	-4.05016	1.20946	3.33233
H	-4.04868	-0.55174	3.59792
H	3.17976	1.52128	4.27938
C	2.74371	1.40869	-1.43853
N	1.80841	0.88995	-0.9899
C	3.92126	2.05235	-2.00865
H	4.1367	1.63368	-2.99698
H	3.74985	3.12885	-2.1082
H	4.78729	1.8891	-1.35929
C	-1.34889	1.84089	-1.88524
C	-1.04083	3.18301	-0.02391
C	-1.94939	2.88027	-2.58697
C	-1.6124	4.27359	-0.64279
H	-0.68052	3.26096	0.9982
H	-2.30561	2.70936	-3.59585
H	-1.71278	5.22587	-0.13464
C	-2.08368	4.13511	-1.96476
N	-0.89631	1.97687	-0.62028
N	-1.25238	-0.58449	-1.48585
C	-1.13277	0.47787	-2.51792
H	-0.11951	0.43313	-2.93341
H	-1.8305	0.33256	-3.35174
O	3.54439	-1.03803	5.25386
C	4.24324	-0.07368	6.06166
H	4.72638	-0.65369	6.84641
H	3.54132	0.63928	6.50583
H	4.9994	0.45066	5.46871
O	-2.6315	5.21543	-2.51395
C	-3.14277	5.16047	-3.85718
H	-3.52462	6.15994	-4.05964
H	-3.95601	4.43131	-3.93164
H	-2.34386	4.91839	-4.56553

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =--2753.13915
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2754.13731
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2755.02792
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2755.38379

Compound G cis-α Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.562668
(Hartree/Particle)
Thermal correction to Energy= 0.592976
Thermal correction to Enthalpy= 0.593921
Thermal correction to Gibbs Free Energy=
0.503571
Sum of electronic and zero-point Energies= -
2526.219633
Sum of electronic and thermal Energies= -
2526.189325
Sum of electronic and thermal Enthalpies= -
2526.188381
Sum of electronic and thermal Free Energies= -
2526.278730

Fe	0.1849217	0.6965412	0.4950874
N	-1.3634283	0.2106812	1.7005974
N	1.7233017	1.1385012	-0.7393426
N	1.2210917	1.0306912	2.0995674
N	-0.2657683	2.5828312	0.4734974
C	-2.4303083	0.9703712	2.0237174
H	-2.4870083	1.9418612	1.5494874
C	-3.3064083	-0.7083288	3.4948474
H	-4.0614283	-1.0687388	4.1867874
C	-2.2069983	-1.5014588	3.1683974
H	-2.0853083	-2.4902888	3.5988674
C	-1.2533783	-1.0086188	2.2804874
C	-0.1202883	1.2685612	-2.2878926
H	-0.5799283	2.2531912	-2.1524026
H	-0.3210883	0.9636412	-3.3213526
C	1.3582117	1.3658212	-2.0239726
C	2.2786317	1.7069512	-3.0123726
H	1.9424417	1.8653312	-4.0320326
C	3.6237617	1.8435512	-2.6715026
H	4.3597917	2.1095812	-3.4236526
C	4.0013517	1.6278612	-1.3457826
C	3.0266217	1.2762912	-0.4191226
H	3.2873717	1.0967412	0.6162474
C	1.7772317	1.3065712	3.0790674
C	-3.4156783	0.5541712	2.9118674
C	-0.4484883	3.7274112	0.5103374
C	-0.6794383	5.1672712	0.5545074
H	-1.5021483	5.4406512	-0.1144826
H	-0.9350883	5.4768312	1.5730974
H	0.2232517	5.7012912	0.2395174
C	2.4784517	1.6509412	4.3112174
H	3.2298817	0.8897412	4.5458574
H	2.9789917	2.6185712	4.2016474
H	1.7677517	1.7138912	5.1419074
N	-0.7545883	0.3319012	-1.3153626
N	0.4871817	-1.3508388	0.5809074
H	5.0346017	1.7234912	-1.0300326
H	-4.2516183	1.2087612	3.1337374
C	-0.9199183	-3.1275188	-3.1693926
C	-0.9867383	-4.0035888	-1.9143126
C	-0.0588283	-3.4472288	-0.8227226
C	-0.4058683	-1.9850788	-0.4785826
C	-0.4160883	-1.0962288	-1.7240326
C	-1.3134383	-1.6801388	-2.8335726
H	-0.1168683	-4.0716388	0.0766174
H	-2.0208983	-4.0473288	-1.5458326
H	-0.6929883	-5.0324588	-2.1449226
H	0.0939417	-3.1563788	-3.5915926
H	-1.5916383	-3.5114388	-3.9439326
H	-1.4152783	-1.9704188	-0.0519626
H	-2.3595183	-1.6810288	-2.5069126
H	-1.2603383	-1.0550788	-3.7325026
H	0.9720217	-3.5105588	-1.1896926
C	0.0002317	-1.7641388	1.9291074
H	0.7836917	-1.5228188	2.6543174
H	-0.1586083	-2.8478688	1.9800274
C	1.9095417	-1.7694388	0.4524874
H	2.2663817	-1.5862388	-0.5608026

H	2.0425217	-2.8287288	0.6919774
H	2.5112017	-1.1792188	1.1448074
H	0.6072317	-1.0488988	-2.1127426
C	-2.2193883	0.5911012	-1.3055026
H	-2.6451983	0.5559412	-2.3124026
H	-2.3936883	1.5852212	-0.8913226
H	-2.7279283	-0.1410288	-0.6785526

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.52268
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.34109
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.15091
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.48445

Compound G cis-α Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.559632 (Hartree/Particle)
Thermal correction to Energy= 0.591577
Thermal correction to Enthalpy= 0.592521
Thermal correction to Gibbs Free Energy= 0.495338
Sum of electronic and zero-point Energies= -2526.203554
Sum of electronic and thermal Energies= -2526.171609
Sum of electronic and thermal Enthalpies= -2526.170665
Sum of electronic and thermal Free Energies= -2526.267848

Fe	0.2364086	0.6802062	0.5028703
N	-1.3464014	0.1445762	1.7809403
N	1.7421486	1.2146462	-0.7738997
N	1.2320586	1.0933162	2.0944103
N	-0.4914014	2.9529662	0.4601503
C	-2.3711714	0.9409162	2.1478103
H	-2.3789914	1.9341962	1.7150503
C	-3.3117214	-0.7580838	3.5505903
H	-4.0768014	-1.1153238	4.2332703
C	-2.2529114	-1.5849438	3.1785203
H	-2.1736114	-2.5959638	3.5655903
C	-1.2806114	-1.1012138	2.3033903
C	-0.1465714	1.2302262	-2.2637197
H	-0.6315314	2.1976762	-2.0938097
H	-0.3775714	0.9304262	-3.2913097
C	1.3350686	1.3828262	-2.0543297
C	2.2221686	1.7190062	-3.0735997
H	1.8618786	1.8384362	-4.0901797
C	3.5713086	1.8976662	-2.7653297
H	4.2822786	2.1584662	-3.5432397
C	3.9912286	1.7293862	-1.4446297
C	3.0480386	1.3876262	-0.4828997
H	3.3311586	1.2433362	0.5528803
C	1.7819386	1.3798162	3.0745503
C	-3.3678114	0.5340162	3.0275003
C	-0.5756914	4.1101562	0.4993803
C	-0.6920514	5.5638762	0.5460403
H	-1.6116214	5.8827362	0.0444003
H	-0.7190614	5.9055662	1.5854003
H	0.1636486	6.0253962	0.0427103
C	2.4683686	1.7420862	4.3088603
H	3.2239386	0.9893962	4.5575703
H	2.9613586	2.7130962	4.1946903
H	1.7487586	1.8061262	5.1318303
N	-0.7185114	0.2644062	-1.2755597
N	0.4710286	-1.5562438	0.6159403
H	5.0306186	1.8564462	-1.1622297
H	-4.1697014	1.2161662	3.2886703
C	-0.8320914	-3.1380738	-3.2405697
C	-0.9651314	-4.0624638	-2.0268597
C	-0.0760014	-3.5614838	-0.8804697
C	-0.4009314	-2.1056538	-0.4834697
C	-0.3634214	-1.1616138	-1.6992797
C	-1.2228814	-1.7009438	-2.8616497
H	-0.1803014	-4.2120838	-0.0038897
H	-2.0144614	-4.1034038	-1.7036297
H	-0.6776814	-5.0862138	-2.2869797
H	0.1995686	-3.1636138	-3.6172697
H	-1.4730514	-3.4790538	-4.0599697
H	-1.4226714	-2.0905038	-0.0857297
H	0.6747486	-1.1008638	-2.0450497
H	-2.2801014	-1.7052938	-2.5721797
H	-1.1354214	-1.0452138	-3.7358997
H	0.9691886	-3.6329538	-1.2042197
C	-0.0610714	-1.9217138	1.9443703
H	0.7229486	-1.7189338	2.6834203
H	-0.2872214	-2.9944338	2.0173503
C	1.8929286	-1.9624638	0.5151703
H	2.2753486	-1.7508838	-0.4848497
H	2.0426786	-3.0267038	0.7298303
H	2.4762986	-1.3823038	1.2347703
C	-2.1909714	0.4888462	-1.2217297
H	-2.6377414	0.4726262	-2.2196797
H	-2.3757514	1.4661262	-0.7732197
H	-2.6664614	-0.2741438	-0.6065997

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.48502
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.32762
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.12022
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = --2527.46564

Compound G cis-α Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.557526 (Hartree/Particle)
Thermal correction to Energy= 0.590471
Thermal correction to Enthalpy= 0.591416
Thermal correction to Gibbs Free Energy= 0.490625
Sum of electronic and zero-point Energies= -2526.223571
Sum of electronic and thermal Energies= -2526.190626
Sum of electronic and thermal Enthalpies= -2526.189681
Sum of electronic and thermal Free Energies= -2526.290472

Fe	0.1935322	0.7840515	0.5513078
N	-1.4891178	0.1901115	1.8390378
N	1.8441022	1.2568815	-0.8210122
N	1.4259322	1.1737415	2.3126278
N	-0.4321878	2.8759915	0.5507578
C	-2.5546678	0.9403515	2.1838978

H	-2.5756178	1.9488615	1.7855778
C	-3.4983278	-0.8410785	3.4750078
H	-4.2807878	-1.2481185	4.1084978
C	-2.4001978	-1.6236885	3.1191478
H	-2.3097978	-2.6470685	3.4692878
C	-1.4084478	-1.0755485	2.3057478
C	-0.0003878	1.2017215	-2.4125122
H	-0.4684578	2.1889915	-2.3178422
H	-0.1531578	0.8844015	-3.4518422
C	1.4782222	1.3409315	-2.1193922
C	2.4055722	1.5994515	-3.1283322
H	2.0808422	1.6493815	-4.1628722
C	3.7446622	1.7931715	-2.7897122
H	4.4821822	1.9958015	-3.5602922
C	4.1198822	1.7162715	-1.4472922
C	3.1401222	1.4432015	-0.5001122
H	3.3857522	1.3664315	0.5537278
C	1.9387222	1.4313515	3.3207778
C	-3.5769978	0.4688515	2.9994578
C	-0.5983778	4.0240115	0.5422978
C	-0.8099078	5.4663415	0.5322078
H	-1.7318978	5.7084915	-0.0065722
H	-0.8875778	5.8410615	1.5577978
H	0.0312722	5.9620715	0.0364278
C	2.5864522	1.7529715	4.5865478
H	3.3294422	0.9879915	4.8350378
H	3.0858422	2.7246515	4.5150378
H	1.8395422	1.7967515	5.3860178
N	-0.6780478	0.2940115	-1.4559322
N	0.3935722	-1.4492085	0.6321878
H	5.1498822	1.8590715	-1.1390522
H	-4.4141178	1.1116715	3.2493178
C	-0.7980478	-3.2094685	-3.2055022
C	-0.9971078	-4.0547185	-1.9443322
C	-0.1390878	-3.5040185	-0.7967322
C	-0.4469678	-2.0223685	-0.4894422
C	-0.3389778	-1.1501585	-1.7607022
C	-1.1639478	-1.7459385	-2.9217022
H	-0.2842178	-4.1085285	0.1066278
H	-2.0584678	-4.0522385	-1.6589622
H	-0.7251378	-5.0989385	-2.1295822
H	0.2450622	-3.2821685	-3.5425522
H	-1.4187278	-3.5847885	-4.0256022
H	-1.4833978	-1.9610785	-0.1347822
H	0.7136022	-1.1396485	-2.0685622
H	-2.2312478	-1.7076285	-2.6738022
H	-1.0284878	-1.1382685	-3.8243522
H	0.9149222	-3.6108585	-1.0801022
C	-0.1533978	-1.8440985	1.9521078
H	0.6121722	-1.6206685	2.7045178
H	-0.3399578	-2.9245685	2.0091478
C	1.8221022	-1.8498485	0.5609578
H	2.2182922	-1.6492285	-0.4352722
H	1.9709722	-2.9100285	0.7931878
H	2.3894322	-1.2561285	1.2816278
C	-2.1362778	0.5722915	-1.4699922
H	-2.5652278	0.5205215	-2.4765322
H	-2.3054378	1.5772415	-1.0749722
H	-2.6598878	-0.1390085	-0.8296622

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = --2525.48079
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.35394
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.13748
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.48004

Compound G cis-β Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.562549 (Hartree/Particle)
Thermal correction to Energy= 0.593086
Thermal correction to Enthalpy= 0.594030
Thermal correction to Gibbs Free Energy= 0.501744
Sum of electronic and zero-point Energies= -2526.213731
Sum of electronic and thermal Energies= -2526.183194
Sum of electronic and thermal Enthalpies= -2526.182250
Sum of electronic and thermal Free Energies= -2526.274536

C	-1.24275	1.37074	-0.85998
C	-2.51021	2.12413	-1.30975
C	-2.15823	3.4894	-1.92144
C	-1.35196	4.33328	-0.92855
C	-0.07863	3.58892	-0.49167
C	-0.41732	2.21751	0.12376
C	-2.6054	0.02865	0.73892
C	1.0929	1.93326	2.03756
C	-1.83018	-1.01792	-1.27728
C	-1.47703	-2.38596	-0.74463
C	-2.16412	-3.54246	-1.10273
C	-1.74073	-4.77119	-0.59526
C	-0.646	-4.79913	0.26806
C	-0.01437	-3.60245	0.58901
C	2.01863	1.58603	-0.15171
C	1.98879	0.72544	-1.38292
C	2.73042	1.02666	-2.52316
C	2.76949	0.10975	-3.57225
C	2.06739	-1.08756	-3.43714
C	1.33589	-1.30938	-2.27602
Fe	0.32645	-0.60254	0.52237
H	-0.63407	1.18602	-1.74956
H	-3.06835	1.5154	-2.03129
H	-3.17182	2.29383	-0.45244
H	-1.58082	3.3495	-2.84574
H	-3.08008	4.00677	-2.2055
H	-1.96852	4.56899	-0.05055
H	-1.07089	5.2914	-1.37731
H	0.488	4.19641	0.22311
H	0.55328	3.45528	-1.3788
H	-1.04024	2.40122	1.00567
H	-3.5549	0.26553	0.2515
H	-2.41332	0.76197	1.52157
H	-2.68822	-0.95674	1.1977
H	1.40038	2.98498	2.01659
H	1.90132	1.33851	2.46655
H	0.21227	1.83516	2.67213
H	-1.24976	-0.8104	-2.18158
H	-2.88835	-0.96966	-1.55768
H	-3.01991	-3.47912	-1.76746
H	-2.26099	-5.68567	-0.86254
H	-0.28607	-5.73001	0.69286
H	2.84934	1.2409	0.47363
H	2.22791	2.63136	-0.39201
H	3.27852	1.96198	-2.57901
H	3.34161	0.32167	-4.47011
H	2.07932	-1.84142	-4.21689
N	-1.48661	0.00904	-0.24914

N	0.78164	1.43022	0.66873
N	1.27169	-0.41737	-1.26471
N	-0.40713	-2.41337	0.09079
N	2.03127	-1.22125	1.20539
N	-0.35037	-0.77233	2.32961
C	3.04948	-1.62008	1.59102
C	-0.6643	-0.95689	3.42973
C	4.33214	-2.12333	2.07038
H	5.02203	-1.29198	2.2488
H	4.774	-2.79411	1.32632
H	4.19605	-2.67373	3.0069
C	-1.07396	-1.17986	4.81157
H	-2.13036	-0.92058	4.93783
H	-0.47566	-0.56077	5.488
H	-0.93592	-2.23205	5.0807
H	0.83493	-3.57978	1.26188
H	0.78239	-2.23079	-2.14185

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2525.50105
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.33220
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.14859
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.46571

Compound G cis-β Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.559622 (Hartree/Particle)
Thermal correction to Energy= 0.591802
Thermal correction to Enthalpy= 0.592746
Thermal correction to Gibbs Free Energy= 0.493915
Sum of electronic and zero-point Energies= -2526.198122
Sum of electronic and thermal Energies= -2526.165942
Sum of electronic and thermal Enthalpies= -2526.164998
Sum of electronic and thermal Free Energies= -2526.263829

C	-1.24633	1.338	-0.89102
C	-2.52683	2.07119	-1.33373
C	-2.19202	3.4149	-2.00145
C	-1.35981	4.29432	-1.06223
C	-0.0763	3.56671	-0.62681
C	-0.4005	2.21859	0.044
C	-2.55875	0.0271	0.78913
C	1.12622	1.95844	1.95003
C	-1.84606	-1.05047	-1.24996
C	-1.52273	-2.42431	-0.71277
C	-2.21888	-3.5707	-1.08625
C	-1.81553	-4.80446	-0.57452
C	-0.7319	-4.85309	0.30343
C	-0.08842	-3.6666	0.63451
C	2.04454	1.58876	-0.24403
C	2.03452	0.77653	-1.51883
C	2.75496	1.17489	-2.64533
C	2.81855	0.31925	-3.74516
C	2.1597	-0.90874	-3.68195
C	1.44877	-1.22091	-2.52674
Fe	0.30204	-0.61673	0.53889
H	-0.6545	1.12503	-1.78503
H	-3.10147	1.4389	-2.0211
H	-3.16743	2.26741	-0.46588
H	-1.63984	3.24122	-2.93535
H	-3.12161	3.92193	-2.27882
H	-1.95433	4.56461	-0.17896
H	-1.09037	5.23418	-1.55465
H	0.50235	4.19855	0.05671
H	0.54114	3.40097	-1.51876
H	-1.00353	2.43514	0.93274
H	-3.52713	0.24986	0.33291
H	-2.33548	0.77877	1.54564
H	-2.61597	-0.94438	1.28014
H	1.40223	3.01911	1.92631
H	1.9585	1.38735	2.36491
H	0.25959	1.82817	2.59827
H	-1.25872	-0.86861	-2.1555
H	-2.9032	-0.97817	-1.52852
H	-3.06418	-3.49793	-1.76318
H	-2.34385	-5.71162	-0.85148
H	-0.39134	-5.7915	0.72739
H	2.86658	1.21595	0.3766
H	2.26759	2.63892	-0.45114
H	3.2651	2.13335	-2.65628
H	3.37487	0.60518	-4.63255
H	2.18993	-1.60976	-4.50921
N	-1.47588	-0.0124	-0.23895
N	0.80701	1.45008	0.5841
N	1.37475	-0.39669	-1.46613
N	-0.46721	-2.47316	0.13658
N	1.97719	-1.23661	1.2548
N	-0.42682	-0.7557	2.80187
C	2.99111	-1.63435	1.65322
C	-0.69106	-0.97088	3.91072
C	4.26815	-2.13444	2.1487
H	4.93214	-1.29849	2.39217
H	4.74936	-2.75575	1.38624
H	4.11511	-2.73539	3.05099
C	-1.03083	-1.23483	5.30489
H	-2.01293	-0.81142	5.53842
H	-0.28422	-0.7832	5.96576
H	-1.05901	-2.31386	5.48662
H	0.75509	-3.65312	1.31535
H	0.9179	-2.16512	-2.43976

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF =-2525.46282
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.32190
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.11280
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.45975

Compound G cis-β Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.557655 (Hartree/Particle)
Thermal correction to Energy= 0.590704
Thermal correction to Enthalpy= 0.591648
Thermal correction to Gibbs Free Energy= 0.489955
Sum of electronic and zero-point Energies= -2526.218280
Sum of electronic and thermal Energies= -2526.185231

Sum of electronic and thermal Enthalpies= -2526.184287
Sum of electronic and thermal Free Energies= -2526.28597

C	-1.26985	1.34962	-0.8898
C	-2.53823	2.08934	-1.36711
C	-2.20581	3.43335	-2.03049
C	-1.40395	4.31954	-1.0728
C	-0.12685	3.59877	-0.61257
C	-0.44256	2.24749	0.05972
C	-2.62642	0.0367	0.74872
C	1.06014	2.06452	1.99579
C	-1.85765	-1.02317	-1.27574
C	-1.57748	-2.41923	-0.75565
C	-2.34645	-3.5195	-1.13036
C	-1.99378	-4.78749	-0.668
C	-0.88332	-4.92001	0.1666
C	-0.17063	-3.776	0.50614
C	2.0239	1.67196	-0.17804
C	2.03975	0.81751	-1.42425
C	2.69265	1.22252	-2.5879
C	2.77665	0.33686	-3.66246
C	2.2023	-0.92811	-3.53815
C	1.55452	-1.24979	-2.34934
Fe	0.42465	-0.67758	0.63266
H	-0.65624	1.13871	-1.77145
H	-3.09496	1.44996	-2.06271
H	-3.19942	2.2808	-0.51321
H	-1.62984	3.265	-2.95113
H	-3.13379	3.93092	-2.33016
H	-2.02017	4.58287	-0.20228
H	-1.13021	5.26279	-1.55662
H	0.43813	4.23679	0.077
H	0.50541	3.43546	-1.49482
H	-1.06582	2.4582	0.93579
H	-3.60279	0.24479	0.29719
H	-2.42062	0.79246	1.50831
H	-2.67627	-0.93561	1.24285
H	1.31774	3.13041	1.97139
H	1.89614	1.51601	2.43693
H	0.18262	1.92729	2.62911
H	-1.22632	-0.84629	-2.15352
H	-2.89985	-0.9555	-1.61371
H	-3.20949	-3.38321	-1.77447
H	-2.58036	-5.65653	-0.95009
H	-0.57702	-5.88691	0.55083
H	2.8454	1.33116	0.46387
H	2.23793	2.71723	-0.41859
H	3.13496	2.21221	-2.64697
H	3.28244	0.6291	-4.57759
H	2.24906	-1.65198	-4.34465
N	-1.53943	0.00885	-0.26058
N	0.77828	1.5327	0.63308
N	1.46481	-0.3983	-1.31007
N	-0.50257	-2.55034	0.05479
N	2.3153	-1.40913	1.41984
N	-0.31641	-0.82132	2.69087
C	3.34799	-1.7993	1.77494
C	-0.64483	-1.00398	3.78768
C	4.64631	-2.28864	2.22081
H	5.44653	-1.78182	1.67189
H	4.72022	-3.36554	2.03724
H	4.77213	-2.10119	3.29194
C	-1.06298	-1.22814	5.16582
H	-2.13339	-1.02459	5.27231
H	-0.50626	-0.56696	5.83778
H	-0.86908	-2.26725	5.4507
H	0.6967	-3.82701	1.15747
H	1.08848	-2.22144	-2.21476

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2525.46245
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2526.34898
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2527.14055
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas HF = -2527.46343

Compound G trans Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.562739 (Hartree/Particle)
Thermal correction to Energy= 0.592976
Thermal correction to Enthalpy= 0.593920
Thermal correction to Gibbs Free Energy= 0.501948
Sum of electronic and zero-point Energies= -2526.200429
Sum of electronic and thermal Energies= -2526.170192
Sum of electronic and thermal Enthalpies= -2526.169248
Sum of electronic and thermal Free Energies= -2526.261220

Fe	0.12717	0.54288	0.30642
N	1.27958	0.698	1.96419
N	0.74917	-1.41193	0.44761
N	-1.34191	0.38804	1.56464
C	1.88004	1.77781	2.49678
H	1.78131	2.70406	1.94042
C	2.71124	0.51135	4.35284
C	2.11387	-0.6189	3.79286
H	2.20424	-1.58952	4.27055
C	1.40424	-0.49521	2.60209
C	0.73201	-1.67098	1.91612
H	1.2402	-2.60789	2.17368
H	-0.30699	-1.76206	2.24382
C	2.1426	-1.68541	-0.01709
C	-0.27252	-2.19498	-0.36175
C	-0.56526	-1.39571	-1.6611
C	-2.54684	-0.05095	-0.96901
C	-2.16814	0.46811	2.37394
C	2.59829	1.73127	3.68764
C	-3.21827	0.56257	3.38154
H	-2.77966	0.7542	4.36623
H	-3.90282	1.38087	3.13498
H	-3.78745	-0.37194	3.42449
H	3.061	2.63214	4.07606
C	2.61212	1.4326	-1.3006
N	1.66905	1.00963	-0.77545
C	3.80426	1.94921	-1.963
H	3.87221	1.55565	-2.9826
H	3.76605	3.04246	-2.00874
H	4.70063	1.65025	-1.40965
C	-0.95706	2.38798	-1.53687
C	-0.65571	3.50219	0.48098
C	-1.42096	3.551	-2.1442
C	-1.10309	4.70335	-0.06083
H	-0.36266	3.43412	1.5234
H	-1.73596	3.53042	-3.18287
H	-1.15381	5.59147	0.5598
C	-1.48514	4.73073	-1.40126
N	-0.56604	2.36712	-0.23568

N	-1.08071	-0.02288	-1.25719
C	-0.86634	1.05776	-2.26243
H	0.12426	0.93079	-2.70726
H	-1.60035	1.01237	-3.07566
H	2.22232	-1.5562	-1.0955
H	2.44491	-2.7039	0.24142
H	2.82583	-0.98959	0.46871
H	-3.11965	-0.19561	-1.889
H	-2.84407	0.89821	-0.5242
H	-2.78824	-0.85247	-0.27227
C	0.11325	-3.66228	-0.63544
H	-1.18364	-2.19604	0.24725
H	1.09967	-3.71188	-1.10824
C	-0.88099	-4.35795	-1.5773
H	0.18845	-4.20166	0.31659
C	-0.97936	-3.59005	-2.89911
H	-1.87309	-4.42533	-1.10996
H	-0.548	-5.38624	-1.75049
C	-1.47654	-2.16003	-2.64129
H	-1.66922	-4.08942	-3.58679
H	0.00065	-3.57405	-3.39572
H	-2.49015	-2.23506	-2.2336
H	-1.55121	-1.59865	-3.58054
H	0.38848	-1.20799	-2.16681
H	-1.84251	5.6486	-1.85766
H	3.26729	0.4355	5.2821

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.48856
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.31900
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.13602
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.45182

Compound G trans Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.557537
(Hartree/Particle)
Thermal correction to Energy= 0.590630
Thermal correction to Enthalpy= 0.592561
Thermal correction to Gibbs Free Energy=
0.490628
Sum of electronic and zero-point Energies= -
2526.212913
Sum of electronic and thermal Energies= -
2526.179820
Sum of electronic and thermal Enthalpies= -
2526.161657
Sum of electronic and thermal Free Energies= -
2526.26359

Fe	0.31443	0.55046	0.09519
N	1.28582	0.71684	1.84544
N	0.76164	-1.41221	0.34794
N	-2.05369	0.22034	2.36303
C	1.8894	1.79156	2.38966
H	1.87405	2.70163	1.80043
C	2.53921	0.54708	4.32899
C	1.94011	-0.57694	3.75912
H	1.95948	-1.5356	4.26749
C	1.32168	-0.46066	2.51901
C	0.62777	-1.60995	1.82244
H	1.03888	-2.57565	2.14034
H	-0.43664	-1.5897	2.07641
C	2.16595	-1.72403	-0.05011
C	-0.26406	-2.19684	-0.46362
C	-0.56564	-1.40238	-1.75598
C	-2.43189	0.04348	-0.91307
C	-2.8043	0.21123	3.24798
C	2.51904	1.7519	3.62799
C	-3.76336	0.21026	4.34965
H	-3.39561	0.83241	5.17167
H	-4.72333	0.60895	4.0071
H	-3.91507	-0.80889	4.71823
H	2.98845	2.64519	4.02535
C	3.14805	1.5926	-1.60588
N	2.21255	1.1457	-1.08125
C	4.32143	2.14008	-2.27358
H	4.37379	1.77673	-3.30507
H	4.2705	3.23358	-2.28141
H	5.23033	1.83781	-1.74343
C	-0.84131	2.3916	-1.667
C	-0.45518	3.49851	0.34337
C	-1.34057	3.54862	-2.25004
C	-0.94133	4.6954	-0.17559
H	-0.12518	3.42946	1.37336
H	-1.70398	3.52884	-3.27257
H	-0.98	5.57877	0.45251
C	-1.37998	4.72548	-1.49747
N	-0.38186	2.36955	-0.38416
N	-0.99832	-0.00686	-1.34044
C	-0.77656	1.05183	-2.37015
H	0.21653	0.90312	-2.80807
H	-1.51372	0.99313	-3.17994
H	2.29096	-1.59408	-1.12537
H	2.4328	-2.74921	0.22208
H	2.84213	-1.03865	0.45979
H	-3.09185	-0.06124	-1.7792
H	-2.63273	0.9952	-0.42346
H	-2.64566	-0.74766	-0.19685
C	0.11306	-3.66158	-0.74889
H	-1.17173	-2.20079	0.15122
H	1.07881	-3.70935	-1.26453
C	-0.93149	-4.34813	-1.64403
H	0.22685	-4.20421	0.19718
C	-1.10037	-3.57945	-2.95913
H	-1.89638	-4.41301	-1.12257
H	-0.61309	-5.37739	-1.83767
C	-1.55005	-2.13557	-2.68483
H	-1.84225	-4.06905	-3.59792
H	-0.15465	-3.58449	-3.51858
H	-2.54237	-2.17313	-2.22152
H	-1.6561	-1.57729	-3.62262
H	0.37682	-1.26243	-2.30079
H	-1.76687	5.64134	-1.93214
H	3.02671	0.47771	5.29601

UPBEPBE/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.45407
UM06/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.30837
UM06L/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.10698
UB3LYP-D3/6-311+G(d,p)-
CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.43799

Compound G trans Quintet

UB3LYP/6-31G(d)-gas

Zero-point correction= 0.557537 (Hartree/Particle)
Thermal correction to Energy= 0.590630
Thermal correction to Enthalpy= 0.591574
Thermal correction to Gibbs Free Energy= 0.487524
Sum of electronic and zero-point Energies= -2526.212913
Sum of electronic and thermal Energies= -2526.179820
Sum of electronic and thermal Enthalpies= -2526.178876
Sum of electronic and thermal Free Energies= -2526.282926

Fe	0.16943	0.70235	0.39302
N	1.42211	0.51104	2.17718
N	0.77354	-1.47086	0.40477
N	-1.4636	0.68007	1.90416
C	2.04093	1.49676	2.85433
H	1.97081	2.49382	2.42788
C	2.81292	-0.02939	4.52795
C	2.18534	-1.05611	3.82283
H	2.23624	-2.08262	4.17226
C	1.49288	-0.7524	2.65198
C	0.75665	-1.81003	1.8493
H	1.19599	-2.79714	2.04392
H	-0.28789	-1.84951	2.18004
C	2.15659	-1.66558	-0.1069
C	-0.25747	-2.23949	-0.38848
C	-0.62966	-1.43802	-1.66074
C	-2.58004	-0.09678	-0.86384
C	-2.23785	0.84159	2.75251
C	2.74198	1.27394	4.03386
C	-3.21774	1.03828	3.81376
H	-2.71257	1.30978	4.74616
H	-3.91	1.84048	3.53826
H	-3.78839	0.1176	3.97299
H	3.22507	2.09964	4.54502
C	2.88075	1.81432	-1.2796
N	1.94978	1.32883	-0.7868
C	4.05395	2.41428	-1.90317
H	4.27206	1.91346	-2.85201
H	3.87572	3.47726	-2.09444
H	4.92082	2.31281	-1.24219
C	-1.11348	2.33981	-1.762
C	-0.768	3.73539	0.06347
C	-1.62875	3.39758	-2.50932
C	-1.25926	4.84069	-0.62157
H	-0.42974	3.82312	1.09243
H	-1.97632	3.22662	-3.52342
H	-1.3043	5.80832	-0.13362
C	-1.69645	4.667	-1.93554
N	-0.68772	2.51079	-0.49073
N	-1.14701	-0.07529	-1.26219
C	-0.97371	0.93939	-2.33117
H	0.03089	0.82274	-2.75445
H	-1.68994	0.79787	-3.15113
H	2.1923	-1.48254	-1.18123
H	2.52374	-2.67765	0.09436
H	2.82383	-0.95384	0.38013
H	-3.23634	-0.2702	-1.72324
H	-2.8442	0.86258	-0.4178
H	-2.75597	-0.87533	-0.12079
C	0.15535	-3.69179	-0.70993
H	-1.14614	-2.28013	0.25284
H	1.11329	-3.69731	-1.24195
C	-0.86999	-4.41298	-1.59576
H	0.30965	-4.24213	0.22607
C	-1.07616	-3.63568	-2.89852
H	-1.82808	-4.51654	-1.06753
H	-0.51607	-5.42842	-1.80123
C	-1.58166	-2.21946	-2.59123
H	-1.80069	-4.14356	-3.54329
H	-0.13307	-3.59296	-3.461
H	-2.56652	-2.31454	-2.12051
H	-1.72775	-1.65334	-3.51906
H	0.29632	-1.24545	-2.21589
H	-2.09423	5.50408	-2.50114
H	3.35787	-0.24521	5.4419

UPBEPBE/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2525.45981
UM06/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2526.34480
UM06L/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = --2527.13737
UB3LYP-D3/6-311+G(d,p)-CPCM(dichloromethane)//UB3LYP/6-31G(d)-gas
HF = -2527.45962

Compound 1-OH_2Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.563301 (Hartree/Particle)
Thermal correction to Energy= 0.596694
Thermal correction to Enthalpy= 0.597638
Thermal correction to Gibbs Free Energy= 0.500938
Sum of electronic and zero-point Energies= -2869.593880
Sum of electronic and thermal Energies= -2869.560488
Sum of electronic and thermal Enthalpies= -2869.559543
Sum of electronic and thermal Free Energies= -2869.656244

C	0.87619	3.95814	-0.84438
C	0.03502	5.03482	-1.07827
C	-1.19115	4.80048	-1.7048
C	-1.52397	3.49493	-2.05195
C	-0.63029	2.45899	-1.77644
C	-0.9895	1.02456	-2.07593
C	-0.19823	-1.16181	-1.15177
C	0.07785	-2.34505	-1.87935
C	-0.15768	-3.57672	-1.3216
C	-0.66367	-3.68693	-0.00198
C	-0.87984	-4.95601	0.59782
C	-1.34221	-5.05457	1.88975
C	-1.60249	-3.88053	2.63412
C	-1.41686	-2.6334	2.07634
C	-0.95243	-2.49095	0.73846
C	-0.73557	-1.20132	0.12796
C	-1.09843	0.0442	0.88275
C	-2.48587	0.33128	1.15718
C	-3.54534	-0.47568	0.65495
C	-4.86169	-0.16712	0.92515
C	-5.19609	0.95762	1.71475
C	-4.19924	1.76809	2.20669
C	-2.8338	1.48732	1.93487
C	-1.80234	2.33418	2.41279
C	-0.48866	2.07097	2.11549
C	-0.13952	0.93727	1.34176
C	1.93773	-0.44413	1.54834
C	2.87548	-1.05596	0.53687
C	3.67251	-2.1527	0.86756

C	4.47956	-2.73414	-0.10524
C	4.46158	-2.20161	-1.39641
C	3.6514	-1.10571	-1.64989
Fe	1.74384	1.09522	-0.96306
H	1.82574	4.10588	-0.34099
H	0.33459	6.032	-0.77451
H	-1.87535	5.61777	-1.91016
H	-2.47476	3.27138	-2.52622
H	0.54781	-0.1532	-2.70451
H	0.46185	-2.27386	-2.89502
H	0.04159	-4.48049	-1.89051
H	-0.66972	-5.84969	0.01648
H	-1.50536	-6.02829	2.34095
H	-1.9592	-3.96252	3.6565
H	-1.63555	-1.74973	2.66486
H	-3.31566	-1.35013	0.05684
H	-5.65201	-0.79936	0.53154
H	-6.23742	1.17852	1.92733
H	-4.44227	2.63873	2.80971
H	-2.06272	3.19628	3.02034
H	0.29462	2.72608	2.49184
H	1.74703	1.57954	1.44132
H	3.64919	-2.54757	1.87871
H	5.10433	-3.58879	0.13456
H	5.06196	-2.62714	-2.19316
H	3.60021	-0.68246	-2.64743
H	-1.84143	0.73312	-1.45827
H	-1.30748	0.91513	-3.11937
H	3.73309	3.03284	-0.52401
H	4.22205	1.64431	-0.03453
H	1.96304	2.26337	-3.38786
H	3.2304	1.36994	-3.33522
H	1.17185	-1.17503	1.8149
H	2.47212	-0.20006	2.4739
N	0.573	2.68582	-1.19424
N	0.1601	0.10155	-1.79615
N	1.27578	0.78765	1.00424
N	2.87472	-0.51966	-0.70847
O	3.42117	2.16495	-0.21808
O	2.33638	1.4694	-2.96785

Compound 1-OH_2Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.561344 (Hartree/Particle)
Thermal correction to Energy= 0.595777
Thermal correction to Enthalpy= 0.596721
Thermal correction to Gibbs Free Energy= 0.495108
Sum of electronic and zero-point Energies= -2869.599159
Sum of electronic and thermal Energies= -2869.564727
Sum of electronic and thermal Enthalpies= -2869.563783
Sum of electronic and thermal Free Energies= -2869.665396

C	0.91984	4.02589	-0.45647
C	0.14401	5.13883	-0.73884
C	-1.01792	4.96853	-1.49616
C	-1.35828	3.68929	-1.92531
C	-0.53531	2.61151	-1.59791
C	-0.89529	1.196	-1.97896
C	-0.13693	-1.0331	-1.10513
C	0.13133	-2.18326	-1.88815
C	-0.11612	-3.43864	-1.39308
C	-0.63296	-3.61003	-0.08407
C	-0.86871	-4.90489	0.44932
C	-1.35234	-5.06259	1.7277
C	-1.61756	-3.92419	2.52369
C	-1.41052	-2.65307	2.03114
C	-0.91815	-2.4495	0.71126
C	-0.67579	-1.13194	0.17285
C	-1.06792	0.06584	0.99529
C	-2.47378	0.35139	1.16662
C	-3.48759	-0.39814	0.50603
C	-4.82182	-0.09443	0.6776
C	-5.22174	0.96776	1.52083
C	-4.2695	1.71921	2.17012
C	-2.88684	1.44021	2.00559
C	-1.89937	2.22168	2.65678
C	-0.56624	1.95636	2.47342
C	-0.14985	0.88743	1.64079
C	1.92725	-0.53817	1.85153
C	2.89125	-1.0322	0.79804
C	3.74993	-2.1048	1.03891
C	4.58954	-2.55274	0.02299
C	4.54493	-1.91592	-1.21987
C	3.67021	-0.85348	-1.39151
Fe	1.70752	1.17906	-0.60047
H	1.82355	4.11342	0.13976
H	0.44278	6.11472	-0.37186
H	-1.64844	5.81739	-1.74153
H	-2.25974	3.51967	-2.50607
H	0.69559	0.06402	-2.58809
H	0.51839	-2.06007	-2.89608
H	0.07869	-4.31531	-2.0045
H	-0.65802	-5.77092	-0.17229
H	-1.53065	-6.05574	2.12793
H	-1.99586	-4.05285	3.53344
H	-1.63522	-1.79667	2.65679
H	-3.20951	-1.22792	-0.13378
H	-5.57576	-0.68426	0.16477
H	-6.27683	1.18603	1.65286
H	-4.56166	2.53981	2.81974
H	-2.20932	3.03261	3.30982
H	0.18155	2.55702	2.98764
H	1.72346	1.49078	1.99673
H	3.75569	-2.58041	2.01483
H	5.26526	-3.38461	0.19552
H	5.17692	-2.23643	-2.04109
H	3.58187	-0.33872	-2.34449
H	-1.77722	0.88405	-1.41425
H	-1.16013	1.13754	-3.04109
H	3.49034	3.14613	-1.31759
H	4.32237	1.87326	-0.92855
H	1.67775	0.90044	-4.85854
H	2.03725	-0.5782	-4.69815
H	1.14629	-1.2857	2.00961
H	2.44214	-0.41115	2.81034
N	0.60384	2.77963	-0.88318
N	0.23227	0.25445	-1.68914
N	1.29171	0.75354	1.43984
N	2.86019	-0.40682	-0.40208
O	3.43305	2.26652	-0.90803
O	1.8221	0.21692	-4.18382

Compound 1-OH_2 Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.560540 (Hartree/Particle)
Thermal correction to Energy= 0.595269
Thermal correction to Enthalpy= 0.596213
Thermal correction to Gibbs Free Energy= 0.491061

Sum of electronic and zero-point Energies= -2869.623226
Sum of electronic and thermal Energies= -2869.588498
Sum of electronic and thermal Enthalpies= -2869.587553
Sum of electronic and thermal Free Energies= -2869.692705

C	0.65736	4.0392	-1.05599
C	-0.13887	5.12411	-1.38956
C	-1.37194	4.87996	-2.0013
C	-1.75653	3.5646	-2.24093
C	-0.90513	2.52286	-1.86503
C	-1.3327	1.08038	-2.0367
C	-0.48639	-1.15015	-1.21535
C	-0.22257	-2.30735	-1.99054
C	-0.3936	-3.55907	-1.45642
C	-0.82923	-3.71967	-0.11693
C	-0.99456	-5.0103	0.45142
C	-1.4015	-5.15755	1.75752
C	-1.6573	-4.01241	2.54675
C	-1.5157	-2.7452	2.02185
C	-1.10378	-2.55285	0.67298
C	-0.93177	-1.23872	0.09964
C	-1.28831	-0.03477	0.92969
C	-2.68189	0.24662	1.18204
C	-3.72932	-0.5246	0.60414
C	-5.05195	-0.22509	0.85396
C	-5.40476	0.85525	1.69548
C	-4.41922	1.62781	2.26554
C	-3.04773	1.35249	2.0212
C	-2.02642	2.15283	2.5924
C	-0.70515	1.88466	2.33947
C	-0.33581	0.79719	1.50854
C	1.73741	-0.61543	1.72623
C	2.87604	-1.0473	0.82652
C	3.77889	-2.0233	1.25068
C	4.76211	-2.47022	0.37284
C	4.82158	-1.922	-0.91036
C	3.90166	-0.94338	-1.2554
Fe	1.5012	1.02041	-0.84716
H	1.62579	4.18198	-0.58423
H	0.19783	6.13324	-1.17811
H	-2.02132	5.7025	-2.28484
H	-2.70957	3.34102	-2.71068
H	0.16377	-0.08527	-2.78032
H	0.10119	-2.19836	-3.02374
H	-0.20175	-4.44052	-2.06162
H	-0.79245	-5.88125	-0.16601
H	-1.52731	-6.14764	2.18436
H	-1.97659	-4.13278	3.5777
H	-1.73101	-1.88414	2.64446
H	-3.48513	-1.36673	-0.0335
H	-5.83291	-0.83135	0.40472
H	-6.45096	1.07066	1.88889
H	-4.67601	2.46196	2.91279
H	-2.30066	2.97984	3.24114
H	0.06958	2.49838	2.79492
H	1.55601	1.41281	1.72336
H	3.70239	-2.43014	2.25442
H	5.46995	-3.23273	0.68316
H	5.5677	-2.24305	-1.62889
H	3.92536	-0.47886	-2.23459
H	-2.10176	0.8495	-1.29683
H	-1.78729	0.93157	-3.02265
H	6.25333	2.13532	-1.46735
H	6.05704	1.95936	-2.98973
H	3.99793	1.96934	-1.9413
H	2.75582	2.84018	-2.41577
H	0.9835	-1.40499	1.74512
H	2.08921	-0.48824	2.75625
N	0.29394	2.75761	-1.29268
N	-0.19178	0.1348	-1.84936
N	1.09343	0.64123	1.24127
N	2.94459	-0.50246	-0.40792
O	5.63347	1.79401	-2.13176
O	3.00054	2.0642	-1.8879

Compound 2-OH_2 Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.619524 (Hartree/Particle)
Thermal correction to Energy= 0.655846
Thermal correction to Enthalpy= 0.656790
Thermal correction to Gibbs Free Energy= 0.553759
Sum of electronic and zero-point Energies= -2948.165605
Sum of electronic and thermal Energies= -2948.129284
Sum of electronic and thermal Enthalpies= -2948.128339
Sum of electronic and thermal Free Energies= -2948.23
1370

C	0.7806	4.1243	-0.7727
C	-0.2019	5.1125	-0.9633
C	-1.4395	4.7834	-1.5393
C	-1.6662	3.4528	-1.9086
C	-0.6611	2.4959	-1.6933
C	-0.9475	1.0619	-2.081
C	-0.1333	-1.1381	-1.1659
C	0.1613	-2.3256	-1.8984
C	-0.0805	-3.5699	-1.3447
C	-0.6062	-3.6833	-0.0221
C	-0.8259	-4.9642	0.5736
C	-1.3086	-5.0686	1.8702
C	-1.5864	-3.8871	2.6194
C	-1.3977	-2.6291	2.0598
C	-0.913	-2.4834	0.7197
C	-0.6961	-1.1851	0.1114
C	-1.0769	0.0649	0.8569
C	-2.473	0.3453	1.1309
C	-3.5313	-0.4829	0.6348
C	-4.861	-0.183	0.9051
C	-5.2073	0.9557	1.6911
C	-4.2081	1.7866	2.1773
C	-2.8325	1.5122	1.9009
C	-1.8022	2.3809	2.3724
C	-0.477	2.1254	2.069
C	-0.1185	0.9782	1.3016
C	1.9628	-0.4214	1.5228
C	2.8346	-1.1235	0.505
C	3.5127	-2.2865	0.9048
C	4.3062	-2.9727	-0.0215
C	4.3942	-2.4649	-1.3276
C	3.7051	-1.2916	-1.684
Fe	1.8092	1.1424	-0.9918
H	0.0089	6.1325	-0.6607
H	-2.6105	3.149	-2.3501
H	0.6412	-0.0857	-2.7156
H	0.5554	-2.2493	-2.9109
H	0.1255	-4.4729	-1.9135
H	-0.6068	-5.8579	-0.0052
H	-1.476	-6.0432	2.3191
H	-1.9575	-3.9759	3.6366
H	-1.6311	-1.7473	2.6467

H	-3.2951	-1.3635	0.047
H	-5.6486	-0.8255	0.5216
H	-6.2512	1.1661	1.9044
H	-4.4607	2.6594	2.7741
H	-2.0703	3.2448	2.975
H	0.3025	2.7898	2.4395
H	1.8006	1.6271	1.3765
H	3.4071	-2.6457	1.924
H	4.9955	-2.972	-2.0744
H	-1.8207	0.7108	-1.5262
H	-1.2182	1.0137	-3.1444
H	3.9355	2.892	-0.3292
H	4.3491	1.3338	-0.1953
H	1.8893	2.6052	-3.2208
H	3.064	1.5282	-3.499
H	1.1889	-1.1124	1.8647
H	2.5606	-0.1655	2.408
N	0.5568	2.8109	-1.1416
N	0.2115	0.1393	-1.8144
N	1.3106	0.8212	0.979
N	2.9256	-0.612	-0.7667
O	3.6151	1.9736	-0.2676
O	2.2819	1.7498	-2.9612
H	-2.2006	5.5425	-1.6908
H	4.8379	-3.8764	0.2598
C	3.8416	-0.7817	-3.1016
H	2.8676	-0.5996	-3.5677
H	4.4478	0.1365	-3.1393
H	4.3631	-1.5188	-3.7171
C	2.1006	4.5331	-0.1574
H	2.3629	3.9083	0.703
H	2.9131	4.5019	-0.8995
H	2.0467	5.5657	0.1959

Compound 2-OH_2 Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.616228 (Hartree/Particle)
Thermal correction to Energy= 0.654452
Thermal correction to Enthalpy= 0.655396
Thermal correction to Gibbs Free Energy= 0.545888
Sum of electronic and zero-point Energies= -2948.177430
Sum of electronic and thermal Energies= -2948.139206
Sum of electronic and thermal Enthalpies= -2948.138262
Sum of electronic and thermal Free Energies= -2948.247770

C	1.0202	4.0335	-0.2272
C	0.2613	5.1673	-0.5195
C	-0.8634	5.0629	-1.3335
C	-1.2173	3.8102	-1.8247
C	-0.4279	2.7082	-1.5074
C	-0.8338	1.3276	-1.9628
C	-0.1004	-0.9572	-1.1824
C	0.2273	-2.0992	-1.959
C	0.004	-3.363	-1.475
C	-0.5452	-3.5567	-0.182
C	-0.759	-4.8611	0.3371
C	-1.271	-5.041	1.6019
C	-1.5861	-3.9149	2.3971
C	-1.4005	-2.6349	1.9172
C	-0.8822	-2.4086	0.6106
C	-0.6627	-1.0801	0.0845
C	-1.0899	0.0954	0.921
C	-2.5011	0.3498	1.0923
C	-3.4964	-0.4009	0.4052
C	-4.837	-0.1265	0.5762
C	-5.2614	0.9062	1.4449
C	-4.3275	1.6577	2.1207
C	-2.9386	1.4082	1.9581
C	-1.9696	2.1873	2.6394
C	-0.6303	1.9525	2.4543
C	-0.1915	0.9202	1.5884
C	1.8915	-0.4586	1.8861
C	2.979	-0.933	0.9536
C	3.8868	-1.8928	1.3874
C	4.7993	-2.423	0.4797
C	4.7495	-1.9876	-0.8397
C	3.8295	-1.0096	-1.2238
Fe	1.7858	1.1483	-0.5827
H	0.5547	6.1238	-0.0994
H	-2.0979	3.6806	-2.4458
H	0.627	0.147	-2.7013
H	0.6501	-1.9602	-2.9505
H	0.2445	-4.2309	-2.0828
H	-0.5084	-5.7168	-0.2841
H	-1.4327	-6.0411	1.9916
H	-1.9859	-4.0595	3.3963
H	-1.6631	-1.7904	2.544
H	-3.1976	-1.2062	-0.2564
H	-5.5773	-0.7152	0.0426
H	-6.3212	1.1018	1.5751
H	-4.6392	2.4553	2.7896
H	-2.2983	2.971	3.316
H	0.103	2.5474	2.995
H	1.6705	1.5698	1.9275
H	3.8657	-2.2271	2.4198
H	5.4199	-2.4024	-1.5856
H	-1.7207	1.0148	-1.4065
H	-1.1044	1.3445	-3.0237
H	3.2408	3.0966	-1.866
H	4.2051	1.864	-1.7409
H	0.1049	-0.4696	-5.1458
H	1.2015	0.5806	-5.3488
H	1.1214	-1.2315	1.9468
H	2.2809	-0.3171	2.9001
N	0.6934	2.8146	-0.7461
N	0.2619	0.3337	-1.7603
N	1.2572	0.8037	1.3954
N	2.9689	-0.4554	-0.3235
O	3.3309	2.2044	-1.4913
O	0.6985	0.1228	-4.6565
H	-1.4573	5.9399	-1.5715
H	5.5203	-3.1726	0.7905
C	2.1815	4.145	0.7316
H	1.8184	4.1015	1.7666
H	2.9274	3.3595	0.5968
H	2.6866	5.1093	0.6244
C	3.785	-0.5853	-2.672
H	2.8782	-0.0385	-2.9283
H	4.6563	0.0253	-2.9462
H	3.8302	-1.47	-3.3145

Compound 2-OH_2 Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.615703 (Hartree/Particle)
Thermal correction to Energy= 0.653855
Thermal correction to Enthalpy= 0.654799
Thermal correction to Gibbs Free Energy= 0.543147
Sum of electronic and zero-point Energies= -2948.205744

Sum of electronic and thermal Energies= -2948.167592
Sum of electronic and thermal Enthalpies= -2948.166648
Sum of electronic and thermal Free Energies= -2948.278300

C	0.4648	4.1325	-0.769
C	-0.4103	5.1679	-1.1505
C	-1.5478	4.8748	-1.919
C	-1.8035	3.5395	-2.2712
C	-0.9054	2.5419	-1.863
C	-1.2356	1.0851	-2.147
C	-0.3405	-1.1247	-1.2558
C	-0.0748	-2.3047	-2.0134
C	-0.2304	-3.5561	-1.4466
C	-0.6524	-3.6878	-0.0891
C	-0.8033	-4.9759	0.5119
C	-1.2082	-5.0976	1.8335
C	-1.4777	-3.9266	2.6015
C	-1.3478	-2.662	2.0398
C	-0.9355	-2.4987	0.6778
C	-0.7796	-1.1893	0.0717
C	-1.1632	0.0288	0.8766
C	-2.5722	0.2956	1.1006
C	-3.6016	-0.5054	0.5084
C	-4.9444	-0.2215	0.7271
C	-5.3338	0.8741	1.5528
C	-4.3626	1.6728	2.1396
C	-2.9742	1.4099	1.9245
C	-1.9708	2.2333	2.5191
C	-0.631	1.978	2.2931
C	-0.2275	0.8841	1.4698
C	1.889	-0.5125	1.7134
C	2.8968	-1.0695	0.7203
C	3.7904	-2.0687	1.1351
C	4.6436	-2.6559	0.1869
C	4.5623	-2.2383	-1.1514
C	3.6524	-1.2283	-1.5181
Fe	1.5659	1.1055	-0.876
H	-0.1981	6.1862	-0.8403
H	-2.6872	3.2746	-2.8437
H	0.3421	-0.0597	-2.8432
H	0.2271	-2.2141	-3.0558
H	-0.0428	-4.4512	-2.034
H	-0.598	-5.8616	-0.0841
H	-1.3253	-6.0779	2.2859
H	-1.7976	-4.0289	3.6348
H	-1.5787	-1.7886	2.6407
H	-3.3335	-1.357	-0.1082
H	-5.7096	-0.845	0.2731
H	-6.3877	1.0745	1.721
H	-4.6476	2.5089	2.7733
H	-2.2712	3.0578	3.1604
H	0.128	2.6002	2.7651
H	1.6775	1.546	1.6865
H	3.808	-2.3866	2.1731
H	5.1883	-2.6935	-1.9121
H	-2.0496	0.7789	-1.4846
H	-1.6107	0.9806	-3.1728
H	6.1992	2.1448	-1.0424
H	6.1267	1.9403	-2.6388
H	4.1039	2.0804	-1.7609
H	2.8358	3.0572	-2.1752
H	1.1183	-1.2687	1.8855
H	2.3745	-0.3344	2.6811
N	0.2279	2.8345	-1.1528
N	-0.0704	0.158	-1.9316
N	1.222	0.7481	1.2344
N	2.8519	-0.6314	-0.5752
O	5.6136	2.0174	-1.8123
O	3.0835	2.2117	-1.7564
H	-2.2248	5.666	-2.2264
H	5.3462	-3.4297	0.4816
C	1.6579	4.4484	0.1086
H	2.2717	5.2485	-0.3237
H	1.3166	4.8132	1.0859
H	2.2983	3.5775	0.2695
C	3.5004	-0.8389	-2.9713
H	2.8275	-1.5457	-3.4773
H	3.0991	0.1702	-3.0927
H	4.4605	-0.8929	-3.4949

Compound 3-OH_2 Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.618020 (Hartree/Particle)
Thermal correction to Energy= 0.655326
Thermal correction to Enthalpy= 0.656270
Thermal correction to Gibbs Free Energy= 0.548991
Sum of electronic and zero-point Energies= -2948.186624
Sum of electronic and thermal Energies= -2948.149318
Sum of electronic and thermal Enthalpies= -2948.148373
Sum of electronic and thermal Free Energies= -2948.255653

C	0.74452	3.88247	-0.79206
C	-0.09488	4.95392	-1.03538
C	-1.33509	4.74092	-1.6629
C	-1.64767	3.41893	-1.99204
C	-0.75863	2.3829	-1.70909
C	-1.12578	0.9482	-2.00022
C	-0.33569	-1.24165	-1.08221
C	-0.06336	-2.42431	-1.81274
C	-0.30201	-3.65708	-1.25856
C	-0.80761	-3.76958	0.06123
C	-1.02785	-5.03988	0.6575
C	-1.48912	-5.14089	1.94985
C	-1.744	-3.96792	2.69824
C	-1.55453	-2.71976	2.1437
C	-1.0915	-2.57471	0.80531
C	-0.87177	-1.28366	0.1983
C	-1.2291	-0.03956	0.95845
C	-2.61514	0.24982	1.23851
C	-3.67829	-0.55333	0.73718
C	-4.99328	-0.24364	1.01346
C	-5.32279	0.8788	1.80882
C	-4.32236	1.6858	2.29974
C	-2.95825	1.40376	2.02142
C	-1.92333	2.2475	2.49795
C	-0.61127	1.98262	2.19468
C	-0.26625	0.85012	1.41678
C	1.80851	-0.53703	1.61575
C	2.75321	-1.14002	0.60451
C	3.55641	-2.22971	0.93694
C	4.38348	-2.82797	-0.01821
C	4.34766	-2.27734	-1.31147
C	3.53441	-1.18971	-1.57219
Fe	1.61195	1.01066	-0.89245
H	1.6932	4.03925	-0.28926
H	0.21191	5.95137	-0.73599
H	-2.5981	3.18637	-2.46433
H	0.41164	-0.22942	-2.63373
H	0.32079	-2.35111	-2.82821
H	-0.10602	-4.55982	-1.8303

H	-0.82206	-5.93257	0.073
H	-1.65571	-6.11538	2.39822
H	-2.09959	-4.05168	3.7209
H	-1.76885	-1.83706	2.73526
H	-3.45238	-1.42578	0.13471
H	-5.78622	-0.87306	0.62052
H	-6.36293	1.10037	2.02664
H	-4.56148	2.55443	2.9073
H	-2.1798	3.10807	3.10941
H	0.17481	2.63544	2.56909
H	1.62413	1.48873	1.50859
H	3.52593	-2.61971	1.95058
H	4.94913	-2.69846	-2.11114
H	3.4849	-0.77494	-2.57368
H	-1.97358	0.66169	-1.37487
H	-1.45181	0.83526	-3.04078
H	3.5845	2.94623	-0.44709
H	4.08853	1.54652	-0.01394
H	1.85315	2.2039	-3.29092
H	3.09249	1.26337	-3.26748
H	1.042	-1.27046	1.8727
H	2.33704	-0.29833	2.54603
N	0.44561	2.60419	-1.12882
N	0.02265	0.02169	-1.72492
N	1.14702	0.6975	1.07668
N	2.74787	-0.60083	-0.6388
O	3.28227	2.07791	-0.13226
O	2.20219	1.38552	-2.89745
C	-2.27177	5.88034	-1.95364
H	-2.51781	6.42489	-1.03474
H	-1.80562	6.60084	-2.63627
H	-3.20359	5.53478	-2.40738
C	5.27029	-3.99597	0.31266
H	5.16956	-4.79035	-0.43455
H	6.32372	-3.68882	0.31345
H	5.04141	-4.4136	1.29604

Compound 3-OH_2 Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.616062 (Hartree/Particle)
Thermal correction to Energy= 0.654448
Thermal correction to Enthalpy= 0.655392
Thermal correction to Gibbs Free Energy= 0.542968
Sum of electronic and zero-point Energies= -2948.191881
Sum of electronic and thermal Energies= -2948.153496
Sum of electronic and thermal Enthalpies= -2948.152551
Sum of electronic and thermal Free Energies= -2948.264975

C	0.9098	4.076	-0.4397
C	0.0953	5.1725	-0.7134
C	-1.0912	4.9999	-1.4732
C	-1.3874	3.6912	-1.9051
C	-0.5338	2.6207	-1.5926
C	-0.8601	1.1985	-1.9989
C	-0.0658	-1.032	-1.0991
C	0.2451	-2.1997	-1.8587
C	0.0023	-3.4611	-1.3469
C	-0.551	-3.6183	-0.0404
C	-0.7865	-4.9175	0.5076
C	-1.3056	-5.0634	1.786
C	-1.6069	-3.9063	2.5634
C	-1.3989	-2.6314	2.0509
C	-0.8719	-2.4427	0.7321
C	-0.6322	-1.1232	0.1777
C	-1.0455	0.0846	0.9815
C	-2.461	0.3706	1.1313
C	-3.4677	-0.3998	0.4641
C	-4.8164	-0.0992	0.6135
C	-5.2355	0.9839	1.441
C	-4.2866	1.7556	2.0965
C	-2.8923	1.4761	1.9519
C	-1.9113	2.2768	2.6117
C	-0.5649	2.0086	2.4504
C	-0.1316	0.9201	1.6341
C	1.9605	-0.5266	1.8718
C	2.8933	-1.0471	0.7953
C	3.7133	-2.1651	1.0144
C	4.5536	-2.6542	-0.0074
C	4.5187	-1.9707	-1.2498
C	3.6863	-0.8631	-1.4118
Fe	1.7426	1.2185	-0.5934
H	1.8097	4.1878	0.1577
H	0.3738	6.1528	-0.3385
H	-2.29	3.4995	-2.4787
H	0.7706	0.0847	-2.6131
H	0.6635	-2.0878	-2.8555
H	0.2261	-4.3456	-1.938
H	-0.5528	-5.7923	-0.0942
H	-1.4861	-6.0518	2.1983
H	-2.0118	-4.027	3.5643
H	-1.6529	-1.7685	2.6574
H	-3.1779	-1.2415	-0.1562
H	-5.5638	-0.7005	0.1032
H	-6.2942	1.1963	1.5564
H	-4.5938	2.5828	2.7315
H	-2.2344	3.0949	3.2502
H	0.1754	2.6173	2.9677
H	1.7666	1.5349	2.0003
H	3.6922	-2.6578	1.9828
H	5.1339	-2.3035	-2.0803
H	3.6253	-0.3378	-2.3602
H	-1.7473	0.8627	-1.4558
H	-1.1055	1.154	-3.0677
H	3.5804	3.1941	-1.1697
H	4.373	1.8803	-0.655
H	1.6779	0.9577	-4.8366
H	1.5975	-0.6364	-4.8713
H	1.176	-1.2632	2.0636
H	2.508	-0.3986	2.8145
N	0.6162	2.8139	-0.8795
N	0.2884	0.2602	-1.7104
N	1.3246	0.7799	1.4689
N	2.8892	-0.3939	-0.4037
O	3.4996	2.2939	-0.8
O	1.5606	0.1525	-4.2945
C	-1.9892	6.1704	-1.7922
H	-2.3236	6.6689	-0.8734
H	-1.4539	6.9233	-2.3855
H	-2.8761	5.8652	-2.3545
C	5.4601	-3.8422	0.2078
H	5.4394	-4.5209	-0.6526
H	6.5016	-3.5143	0.3322
H	5.1835	-4.4104	1.1008

Compound 3-OH_2 Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.615413 (Hartree/Particle)
Thermal correction to Energy= 0.653190
Thermal correction to Enthalpy= 0.654134

Thermal correction to Gibbs Free Energy= 0.542178
Sum of electronic and zero-point Energies= -2948.217223
Sum of electronic and thermal Energies= -2948.179446
Sum of electronic and thermal Enthalpies= -2948.178502
Sum of electronic and thermal Free Energies= -2948.290458

C	1.1136	3.9643	-0.9248
C	0.4559	5.1537	-1.1788
C	-0.8504	5.1278	-1.7004
C	-1.4138	3.8687	-1.931
C	-0.6983	2.7072	-1.6442
C	-1.3309	1.3421	-1.8266
C	-0.6819	-1.0627	-1.3483
C	-0.4534	-2.121	-2.2648
C	-0.6723	-3.4249	-1.8982
C	-1.1198	-3.7429	-0.5915
C	-1.3285	-5.09	-0.1933
C	-1.7458	-5.3897	1.0827
C	-1.9667	-4.3469	2.0126
C	-1.7825	-3.0287	1.6546
C	-1.362	-2.6785	0.3409
C	-1.1496	-1.3084	-0.0613
C	-1.4762	-0.2058	0.9048
C	-2.8607	0.0627	1.2157
C	-3.9308	-0.6322	0.5849
C	-5.2429	-0.348	0.8972
C	-5.563	0.6418	1.8554
C	-4.5556	1.3441	2.4754
C	-3.1938	1.0834	2.1691
C	-2.1503	1.8206	2.7833
C	-0.8394	1.5731	2.4645
C	-0.5014	0.5667	1.5242
C	1.5751	-0.8505	1.6128
C	2.9985	-0.8583	1.1028
C	4.0056	-1.5447	1.7732
C	5.3097	-1.5701	1.2638
C	5.5337	-0.8683	0.0682
C	4.4895	-0.1977	-0.5455
Fe	1.538	0.8794	-0.8268
H	2.1243	3.9645	-0.5245
H	0.9535	6.0968	-0.9753
H	-2.4199	3.7887	-2.3332
H	0.0474	0.165	-2.7531
H	-0.1199	-1.8904	-3.2747
H	-0.5079	-4.227	-2.6122
H	-1.1507	-5.8808	-0.917
H	-1.9048	-6.4216	1.3795
H	-2.2909	-4.5883	3.0205
H	-1.9662	-2.2479	2.3838
H	-3.7123	-1.4002	-0.148
H	-6.0415	-0.8944	0.4043
H	-6.6018	0.8455	2.096
H	-4.787	2.1116	3.2089
H	-2.3992	2.5852	3.5137
H	-0.0477	2.1416	2.9486
H	1.3915	1.1634	1.7432
H	3.7718	-2.0615	2.6993
H	6.5218	-0.8393	-0.3803
H	4.6503	0.3425	-1.4707
H	-2.0401	1.1665	-1.0158
H	-1.9012	1.3042	-2.7621
H	5.1205	0.6703	-4.5731
H	4.5147	-0.7442	-4.4386
H	3.2209	0.76	-3.2196
H	2.3389	2.0707	-3.1188
H	1.0114	-1.6757	1.1695
H	1.5477	-0.9792	2.7004
N	0.5609	2.7487	-1.154
N	-0.2979	0.2695	-1.7987
N	0.918	0.4285	1.2126
N	3.2307	-0.1836	-0.0492
O	4.5601	0.1211	-4.0009
O	2.479	1.2006	-2.7135
C	-1.5995	6.3987	-1.9884
H	-1.7758	6.958	-1.0616
H	-1.0192	7.0523	-2.6495
H	-2.5666	6.204	-2.4576
C	6.4205	-2.3041	1.9605
H	6.8266	-3.0913	1.3142
H	7.248	-1.6243	2.1942
H	6.0825	-2.7667	2.8907

Compound 4-OH_2 Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.543545 (Hartree/Particle)
Thermal correction to Energy= 0.579499
Thermal correction to Enthalpy= 0.580443
Thermal correction to Gibbs Free Energy= 0.476666
Sum of electronic and zero-point Energies= -3788.792479
Sum of electronic and thermal Energies= -3788.756525
Sum of electronic and thermal Enthalpies= -3788.755580
Sum of electronic and thermal Free Energies= -3788.859357

C	2.60356	-3.18207	0.62835
C	3.88609	-3.39785	0.15566
C	4.2144	-2.89981	-1.11064
C	3.24868	-2.19839	-1.83162
C	1.98406	-2.01821	-1.27651
C	0.93875	-1.20536	-2.00127
C	-1.08527	0.04821	-1.23154
C	-2.35644	0.08423	-1.85476
C	-3.12832	1.21775	-1.79752
C	-2.67641	2.36403	-1.0963
C	-3.48172	3.52979	-0.99905
C	-3.04926	4.62687	-0.29042
C	-1.78999	4.59618	0.3527
C	-0.97747	3.48563	0.26515
C	-1.38486	2.33632	-0.4689
C	-0.56606	1.15238	-0.56882
C	0.81031	1.15048	0.02956
C	1.83578	1.9887	-0.54338
C	1.62126	2.7591	-1.72081
C	2.62645	3.54041	-2.25008
C	3.89793	3.60278	-1.63386
C	4.14599	2.86187	-0.50143
C	3.1376	2.03499	0.06114
C	3.39457	1.24332	1.20876
C	2.42252	0.42233	1.72363
C	1.13873	0.36769	1.12813
C	-1.04869	0.00832	2.28878
C	-2.27212	-0.80405	1.93962
C	-3.20572	-2.52555	0.70184
C	-3.51936	-0.46136	2.45609
C	-4.64085	-1.19309	2.06706
C	-4.4814	-2.24726	1.16011
Cl	5.79101	-3.14153	-1.76465
Cl	-6.20127	-0.79905	2.68523
Fe	-0.23149	-2.20991	0.51869

H	2.32875	-3.54018	1.61475
H	4.61272	-3.93628	0.75316
H	3.48145	-1.78864	-2.80892
H	-0.97687	-1.86376	-1.79434
H	-2.71291	-0.78793	-2.39935
H	-4.09549	1.24528	-2.29146
H	-4.44959	3.53747	-1.49286
H	-3.67055	5.51422	-0.22044
H	-1.45601	5.46129	0.91776
H	-0.01161	3.49276	0.75732
H	0.652	2.73859	-2.20577
H	2.4377	4.12035	-3.14856
H	4.67389	4.23228	-2.05804
H	5.12043	2.89547	-0.02181
H	4.37227	1.29367	1.6796
H	2.63077	-0.17667	2.60796
H	0.68689	-1.03976	2.46992
H	-3.05653	-3.32423	-0.01688
H	-1.31242	-4.65184	-0.35662
H	0.07502	-4.41586	-1.00706
H	0.37774	-4.16919	2.45089
H	-0.91838	-3.41207	2.84024
H	1.28413	-0.1731	-2.08491
H	0.80247	-1.57518	-3.02415
H	-3.61714	0.37106	3.14509
H	-5.33015	-2.83047	0.82198
N	1.64584	-2.51948	-0.06221
N	-0.37247	-1.22899	-1.27261
N	0.19298	-0.59234	1.69782
N	-2.10136	-1.84037	1.08144
O	-0.68089	-3.95564	-0.60317
O	-0.10145	-3.33435	2.318
H	-1.17344	1.02386	1.90807
H	-0.93874	0.09216	3.37622

Compound 4-OH_2 Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.541622 (Hartree/Particle)
Thermal correction to Energy= 0.578569
Thermal correction to Enthalpy= 0.579513
Thermal correction to Gibbs Free Energy= 0.471106
Sum of electronic and zero-point Energies= -3788.797903
Sum of electronic and thermal Energies= -3788.760956
Sum of electronic and thermal Enthalpies= -3788.760012
Sum of electronic and thermal Free Energies= -3788.868419

C	2.3379	-3.2449	0.3766
C	3.6224	-3.5593	-0.033
C	4.067	-3.0551	-1.2613
C	3.211	-2.2557	-2.0193
C	1.9341	-1.9832	-1.536
C	0.9857	-1.0857	-2.2975
C	-1.0789	0.1485	-1.5219
C	-2.3251	0.2804	-2.1846
C	-3.0953	1.4016	-2.0082
C	-2.6658	2.4445	-1.1493
C	-3.4653	3.5996	-0.9416
C	-3.0503	4.5998	-0.0928
C	-1.8146	4.4782	0.5834
C	-1.0098	3.3742	0.3946
C	-1.4012	2.3225	-0.4811
C	-0.5876	1.1465	-0.687
C	0.7644	1.0863	-0.0289
C	1.8155	1.9425	-0.5252
C	1.6503	2.7588	-1.6794
C	2.6784	3.5547	-2.1389
C	3.925	3.5866	-1.4718
C	4.1238	2.8054	-0.3568
C	3.0898	1.9659	0.136
C	3.2915	1.1449	1.274
C	2.2934	0.319	1.7262
C	1.0377	0.2803	1.0708
C	-1.1809	-0.1163	2.1764
C	-2.3967	-0.9085	1.76
C	-3.3058	-2.5042	0.3352
C	-3.6459	-0.6599	2.3218
C	-4.7533	-1.3698	1.8577
C	-4.581	-2.3103	0.8345
Cl	5.6548	-3.4161	-1.8295
Cl	-6.3157	-1.0874	2.5293
Fe	-0.3718	-2.123	0.1774
H	1.9562	-3.5953	1.3316
H	4.2643	-4.1792	0.5823
H	3.5357	-1.8507	-2.9719
H	-0.9704	-1.6766	-2.3337
H	-2.6609	-0.5076	-2.856
H	-4.0412	1.5016	-2.533
H	-4.4134	3.6784	-1.4665
H	-3.6662	5.4806	0.0597
H	-1.491	5.2685	1.2543
H	-0.06	3.3142	0.9138
H	0.7	2.7632	-2.2012
H	2.5268	4.1703	-3.0205
H	4.72	4.2264	-1.8419
H	5.0774	2.8183	0.1638
H	4.2472	1.1801	1.7896
H	2.4518	-0.2985	2.6062
H	0.5291	-1.228	2.3217
H	-3.1356	-3.2159	-0.4672
H	-1.4033	-4.656	0.4434
H	0.0047	-4.7877	-0.2307
H	1.9144	-2.6595	3.9619
H	0.4463	-2.9606	4.276
H	1.3572	-0.0587	-2.2708
H	0.9455	-1.3812	-3.3517
H	-3.7571	0.0827	3.1049
H	-5.4206	-2.8711	0.4403
N	1.494	-2.4787	-0.355
N	-0.3872	-1.1264	-1.7035
N	0.0667	-0.6882	1.5775
N	-2.2174	-1.8346	0.7858
O	-0.6944	-4.1544	0.0066
O	1.0302	-2.6609	3.5599
H	-1.2966	0.9187	1.8456
H	-1.0896	-0.0941	3.2685

Compound 4-OH_2 Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.540709 (Hartree/Particle)
Thermal correction to Energy= 0.578125
Thermal correction to Enthalpy= 0.579070
Thermal correction to Gibbs Free Energy= 0.469391
Sum of electronic and zero-point Energies= -3788.817048
Sum of electronic and thermal Energies= -3788.779632
Sum of electronic and thermal Enthalpies= -3788.778688

Sum of electronic and thermal Free Energies= -3788.888366

C	2.389	-3.8853	0.1108
C	3.5487	-4.3241	-0.5047
C	3.9713	-3.6515	-1.6576
C	3.2159	-2.5788	-2.1335
C	2.0669	-2.1966	-1.4431
C	1.2765	-0.9893	-1.8981
C	-0.8668	0.23	-1.4441
C	-2.0473	0.2137	-2.2294
C	-2.8629	1.3157	-2.2887
C	-2.5486	2.4867	-1.5549
C	-3.3982	3.6241	-1.5883
C	-3.1	4.7466	-0.8511
C	-1.9379	4.7697	-0.045
C	-1.0867	3.6864	0.0009
C	-1.3531	2.5132	-0.7596
C	-0.4878	1.3577	-0.7263
C	0.7804	1.4115	0.0747
C	1.8582	2.267	-0.3622
C	1.7952	3.0139	-1.5721
C	2.845	3.8154	-1.966
C	4.0149	3.9198	-1.1776
C	4.1181	3.2012	-0.0093
C	3.0594	2.3573	0.4199
C	3.1682	1.5919	1.6076
C	2.1482	0.762	2.0005
C	0.9601	0.6648	1.2332
C	-1.3595	0.2216	2.0727
C	-2.3909	-0.8831	2.1609
C	-3.1003	-2.9936	1.5105
C	-3.5642	-0.6847	2.8868
C	-4.5348	-1.6865	2.8981
C	-4.2985	-2.8734	2.1934
Cl	5.4022	-4.1449	-2.4816
Cl	-6.0027	-1.4696	3.7749
Fe	-0.2182	-2.1256	0.4993
H	2.0201	-4.3807	1.0017
H	4.1069	-5.1635	-0.1064
H	3.5221	-2.0446	-3.0265
H	-0.629	-1.6921	-1.9582
H	-2.2951	-0.6752	-2.8065
H	-3.7585	1.2991	-2.9033
H	-4.2913	3.5896	-2.2061
H	-3.7536	5.6126	-0.8823
H	-1.7112	5.6545	0.5422
H	-0.1994	3.7323	0.6216
H	0.9074	2.9569	-2.1913
H	2.7716	4.378	-2.892
H	4.8276	4.5637	-1.4989
H	5.0136	3.2661	0.6026
H	4.0696	1.6706	2.2088
H	2.2408	0.1883	2.9208
H	0.3674	-0.7462	2.5274
H	-2.8711	-3.903	0.9629
H	-1.9232	-4.1554	-0.9828
H	-0.4248	-4.5675	-1.1205
H	1.092	-3.5957	2.8272
H	-0.4532	-3.5949	3.0368
H	1.7603	-0.0901	-1.5105
H	1.2822	-0.915	-2.9917
H	-3.7229	0.2402	3.4313
H	-5.0267	-3.6762	2.1853
N	1.645	-2.8441	-0.3302
N	-0.1199	-1.022	-1.3799
N	-0.0236	-0.3131	1.6891
N	-2.15	-2.0286	1.4776
O	-1.0144	-3.8714	-0.7857
O	0.2556	-3.2621	2.4615
H	-1.6738	0.9336	1.3068
H	-1.3	0.7727	3.0184

Compound 5-OH_2 Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.710412 (Hartree/Particle)
Thermal correction to Energy= 0.752955
Thermal correction to Enthalpy= 0.753899
Thermal correction to Gibbs Free Energy= 0.636174
Sum of electronic and zero-point Energies= -3137.427403
Sum of electronic and thermal Energies= -3137.384860
Sum of electronic and thermal Enthalpies= -3137.383916
Sum of electronic and thermal Free Energies= -3137.501641

C	0.5755	3.78	-0.689
C	-0.219	4.8706	-0.9545
C	-1.4724	4.6909	-1.6082
C	-1.8083	3.3444	-1.9164
C	-0.9492	2.3102	-1.5971
C	-1.3574	0.876	-1.8475
C	-0.5783	-1.3396	-0.9909
C	-0.3338	-2.5084	-1.7531
C	-0.5774	-3.7513	-1.2262
C	-1.0602	-3.8904	0.0993
C	-1.2856	-5.1718	0.6688
C	-1.7239	-5.2992	1.9664
C	-1.9494	-4.1421	2.7477
C	-1.7544	-2.8837	2.2199
C	-1.3155	-2.711	0.8766
C	-1.0923	-1.408	0.2976
C	-1.4243	-0.1798	1.0948
C	-2.803	0.1124	1.4055
C	-3.8803	-0.6722	0.905
C	-5.188	-0.3621	1.2117
C	-5.4965	0.7431	2.0385
C	-4.4824	1.5327	2.5289
C	-3.1254	1.2498	2.2195
C	-2.0769	2.0775	2.694
C	-0.773	1.8109	2.3615
C	-0.4467	0.6932	1.5546
C	1.6143	-0.7139	1.7003
C	2.5854	-1.278	0.688
C	3.4135	-2.3307	1.0287
C	4.2682	-2.9266	0.0617
C	4.19	-2.3669	-1.2464
C	3.3446	-1.3094	-1.4874
Fe	1.4019	0.8835	-0.7808
H	1.5203	3.9287	-0.1746
H	0.1256	5.8512	-0.6542
H	-2.7525	3.1047	-2.3897
H	0.1609	-0.3013	-2.5273
H	0.0365	-2.4139	-2.7719
H	-0.4019	-4.642	-1.8231
H	-1.1022	-6.0522	0.0585
H	-1.8951	-6.2823	2.3938
H	-2.2864	-4.2461	3.7749
H	-1.944	-2.0127	2.8366
H	-3.6701	-1.5306	0.2774
H	-5.9913	-0.9781	0.8185
H	-6.5311	0.9653	2.2809
H	-4.7047	2.3888	3.1603
H	-2.3169	2.9277	3.3262
H	0.0236	2.4529	2.7319
H	1.4482	1.3162	1.6291

H	3.3827	-2.7045	2.0447
H	4.7804	-2.7583	-2.0642
H	3.2822	-0.9027	-2.4924
H	-2.1754	0.6159	-1.1739
H	-1.7364	0.7485	-2.8679
H	3.4186	2.7912	-0.29
H	3.8843	1.3531	0.0817
H	1.6177	2.1172	-3.137
H	2.8343	1.149	-3.194
H	0.8424	-1.4573	1.9052
H	2.1155	-0.5083	2.6529
N	0.262	2.498	-1.0056
N	-0.216	-0.0687	-1.6088
N	0.9578	0.5364	1.1921
N	2.5464	-0.728	-0.5563
O	3.0972	1.9151	-0.0208
O	1.9578	1.2729	-2.7945
N	-2.2859	5.7281	-1.9075
N	5.0932	-3.9554	0.3587
C	-3.5716	5.4925	-2.5681
H	-4.229	4.8691	-1.9503
H	-4.0674	6.4481	-2.733
H	-3.4342	5.0089	-3.5423
C	-1.8997	7.097	-1.5551
H	-0.9615	7.3831	-2.0445
H	-2.6769	7.7826	-1.8896
H	-1.7864	7.2133	-0.4708
C	5.9443	-4.5445	-0.6785
H	6.6326	-3.8009	-1.0966
H	6.5388	-5.3439	-0.2385
H	5.3454	-4.9729	-1.4908
C	5.1287	-4.5068	1.7151
H	4.1536	-4.9165	2.0047
H	5.8598	-5.3131	1.7525
H	5.4261	-3.7449	2.4452

Compound 5-OH_2 Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.708727
(Hartree/Particle)
Thermal correction to Energy= 0.752334
Thermal correction to Enthalpy= 0.753278
Thermal correction to Gibbs Free Energy=
0.630346
Sum of electronic and zero-point Energies= -
3137.432729
Sum of electronic and thermal Energies= -
3137.389122
Sum of electronic and thermal Enthalpies= -
3137.388178
Sum of electronic and thermal Free Energies= -
3137.511110

C	1.0415	4.183	-0.5743
C	0.3217	5.2911	-0.9496
C	-0.8513	5.1394	-1.746
C	-1.2003	3.7989	-2.0694
C	-0.4244	2.7435	-1.6336
C	-0.8509	1.3141	-1.8703
C	-0.091	-0.9379	-1.0862
C	0.1541	-2.0506	-1.929
C	-0.1104	-3.3261	-1.4999
C	-0.6226	-3.5573	-0.1984
C	-0.8775	-4.8741	0.2686
C	-1.3549	-5.0908	1.5405
C	-1.5927	-3.9915	2.3978
C	-1.3668	-2.7005	1.9706
C	-0.883	-2.4356	0.6582
C	-0.6261	-1.0954	0.1873
C	-0.9867	0.0663	1.0731
C	-2.3849	0.3601	1.2886
C	-3.4237	-0.3532	0.626
C	-4.7499	-0.0433	0.8417
C	-5.1176	0.9912	1.7325
C	-4.1409	1.7098	2.3825
C	-2.7659	1.4234	2.1735
C	-1.7538	2.1739	2.8232
C	-0.4296	1.8999	2.5985
C	-0.0412	0.854	1.7225
C	2.0194	-0.601	1.8026
C	3.0095	-1.0014	0.7297
C	3.8902	-2.0456	0.9362
C	4.7829	-2.4582	-0.091
C	4.6926	-1.7267	-1.3112
C	3.7896	-0.6952	-1.4261
Fe	1.7791	1.2922	-0.5687
H	1.9235	4.3038	0.0484
H	0.6602	6.2656	-0.6237
H	-2.0916	3.5825	-2.6449
H	0.7467	0.2193	-2.5159
H	0.5405	-1.8795	-2.9303
H	0.0679	-4.1728	-2.1571
H	-0.6868	-5.7095	-0.3998
H	-1.5488	-6.1005	1.889
H	-1.9641	-4.1664	3.4032
H	-1.5669	-1.8741	2.643
H	-3.1704	-1.159	-0.0533
H	-5.5222	-0.6065	0.326
H	-6.1667	1.2145	1.8998
H	-4.4072	2.5101	3.0678
H	-2.0386	2.9674	3.5084
H	0.3376	2.4778	3.1102
H	1.8469	1.4196	2.0578
H	3.8821	-2.5465	1.8962
H	5.323	-1.9645	-2.1579
H	3.7064	-0.1429	-2.3586
H	-1.6692	1.0708	-1.1896
H	-1.2266	1.1736	-2.8902
H	3.6707	3.2088	-0.9397
H	4.373	1.8819	-0.4873
H	1.6407	1.1593	-4.7796
H	2.1369	-0.2857	-4.6528
H	1.2387	-1.3602	1.8777
H	2.5108	-0.5545	2.7809
N	0.7173	2.9066	-0.9094
N	0.283	0.3711	-1.6102
N	1.3865	0.7134	1.485
N	2.9479	-0.3041	-0.4347
O	3.5281	2.364	-0.4816
O	1.8457	0.4739	-4.1234
N	-1.5843	6.1973	-2.1563
N	5.659	-3.474	0.0777
C	-2.7957	5.9932	-2.9541
H	-3.5424	5.4092	-2.403
H	-3.2319	6.9621	-3.193
H	-2.5675	5.482	-3.8966
C	-1.1937	7.5596	-1.7816
H	-0.1907	7.7996	-2.1521
H	-1.8948	8.2648	-2.2258
H	-1.2153	7.6962	-0.694
C	6.5631	-3.8596	-1.0086
H	7.2206	-3.0297	-1.2927
H	7.1886	-4.686	-0.6739
H	6.0054	-4.1914	-1.8923
C	5.7142	-4.2	1.3488
H	4.7549	-4.6806	1.5738
H	6.4744	-4.9769	1.2821
H	5.9814	-3.5328	2.1767

Compound 5-OH_2 Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.708638 (Hartree/Particle)
Thermal correction to Energy= 0.752295
Thermal correction to Enthalpy= 0.753240
Thermal correction to Gibbs Free Energy= 0.628657
Sum of electronic and zero-point Energies= -3137.460082
Sum of electronic and thermal Energies= -3137.416425
Sum of electronic and thermal Enthalpies= -3137.415480
Sum of electronic and thermal Free Energies= -3137.540063

C	1.2605	3.9339	-0.8818
C	0.6491	5.1395	-1.128
C	-0.6478	5.165	-1.7213
C	-1.2144	3.8925	-2.0145
C	-0.5282	2.7314	-1.7169
C	-1.1787	1.38	-1.9479
C	-0.555	-1.0423	-1.5319
C	-0.3384	-2.0884	-2.4672
C	-0.5684	-3.3968	-2.1264
C	-1.0183	-3.7367	-0.8263
C	-1.2388	-5.0891	-0.4535
C	-1.6597	-5.4094	0.8162
C	-1.8723	-4.382	1.7646
C	-1.6763	-3.0592	1.4308
C	-1.2512	-2.6874	0.1242
C	-1.0277	-1.3107	-0.2509
C	-1.3547	-0.2319	0.7418
C	-2.7406	0.0366	1.0468
C	-3.8089	-0.6327	0.3859
C	-5.1225	-0.3496	0.6929
C	-5.4463	0.6142	1.6759
C	-4.4405	1.2916	2.3254
C	-3.0771	1.031	2.0255
C	-2.0348	1.7425	2.6714
C	-0.723	1.4934	2.3596
C	-0.3797	0.5125	1.3939
C	1.6903	-0.9152	1.4738
C	3.112	-0.9167	0.9552
C	4.1086	-1.6074	1.6107
C	5.4304	-1.6451	1.0797
C	5.6264	-0.9208	-0.132
C	4.5747	-0.2495	-0.7086
Fe	1.683	0.8741	-0.9493
H	2.2504	3.9161	-0.432
H	1.1677	6.052	-0.8657
H	-2.1976	3.8152	-2.4618
H	0.1543	0.1922	-2.9347
H	0.0001	-1.8374	-3.4697
H	-0.4123	-4.1871	-2.8556
H	-1.0671	-5.8676	-1.192
H	-1.8279	-6.4454	1.0937
H	-2.1994	-4.6386	2.768
H	-1.8529	-2.2906	2.1744
H	-3.5872	-1.3805	-0.3666
H	-5.9192	-0.8772	0.1768
H	-6.4861	0.8173	1.9125
H	-4.6741	2.0389	3.0789
H	-2.2861	2.4879	3.4207
H	0.0681	2.0423	2.8665
H	1.5138	1.0989	1.6302
H	3.866	-2.1206	2.5325
H	6.5949	-0.8793	-0.6123
H	4.717	0.3055	-1.6291
H	-1.8825	1.1824	-1.1383
H	-1.7563	1.3826	-2.8795
H	1.6466	0.0885	-5.7097
H	2.2011	-1.1415	-4.964
H	2.5455	0.6931	-3.6054
H	2.8683	2.1436	-3.0809
H	1.1231	-1.7295	1.0161
H	1.664	-1.0617	2.5594
N	0.7124	2.723	-1.1624
N	-0.1616	0.291	-1.9687
N	1.0371	0.3712	1.0934
N	3.3157	-0.2253	-0.1994
O	1.7872	-0.2743	-4.8189
O	2.7735	1.2209	-2.7947
N	-1.2927	6.3212	-1.9887
N	6.4312	-2.316	1.6884
C	-2.6264	6.3027	-2.5947
H	-3.3464	5.7796	-1.9545
H	-2.9717	7.3271	-2.726
H	-2.6086	5.8208	-3.5792
C	-0.6703	7.6089	-1.6661
H	0.2711	7.7425	-2.2112
H	-1.3459	8.4122	-1.9563
H	-0.4764	7.6981	-0.5911
C	7.7809	-2.3114	1.1159
H	8.1849	-1.2941	1.0606
H	8.4381	-2.9031	1.7515
H	7.7874	-2.7536	0.1132
C	6.1852	-3.0463	2.9347
H	5.4232	-3.8217	2.7953
H	7.1075	-3.5319	3.2501
H	5.8649	-2.37	3.7359

Compound 7-OH_2 Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.542427 (Hartree/Particle)
Thermal correction to Energy= 0.578878
Thermal correction to Enthalpy= 0.579822
Thermal correction to Gibbs Free Energy= 0.473768
Sum of electronic and zero-point Energies= -8011.813078
Sum of electronic and thermal Energies= -8011.776626
Sum of electronic and thermal Enthalpies= -8011.775682
Sum of electronic and thermal Free Energies= -8011.881737

C	0.85681	3.95403	-0.83635
C	-0.00349	5.02035	-1.02723
C	-1.24244	4.77055	-1.62617
C	-1.56162	3.46461	-1.99157
C	-0.64021	2.4472	-1.75798
C	-0.9807	1.01557	-2.0922
C	-0.18488	-1.16276	-1.15618
C	0.09704	-2.34891	-1.87593
C	-0.13619	-3.57747	-1.31132
C	-0.64628	-3.68153	0.00686
C	-0.86094	-4.94728	0.61319
C	-1.32744	-5.03951	1.90362
C	-1.59354	-3.86239	2.64001
C	-1.40936	-2.61827	2.07603
C	-0.94084	-2.48243	0.73937
C	-0.72485	-1.19638	0.12204
C	-1.08905	0.05324	0.8686

C	-2.47642	0.34334	1.13792
C	-3.53513	-0.46532	0.63813
C	-4.85137	-0.15345	0.90298
C	-5.18632	0.9762	1.6844
C	-4.19022	1.78813	2.17408
C	-2.8248	1.50408	1.90781
C	-1.79368	2.35173	2.38387
C	-0.47986	2.08501	2.0921
C	-0.13056	0.94708	1.32557
C	1.9416	-0.43752	1.54173
C	2.86307	-1.06627	0.52574
C	3.626	-2.18194	0.8601
C	4.43286	-2.77147	-0.1106
C	4.44862	-2.22454	-1.3975
C	3.66523	-1.11134	-1.64424
Fe	1.75377	1.09825	-0.97673
H	1.81283	4.117	-0.3504
H	0.27899	6.01907	-0.71546
H	-2.521	3.23897	-2.44475
H	0.55797	-0.16025	-2.71274
H	0.48332	-2.28261	-2.89104
H	0.06784	-4.484	-1.87405
H	-0.64604	-5.84368	0.03789
H	-1.48931	-6.01107	2.35983
H	-1.95376	-3.93943	3.66152
H	-1.63301	-1.73184	2.65848
H	-3.30487	-1.34403	0.04653
H	-5.64138	-0.7872	0.51127
H	-6.2279	1.19988	1.89265
H	-4.43372	2.66282	2.77096
H	-2.05444	3.21746	2.98601
H	0.30313	2.7408	2.46787
H	1.75401	1.58446	1.43423
H	3.58516	-2.59066	1.86411
H	5.05452	-2.65727	-2.18476
H	3.64889	-0.67987	-2.63857
H	-1.84607	0.70446	-1.50374
H	-1.26939	0.92668	-3.14596
H	3.75834	3.05749	-0.52559
H	4.23794	1.6677	-0.02009
H	1.99737	2.29011	-3.3693
H	3.23057	1.35363	-3.33771
H	1.17372	-1.15821	1.82873
H	2.492	-0.18668	2.45597
N	0.5734	2.68105	-1.20003
N	0.17076	0.09801	-1.80547
N	1.28568	0.79418	0.99165
N	2.88471	-0.51567	-0.71346
O	3.44611	2.1741	-0.26893
O	2.33161	1.46203	-2.98387
Br	-2.45928	6.16899	-1.92049
Br	5.47651	-4.27702	0.29851

Compound 7-OH_2 Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.540466 (Hartree/Particle)
Thermal correction to Energy= 0.577966
Thermal correction to Enthalpy= 0.578910
Thermal correction to Gibbs Free Energy= 0.467834
Sum of electronic and zero-point Energies= -8011.818471
Sum of electronic and thermal Energies= -8011.780972
Sum of electronic and thermal Enthalpies= -8011.780028
Sum of electronic and thermal Free Energies= -8011.891103

C	0.9137	4.0408	-0.4623
C	0.1576	5.159	-0.776
C	-0.991	4.986	-1.5617
C	-1.3384	3.6992	-1.9789
C	-0.533	2.6217	-1.6115
C	-0.9159	1.202	-1.9561
C	-0.1575	-1.0338	-1.0946
C	0.1255	-2.1808	-1.8814
C	-0.1265	-3.4411	-1.3953
C	-0.66	-3.6204	-0.0919
C	-0.9008	-4.9206	0.4308
C	-1.3962	-5.0871	1.706
C	-1.6667	-3.9523	2.5093
C	-1.454	-2.6759	2.0265
C	-0.9523	-2.4637	0.7096
C	-0.7051	-1.1412	0.1809
C	-1.0891	0.0534	1.0124
C	-2.4931	0.3467	1.1975
C	-3.518	-0.3941	0.5402
C	-4.8508	-0.0819	0.7237
C	-5.2376	0.981	1.5762
C	-4.2738	1.7247	2.2221
C	-2.8927	1.4362	2.0451
C	-1.8939	2.2102	2.6922
C	-0.562	1.9371	2.4957
C	-0.1591	0.8683	1.6529
C	1.9146	-0.5739	1.8272
C	2.9086	-1.0277	0.7815
C	3.7934	-2.0773	1.0271
C	4.6497	-2.5012	0.0077
C	4.5967	-1.8589	-1.2379
C	3.6964	-0.8174	-1.4032
Fe	1.7043	1.1831	-0.5994
H	1.8025	4.1386	0.1545
H	0.4525	6.1389	-0.4188
H	-2.2294	3.5349	-2.5756
H	0.6679	0.0626	-2.5758
H	0.5345	-2.0506	-2.8799
H	0.0788	-4.3147	-2.0079
H	-0.6848	-5.783	-0.1943
H	-1.5786	-6.0828	2.0983
H	-2.0522	-4.0884	3.5154
H	-1.6811	-1.8241	2.6577
H	-3.2507	-1.2218	-0.1073
H	-5.6133	-0.6634	0.2138
H	-6.2903	1.2057	1.7169
H	-4.5559	2.5448	2.8768
H	-2.1937	3.0201	3.3515
H	0.1938	2.5317	3.0059
H	1.7253	1.4591	1.9984
H	3.8127	-2.5591	1.999
H	5.2434	-2.1634	-2.0528
H	3.6127	-0.2949	-2.3523
H	-1.7811	0.9128	-1.3543
H	-1.2161	1.1211	-3.0072
H	3.4153	3.1889	-1.3369
H	4.311	1.9247	-1.0107
H	1.7904	0.7583	-4.9034
H	2.2478	-0.6495	-4.5421
H	1.1319	-1.3291	1.9286
H	2.3977	-0.4836	2.8066
N	0.598	2.7874	-0.8765
N	0.2153	0.2596	-1.6722
N	1.2834	0.7295	1.4372
N	2.8658	-0.3953	-0.4177
O	3.4107	2.2927	-0.9568
O	1.8712	0.1537	-4.1477

Br	-2.0506	6.4642	-2.0382
Br	5.8573	-3.9127	0.2997

Compound 7-OH_2 Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.539764
(Hartree/Particle)
Thermal correction to Energy= 0.577484
Thermal correction to Enthalpy= 0.578428
Thermal correction to Gibbs Free Energy=
0.463921
Sum of electronic and zero-point Energies= -
8011.842919
Sum of electronic and thermal Energies= -
8011.805199
Sum of electronic and thermal Enthalpies= -
8011.804255
Sum of electronic and thermal Free Energies= -
8011.918762

C	0.6545	4.0176	-0.8713
C	-0.1521	5.11	-1.1356
C	-1.3836	4.8803	-1.7608
C	-1.7507	3.5754	-2.0827
C	-0.8789	2.5325	-1.774
C	-1.2796	1.0983	-2.0541
C	-0.4389	-1.1336	-1.2234
C	-0.1458	-2.29	-1.9891
C	-0.3195	-3.5416	-1.4571
C	-0.7889	-3.7036	-0.1297
C	-0.9624	-4.9943	0.4349
C	-1.4053	-5.1429	1.7286
C	-1.6899	-3.9991	2.5088
C	-1.5403	-2.7318	1.9874
C	-1.092	-2.5381	0.651
C	-0.9126	-1.2234	0.0812
C	-1.2934	-0.0224	0.9045
C	-2.6925	0.2572	1.1213
C	-3.724	-0.5116	0.5131
C	-5.0523	-0.2117	0.7274
C	-5.4271	0.8662	1.5617
C	-4.4573	1.6355	2.1613
C	-3.0802	1.3599	1.9542
C	-2.0743	2.1561	2.557
C	-0.7471	1.8882	2.3393
C	-0.3564	0.8058	1.5127
C	1.7087	-0.6025	1.788
C	2.8838	-1.0223	0.9308
C	3.7843	-1.9722	1.4062
C	4.8063	-2.4133	0.5683
C	4.9027	-1.8852	-0.7229
C	3.9755	-0.934	-1.1111
Fe	1.5347	1.0078	-0.8042
H	1.6187	4.1532	-0.3881
H	0.1628	6.1112	-0.8657
H	-2.7025	3.3737	-2.5624
H	0.2217	-0.0698	-2.7828
H	0.2013	-2.1802	-3.0146
H	-0.1054	-4.4225	-2.0555
H	-0.7382	-5.8646	-0.1758
H	-1.5375	-6.1333	2.1525
H	-2.0382	-4.1205	3.5302
H	-1.7786	-1.8716	2.6028
H	-3.4632	-1.3531	-0.1189
H	-5.821	-0.8163	0.2555
H	-6.4779	1.082	1.7269
H	-4.7313	2.4674	2.8044
H	-2.3656	2.9798	3.2025
H	0.0152	2.4987	2.8193
H	1.5303	1.4248	1.7641
H	3.6859	-2.3673	2.4116
H	5.682	-2.2053	-1.4043
H	4.0386	-0.4889	-2.0975
H	-2.0944	0.8198	-1.3829
H	-1.667	1.0072	-3.0751
H	6.2449	1.8973	-2.2435
H	5.6978	1.6935	-3.6785
H	3.9458	1.8725	-2.2001
H	2.7144	2.859	-2.3827
H	0.9602	-1.3971	1.773
H	2.0189	-0.4775	2.8314
N	0.3158	2.7468	-1.187
N	-0.1427	0.1509	-1.8562
N	1.0781	0.6493	1.2786
N	2.9796	-0.4933	-0.3088
O	5.4893	1.5439	-2.7414
O	2.9916	2.0433	-1.938
Br	-2.5265	6.3156	-2.1581
Br	6.038	-3.6984	1.1654

Compound 8-OH_2 Singlet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.546639
(Hartree/Particle)
Thermal correction to Energy= 0.581797
Thermal correction to Enthalpy= 0.582741
Thermal correction to Gibbs Free Energy=
0.481767
Sum of electronic and zero-point Energies= -
3068.067781
Sum of electronic and thermal Energies= -
3068.032623
Sum of electronic and thermal Enthalpies= -
3068.031679
Sum of electronic and thermal Free Energies= -
3068.132654

C	0.86101	3.9473	-0.86138
C	0.00557	5.01694	-1.04898
C	-1.22373	4.74647	-1.63408
C	-1.56624	3.45774	-1.99839
C	-0.64279	2.44342	-1.77081
C	-0.98421	1.01608	-2.10312
C	-0.20374	-1.15641	-1.16823
C	0.05837	-2.34007	-1.89636
C	-0.17537	-3.56893	-1.33347
C	-0.6685	-3.6769	-0.01107
C	-0.88135	-4.94196	0.59415
C	-1.33055	-5.03753	1.89011
C	-1.57934	-3.86289	2.633
C	-1.39598	-2.61803	2.07102
C	-0.94596	-2.47882	0.72982
C	-0.72992	-1.193	0.11457
C	-1.08666	0.05096	0.87202
C	-2.47273	0.33903	1.14403
C	-3.53226	-0.45844	0.63259
C	-4.84794	-0.1474	0.89987
C	-5.18125	0.97036	1.69559
C	-4.18326	1.77215	2.19712
C	-2.81925	1.48952	1.93012
C	-1.78696	2.32652	2.41677
C	-0.47359	2.06159	2.12292
C	-0.12716	0.9364	1.33976
C	1.94769	-0.42862	1.55449
C	2.87029	-1.05452	0.54522
C	3.62826	-2.16932	0.8861
C	4.42808	-2.73753	-0.0879
C	4.46535	-2.21007	-1.37103

C	3.67769	-1.10052	-1.61653
Fe	1.74257	1.09081	-0.97101
H	1.81986	4.10959	-0.38536
H	0.27331	6.02413	-0.75052
H	-2.5351	3.25539	-2.44326
H	0.50298	-0.17818	-2.72317
H	0.43534	-2.2725	-2.91486
H	0.01825	-4.47329	-1.90314
H	-0.67664	-5.83435	0.00922
H	-1.4886	-6.01127	2.34266
H	-1.92416	-3.93623	3.65998
H	-1.60283	-1.73165	2.65916
H	-3.30162	-1.32667	0.02645
H	-5.63522	-0.77568	0.49443
H	-6.22149	1.19742	1.90609
H	-4.42052	2.64058	2.80536
H	-2.04483	3.18608	3.02875
H	0.31022	2.71219	2.50555
H	1.73213	1.56183	1.47886
H	3.59811	-2.59404	1.88422
H	5.08301	-2.65623	-2.1421
H	3.66216	-0.67015	-2.60691
H	-1.85676	0.7069	-1.52415
H	-1.25934	0.92476	-3.15939
H	3.77402	3.04554	-0.5412
H	4.23942	1.6979	-0.00446
H	1.99127	2.24459	-3.43769
H	3.2253	1.34599	-3.38789
H	1.18888	-1.15311	1.85631
H	2.50045	-0.15791	2.46054
N	0.58075	2.66765	-1.21952
N	0.16835	0.10705	-1.8038
N	1.28595	0.78947	0.98649
N	2.88989	-0.4956	-0.6951
O	3.42686	2.17987	-0.2508
O	2.34229	1.45679	-2.98109
F	-2.14848	5.80951	-1.85727
F	5.22061	-3.88068	0.23064

Compound 8-OH_2 Triplet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.544719
(Hartree/Particle)
Thermal correction to Energy= 0.580905
Thermal correction to Enthalpy= 0.581849
Thermal correction to Gibbs Free Energy=
0.475926
Sum of electronic and zero-point Energies= -
3068.073355
Sum of electronic and thermal Energies= -
3068.037169
Sum of electronic and thermal Enthalpies= -
3068.036225
Sum of electronic and thermal Free Energies= -
3068.142148

C	0.9109	4.0296	-0.4982
C	0.1157	5.1226	-0.7379
C	-1.0621	4.9105	-1.4471
C	-1.4046	3.6427	-1.8818
C	-0.5448	2.5975	-1.5942
C	-0.8793	1.1814	-1.9987
C	-0.1194	-1.0369	-1.1001
C	0.1348	-2.1863	-1.8826
C	-0.0968	-3.4317	-1.3805
C	-0.586	-3.5989	-0.065
C	-0.8023	-4.8875	0.477
C	-1.2656	-5.0394	1.7536
C	-1.5323	-3.9024	2.5443
C	-1.3448	-2.6393	2.0473
C	-0.8693	-2.4401	0.7271
C	-0.6429	-1.1291	0.1808
C	-1.0475	0.0733	0.9879
C	-2.4522	0.3513	1.1447
C	-3.4535	-0.4108	0.4919
C	-4.7817	-0.1107	0.6488
C	-5.1915	0.9605	1.4691
C	-4.2549	1.7225	2.1099
C	-2.8752	1.4484	1.9615
C	-1.9001	2.2426	2.6069
C	-0.5732	1.9833	2.4412
C	-0.1435	0.9069	1.63
C	1.941	-0.4981	1.8777
C	2.846	-1.0524	0.8013
C	3.6258	-2.1724	1.032
C	4.4196	-2.6403	-0.0018
C	4.4264	-2.0013	-1.2374
C	3.6187	-0.8981	-1.3822
Fe	1.715	1.1875	-0.6051
H	1.8339	4.1376	0.0612
H	0.3857	6.1119	-0.3877
H	-2.3286	3.4838	-2.4271
H	0.7258	0.0557	-2.5762
H	0.4922	-2.0673	-2.9017
H	0.0887	-4.3096	-1.9922
H	-0.5922	-5.7556	-0.141
H	-1.4293	-6.0314	2.1616
H	-1.8982	-4.0295	3.5583
H	-1.5709	-1.7819	2.6709
H	-3.1685	-1.2493	-0.1328
H	-5.5291	-0.7117	0.1404
H	-6.248	1.1763	1.5891
H	-4.5568	2.5515	2.7434
H	-2.2194	3.0614	3.2447
H	0.165	2.5962	2.9538
H	1.7116	1.5256	2.0081
H	3.6249	-2.6779	1.9916
H	5.044	-2.3672	-2.0492
H	3.5592	-0.3716	-2.3296
H	-1.7771	0.8547	-1.4686
H	-1.1052	1.1347	-3.0703
H	3.5735	3.0922	-1.3194
H	4.3382	1.8926	-0.7172
H	1.6815	1.1159	-4.7463
H	1.9589	-0.3888	-4.8074
H	1.1648	-1.2283	2.1193
H	2.5142	-0.3284	2.7961
N	0.6119	2.7852	-0.9178
N	0.2493	0.2497	-1.6864
N	1.3019	0.7842	1.4416
N	2.8442	-0.4164	-0.3901
O	3.4613	2.2569	-0.864
O	1.8592	0.3464	-4.1765
F	-1.8647	5.9298	-1.7058
F	5.1791	-3.708	0.1891

Compound 8-OH_2 Quintet

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.544037
(Hartree/Particle)
Thermal correction to Energy= 0.580444
Thermal correction to Enthalpy= 0.581388
Thermal correction to Gibbs Free Energy=
0.471988
Sum of electronic and zero-point Energies= -
3068.098406

Sum of electronic and thermal Energies= -3068.061999

Sum of electronic and thermal Enthalpies= -3068.061054

Sum of electronic and thermal Free Energies= -3068.170455

C	0.5709	4.0626	-0.9479
C	-0.3074	5.1255	-1.1673
C	-1.5506	4.8116	-1.7394
C	-1.8964	3.4999	-2.0725
C	-0.9561	2.4882	-1.8127
C	-1.2937	1.0387	-2.1212
C	-0.3783	-1.162	-1.2223
C	-0.0769	-2.3483	-1.9567
C	-0.2281	-3.5929	-1.3732
C	-0.6818	-3.7105	-0.0242
C	-0.8323	-4.9917	0.5913
C	-1.2637	-5.0992	1.906
C	-1.5606	-3.9207	2.6522
C	-1.4315	-2.6623	2.0762
C	-0.9938	-2.514	0.7204
C	-0.8378	-1.2122	0.0989
C	-1.2234	0.0196	0.8802
C	-2.6301	0.3026	1.0942
C	-3.6643	-0.5075	0.5233
C	-5.0053	-0.2069	0.7323
C	-5.387	0.9153	1.5253
C	-4.4106	1.724	2.0899
C	-3.024	1.4444	1.8844
C	-2.0147	2.279	2.4537
C	-0.6758	2.0059	2.2402
C	-0.2817	0.8821	1.4535
C	1.8045	-0.5536	1.7283
C	2.8015	-1.1287	0.7359
C	3.6015	-2.226	1.0962
C	4.469	-2.7424	0.1306
C	4.5545	-2.1904	-1.1569
C	3.733	-1.0947	-1.4291
Fe	1.5469	1.0727	-0.8879
H	1.5459	4.2385	-0.5053
H	-0.0486	6.1464	-0.9105
H	-2.865	3.2807	-2.5105
H	0.2725	-0.1123	-2.8327
H	0.2522	-2.2703	-2.9919
H	-0.0133	-4.4938	-1.942
H	-0.6054	-5.8835	0.0126
H	-1.3805	-6.0743	2.3693
H	-1.9011	-4.0125	3.6798
H	-1.6841	-1.7832	2.6601
H	-3.4018	-1.3796	-0.0666
H	-5.775	-0.8377	0.2964
H	-6.4395	1.1285	1.6863
H	-4.6904	2.5804	2.6981
H	-2.3094	3.1263	3.0673
H	0.0862	2.6381	2.6939
H	1.6347	1.5088	1.6874
H	3.5489	-2.6719	2.0843
H	5.2274	-2.6023	-1.9003
H	3.7535	-0.6173	-2.4023
H	-2.1168	0.7185	-1.4779
H	-1.6541	0.9571	-3.1549
H	6.1295	2.3394	-1.0431
H	6.1455	1.8791	-2.5857
H	4.0801	2.0371	-1.8122
H	2.792	2.8459	-2.4536
H	1.0211	-1.2915	1.9164
H	2.3018	-0.3719	2.6898
N	0.262	2.7684	-1.2655
N	-0.1229	0.1151	-1.9157
N	1.1682	0.7181	1.2331
N	2.8742	-0.5686	-0.5061
O	5.5898	2.0416	-1.7997
O	3.0544	2.1107	-1.868
F	-2.4529	5.8215	-1.9755
F	5.2593	-3.8219	0.4504

Appendix 2: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 2 (Mechanism of Iminium Salt-Catalyzed C(sp^3)-H Amination: Factors Controlling Hydride Transfer versus H-atom Abstraction)

A2.1 Methods

All optimizations of intermediates and transition states were calculated without constraints using unrestricted M06-2X/6-31+G(d,p)-LANL2DZ(I) level of the theory in implicit solvent (dichloromethane) using CPCM as solvation model with the "guess=mix, always" keywords as implemented in Gaussian 16.[219] Frequency calculations, at the same level of theory, were used to obtain thermal corrections (at 298K) and to characterize optimized structures as transition states (only a single imaginary frequency) or intermediate (if no imaginary frequencies were found). Intrinsic reaction coordinate (IRCs) calculations were undertaken to ensure transition states connected illustrated ground states. Single point energy calculations in implicit solvent (dichloromethane) using SMD as solvation model[220] with unrestricted M06-2X/6-311+G(d,p)-LANL2DZ (I) were also performed on all structures.[221] For comparison, single point energy calculations in implicit solvent (dichloromethane) using CPCM as solvation model with unrestricted B3LYP-D3/6-311+G(d,p)-SDD(I) were also performed on all structures.[222] All 3-D structures were generated using CYLview.[223] Kinetic isotope effects were calculated using PyQuiver.[224]

Molecular dynamics (MD) simulations were performed in the gas phase on the truncated open- shell singlet and triplet transition states $\mathbf{TS_{D\text{-}F}}$ and $\mathbf{^tTS_{D\text{-}F}}$. The truncated singlet $\mathbf{TS_{D\text{-}F}}$ and triplet $\mathbf{^tTS_{D\text{-}F}}$ were located at the UB3LYP/6-31G(d) level of theory using Gaussian 09 with HOMO−LUMO mixing for the initial guess in both transition state optimization and dynamics simulation. Quasi-classical direct-dynamics simulations were then

initialized within the region of the potential energy surface near $\mathbf{TS_{D\text{-}F}}$ and $^{t}\mathbf{TS_{D\text{-}F}}$, adding zero-point energy for each real normal mode in $\mathbf{TS_{D\text{-}F}}$ and $^{t}\mathbf{TS_{D\text{-}F}}$, plus a Boltzmann sampling of thermal energy available at 300 K with a random phase. The trajectories were propagated forward and backward until the emergence of the intermediate **F** (N−H< 1.15 Å and N−C > 5.00 Å), reactant **D** (N−H >5.00 Å), or product **P** (N−H < 1.20 Å and N−C < 1.60 Å). The classical equations of motion were integrated with a velocity-Verlet algorithm using Singleton's program Progdyn[225], with the energies and derivatives computed using the UB3LYP/6-31G(d) method with Gaussian 09. The step length for integration was 1 fs.

Input Parameters for Progdyn

The configuration file progdyn.conf for trajectory initialization for the singlet transition state is
given below. For the simulation from the triplet transition state, the multiplicity line is modified
to read multiplicity 3.

/#This is the configuration file for PROGDYN. This file is read by progdynstarterHP and

the awk programs proggenHP, prog1stpoint, prog2ndpoint, and progdynb.

#The programs won't read anything past the first blank line,

#and this file must end with a blank line.

#The program has a number of default values but they are unlikely to be what you want.

#Do not delete lines - rather, comment out lines for unwanted options.

#The values here are read repeatedly and most can be changed in the middle of running jobs

#***The keywords are case sensitive. The following keywords should always be defined:***

#***method, charge, multiplicity, memory, processors, title

#*** method --The following word is copied exactly to the gaussian input file.

method ub3lyp/6-31g(d)

#To do a nonstandard route, make nonstandard 1. For normal calcs, use nonstandard 0 or else
leave it out.

#Then make a file called "nonstandard" containing the nonstandard route with no extra lines.

nonstandard 0

NMRoptions As is NMR=1 will add a section for an NMR calc at every NMRevery intervals. If you want to combine the two use nonstandard

#NMRtype 1

#NMRmethod B3LYP/cc-pvtz

#NMRevery 4

#geometry linear

rotationmode 1

#*** method2 --The options here are restricted, unrestricted, and read. restricted is the default

#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.

#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things
faster, sometimes not.

#The use of read requires a specifically defined checkpoint file name using the keyword checkpoint.

method2 unrestricted

charge 1

multiplicity 1

processors 32

#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.memory 64gb

#*** killcheck and checkpoint -- You can use a specifically defined checkpoint file name by putting

#the name after the keyword checkpoint. This is necessary if you use the read option with method2.

#Defined checkpoint names are an unnecessary modest hastle and if you do not want to bother, use killcheck 1

killcheck 1

#checkpoint g09.chk

#*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra stuff to a

#file "diagnostics", 2 adds more stuff, 3 adds velocities to a file "vellist"

#4 adds the apparent temperature to vellist, but this is meaningless with quasiclassical calculations

diagnostics 1

#*** title -- the title keyword must be followed by exactly four words

title j j j C_TS_down_alkene

#*** initialdis -- 0 (default) turns off displacement of the normal modes, so that all trajectories start from the same place

and only the energies and signs of the motion in the modes are randomized

1 gives a flat distribution of displacements where all of the possible values are equally likely

2 (recommended) gives a QM-like gaussian distribution of displacements, so that displacements in the middle are more likely that

those at the end by 1/e

initialdis 2

#*** timestep -- this is the time bet*-ween points in the trajectory. Typical values would be 1E-15 or 0.5E-15 or 0.25E-15

timestep 1E-15

#*** scaling -- this lets you scale the gaussian frequencies by a constant

scaling 1.0

temperature 298.15

#*** method3, method4, method5, and method6 -- These keywords let you add extra lines to the gaussian input file.

#method3 and method4 add lines at the top of the input after the lines defining the method, and

#this is useful to implement things like the iop for mPW1k

#method5 and method6 add lines after the geometry, after a blank line of course

#only a single term with no spaces can be added, one per method line. Here are some examples to uncomment if needed

#method4 IOp(3/76=0572004280)

#method3 scrf=(cpcm,solvent=dichloromethane)
#add the line below with big structures to get it to put out the distance matrix and the input Orientation

#method3 iop(2/9=2000)

#method4 iop(3/124=3)

#method5 eps=32.63

#method6 rsolv=1.329

#*** methodfile -- This keyword lets you add more complicated endings to gaussian input files

#such as a gen basis set. Put after the keyword the number of lines in a file you create called

#methodfile that contains the test you want to add to the end of the gaussian input

methodfile 0

#*** numimag --This tells the program the number of imaginary frequencies in the starting structure.

#if 0, treats as ground state and direction of all modes is random

#if 1, motion along the reaction coordinate will start out in the direction defined by searchdir

#if 2, only lowest freq will go direction of searchdir and other imag mode will go in random direction

numimag 2

#*** searchdir -- This keyword says what direction to follow the mode associated with the imaginary frequency.

#The choices are "negative" and "positive". Positive moves in the direction defined in the gaussian frequency calculation

#for the imaginary frequency, while negative moves in the opposite direction. The correct choice can be made either

#by a careful inspection of the normal modes and standard orientation geometry, or by trial and error.

searchdir positive

#*** classical -- for quassiclassical dynamics, the default, use 0. for classical dynamics, use 1

#if there are no normal modes and the velocities are to be generated from scratch, use classical 2

classical 0

#*** DRP, saddlepoint, and maxAtomMove --to run a DRP use 'DRP 1' in the line below, otherwise leave it at 0 or comment it out

#the treatment of starting saddlepoints is not yet implemented so use saddlepoint no

#if DRP shows oscillations then decrease maxAtomMove

#DRP 1

#saddlepoint no

#maxAtomMove 0.01

#*** cannonball -- The program can "fire" a trajectory from a starting position toward a particular target, such as toward

#a ts. To use this, make a file cannontraj with numAtom lines and three numbers per line that defines the vector

#for firing the trajectory, relative to the starting geometry's standard orientation. The number following cannonball sets

#the extra energy being put into the structure in kcal/mol

#cannonball 10

#*** keepevery --This tells the program how often to write the gaussian output file to file dyn, after the first two points.

#Use 1 for most dynamics to start with, but use a higher number to save on disk space or molden loading time.

keepevery 1

#*** highlevel --For ONIOM jobs, the following line states the number of highlevel atoms,

#which must come before the medium level atoms. Use some high value such as 999 if not using ONIOM

highlevel 999

#*** fixedatom1, fixedatom2, fixedatom3, and fixedatom4 - These fix atoms in space.

#Fixing one atom serves no useful purpose and messes things up, while fixing two atoms

#fixes one distance and fixing three has the effect of fixing three distances, not just two

#in current form fixed atoms only are meant to work with no displacements, that is, initialdis=0

#fixedatom1 2

#fixedatom2 3

#fixedatom3 19

#*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that reach the edge

#are reflected back toward the middle. Useful for dynamics with solvent molecules. This is a crude

#implementation that is ok for a few thousand femtoseconds but will not conserve energy long term.

#Set the box size so as to fit the entire initial molecule but not have too much extra room.

#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5 leads to a box that is 15 x 15 x 15 angstroms

boxon 0

boxsize 7.5

#*** displacements -- This keyword lets you set the initialdis of particular modes by using a series of lines of the format

displacements NumberOfMode InitialDisForThatMode, as in the example below. You should be able to do as many of these as you like

you might consider this for rotations where a straight-line displacement goes wrong at large displacements

The choices for InitialDisForThatMode are 0, 1, 2, and 10, where 10 does the same thing as 0 but is maintained for now because

a previous version of the program had a bug that made 0 not work.

#displacements 2 0

#displacements 3 0

#*** etolerance --This sets the allowable difference between the desired energy in a trajectory and the actual

#energy, known after point 1 from the potential energy + the kinetic energy in the initial velocities.

#The unit is kcal/mol and 1 is a normal value for mid-sized organic systems. For very large and floppy molecules, a larger value

#may be needed, but the value must stay way below the average thermal energy in the molecule (not counting zpe).

#If initialdis is not 0 and few trajectories are being rejected, decrease the value.

etolerance 0.5

#*** controlphase --It is sometimes useful to set the phase of particular modes in the initialization of trajectories.

#The format is controlphase numberOfModeToControl positive or controlphase numberOfModeToControl negative.

#controlphase 2 positive

#*** damping -- The damping keyword lets you add or subtract energy from the system at each point, by multiplying the velocities

#by the damping factor. A damping of 1 has no effect, and since you mostly want to change the energy slowly, normal values range

#from 0.95 to 1.05. The use of damping lets one do simulated annealing - you add energy until the structure is moving enough

#to sample the kinds of possibilities you are interested in, then you take away the energy slowly.

damping 1

#*** reversetraj --This keyword sets the trajectories so that both directions from a transition state are explored.

reversetraj true

#updated Aug 9, 2007 to include the possibility of classical dynamics by the keyword classical

#updated Jan 2008 to include fixed atoms, ONIOM jobs, keepevery, and box size

#update Feb 2008 to include methodfile parameter

updated Nov 2008 to allow for start without an initial freq calc using classical = 2

update Aug 2010 to include etolerance, damping controlphase and reversetraj

A2.2 Supplementary Figures

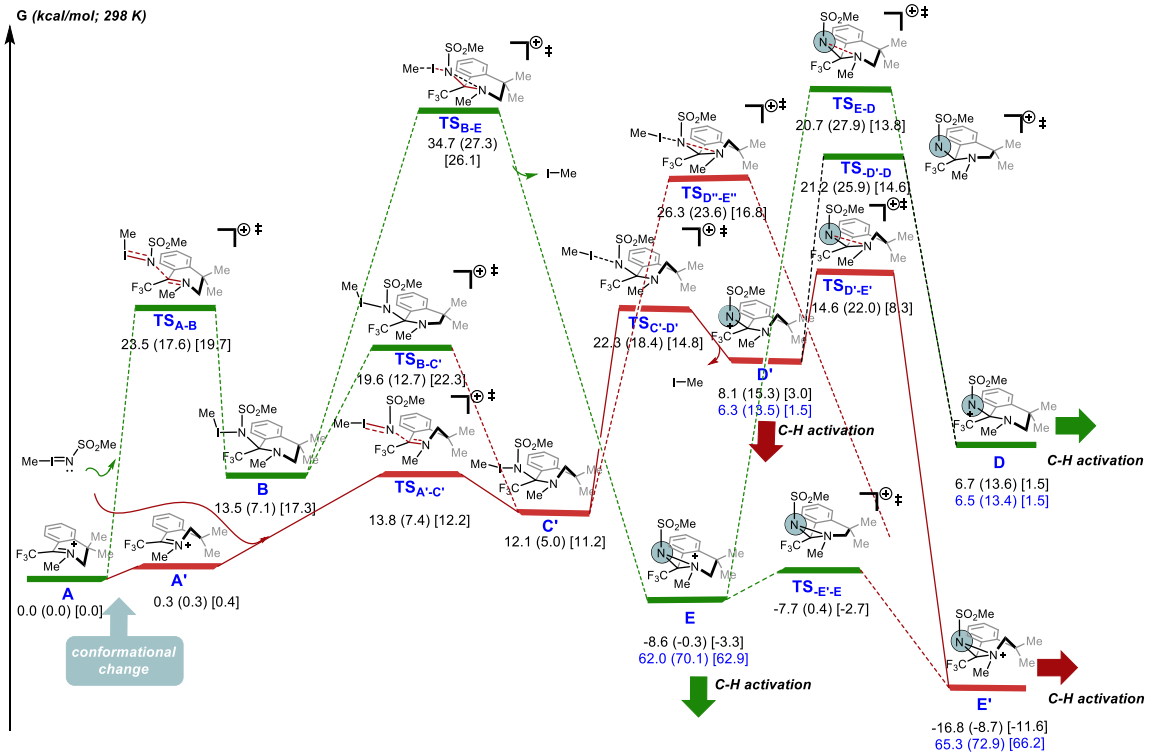


Figure A2.1 Energetics of reaction coordinate pathway leading to the formation of open-diaminium (**D** and **D'**) and closed-formed (**E** and **E'**) diaziridinium intermediates. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory. Singlet energies are given in black and triplet energies are in blue.

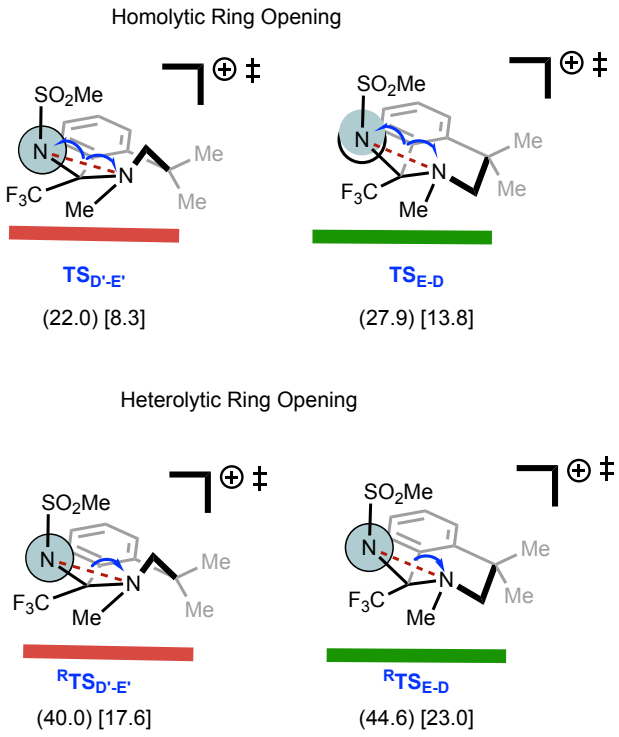


Figure A2.2 Comparison between homolytic (open-shell) and heterolytic (closed-shell) ring opening transition states $\mathbf{TS_{D'\text{-}E'}}$ and $\mathbf{TS_{E\text{-}D}}$. The heterolytic ring opening leading to the closed-shell nitrenium intermediates is significantly higher in energy. Free energies (kcal/mol) are computed at the UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane) (brackets) levels of theory.

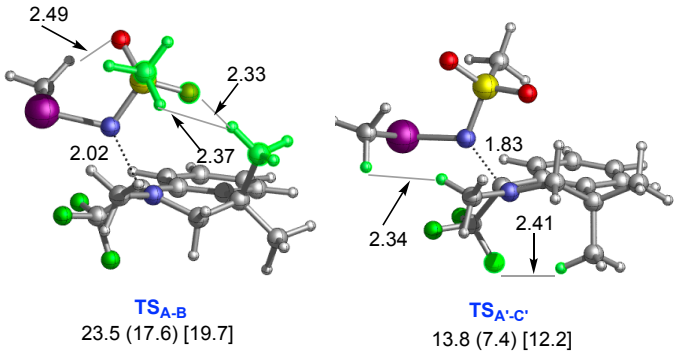


Figure A2.3 Comparison between $\mathbf{TS_{A\text{-}B}}$ and $\mathbf{TS_{A'\text{-}C'}}$. $\mathbf{TS_{A\text{-}B}}$ is ~10 kcal/mol higher in energy than $\mathbf{TS_{A'\text{-}C'}}$ as a result of the negative steric interaction between the axial groups (highlighted in green) which is not present in $\mathbf{TS_{A'\text{-}C'}}$. Key bond distances are given. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory.

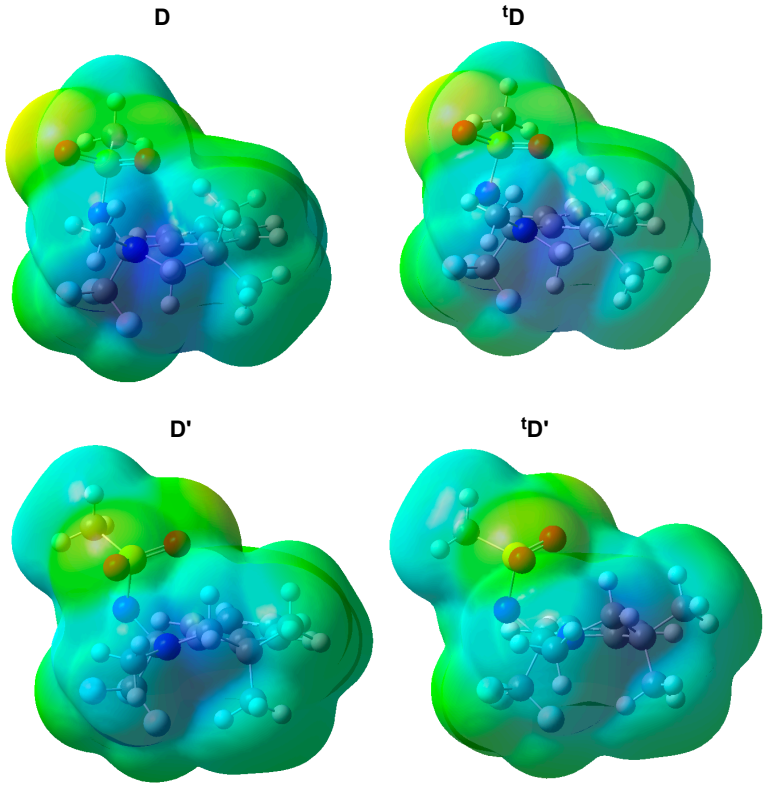


Figure A2.4 Electrostatic potential maps (EPM) of singlet **D** and **D'** (left) and triplet **D** and **D'** (right) states, with positive charge observed in the blue color. Diagrams are generated at the UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory.

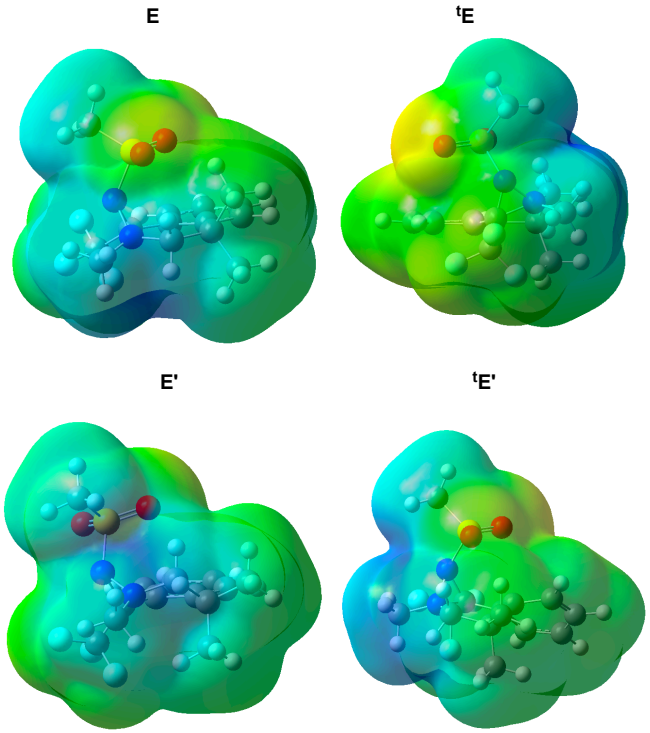


Figure A2.5 Electrostatic potential maps (EPM) of singlet **E** and **E'** (left) and triplet **E** and **E'** (right) states, with positive charge observed in the blue color. Diagrams are generated at the UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory.

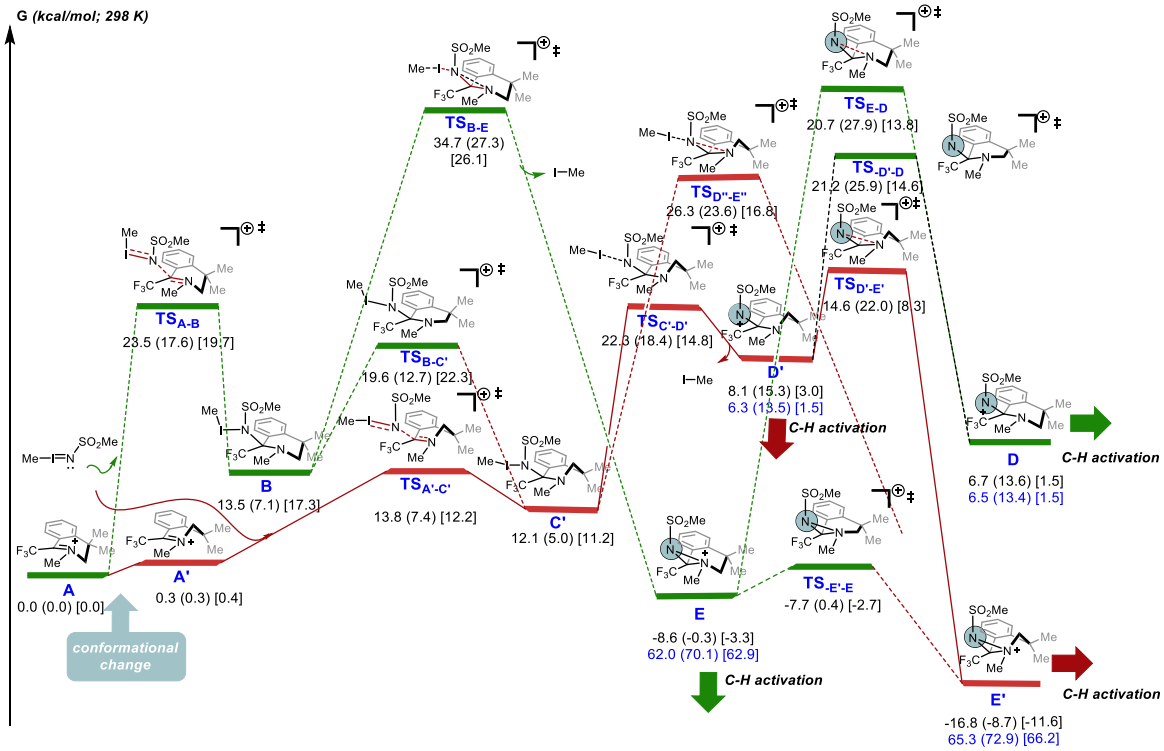


Figure A2.6 Energetics of reaction coordinate pathway leading to the formation of open-diaminium (**D** and **D'**) and closed-formed (**E** and **E'**) diaziridinium intermediates. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory. Singlet energies are given in black and triplet energies are in blue.

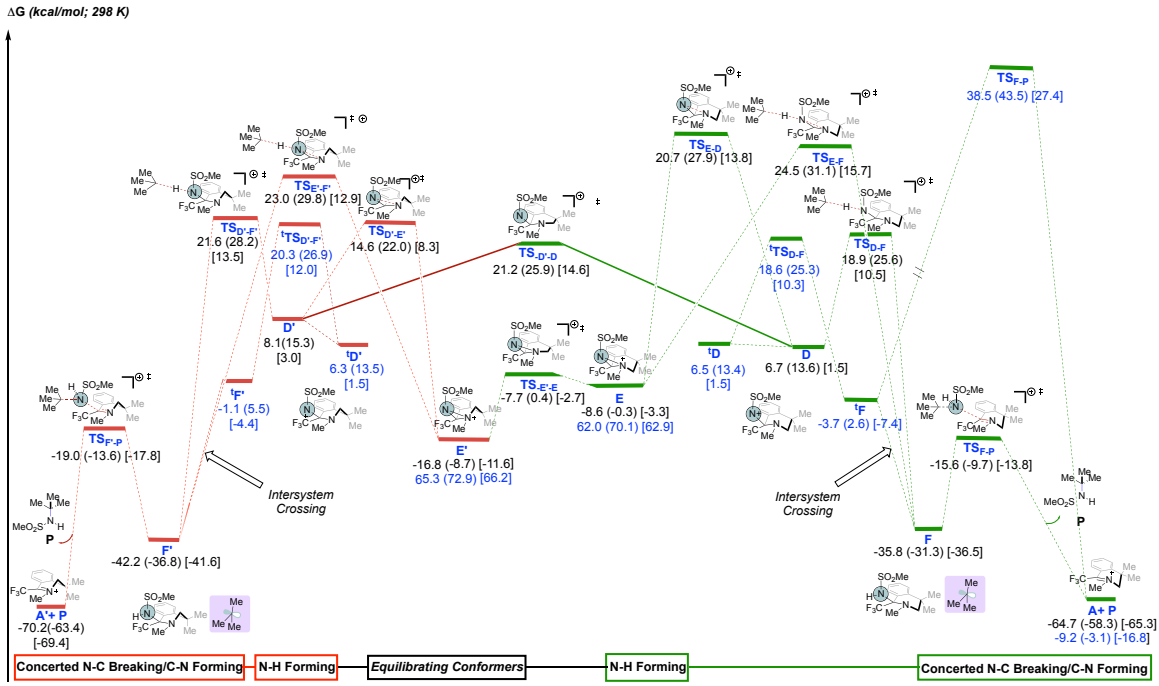


Figure A2.7 Pathways leading to C-H activation via open diaminium species **D** and **D'** and closed diaziridinium species **E** and **E'** which undergo N-H bond formation with the tertiary substrate to give F and F' respectively. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory. Singlet energies are given in black and triplet energies are in blue.

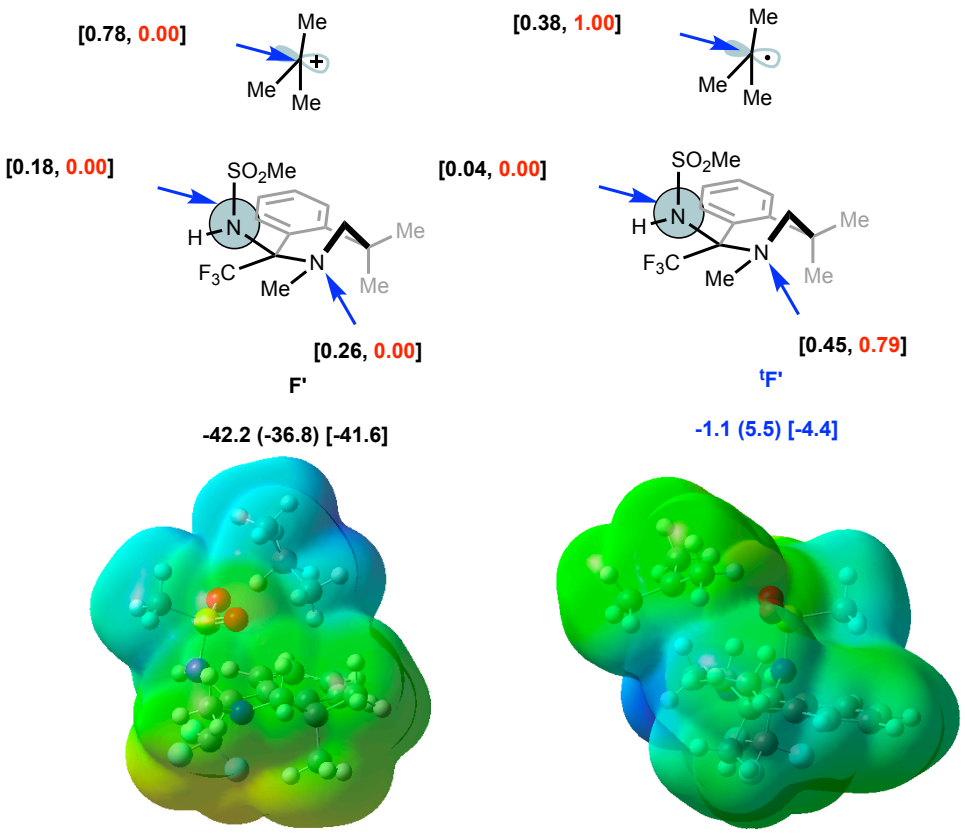


Figure A2.8 Comparison of singlet (left) and triplet (right) states of intermediate **F'**. Mulliken charges and spins for select atoms are given in black and red respectively. Electrostatic potential maps (EPM) are given as well. The singlet state of intermediate **F'** has a positive charge of 0.78 on the carbon substrate, which can be visually observed in the blue color on the EPM. The triplet state is characterized by a Mulliken spin of 1.00 on the carbon substrate, which is neutral (green) on the EPM. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory.

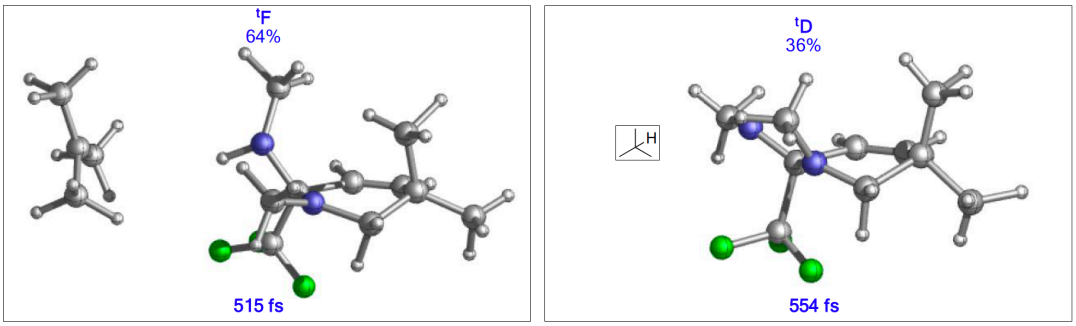


Figure A2.9 Summary of results from 28 MD simulations from the open-shell triplet transition state located using UM06-2X/6-31+G(d,p)-CPCM(dichloromethane) in Gaussian 09 propagated in the gas phase using UB3LYP/6-31G(d).

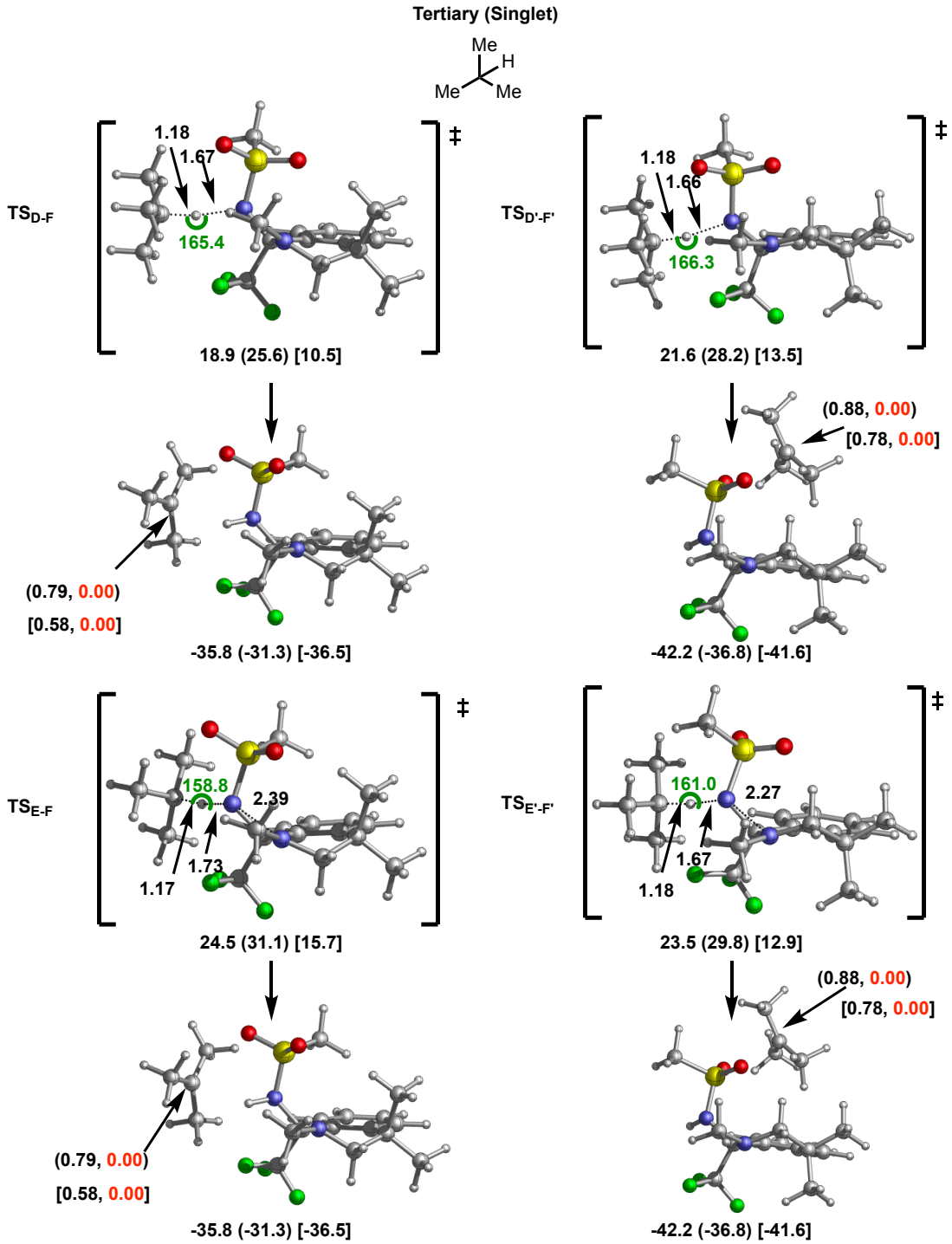


Figure A2.10 Transition states **TS$_{D'-F'}$**, **TS$_{E'-F'}$**, **TS$_{D-F}$**, and **TS$_{D'-F'}$** for the tertiary singlet substrate. All singlet transition states with a tertiary substrate proceed through a hydride transfer mechanism to intermediate **F**. Bond lengths (Å) are given as well as Mulliken charge (black) and spin (red) of the central carbon atom of the substrate. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-

CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory.

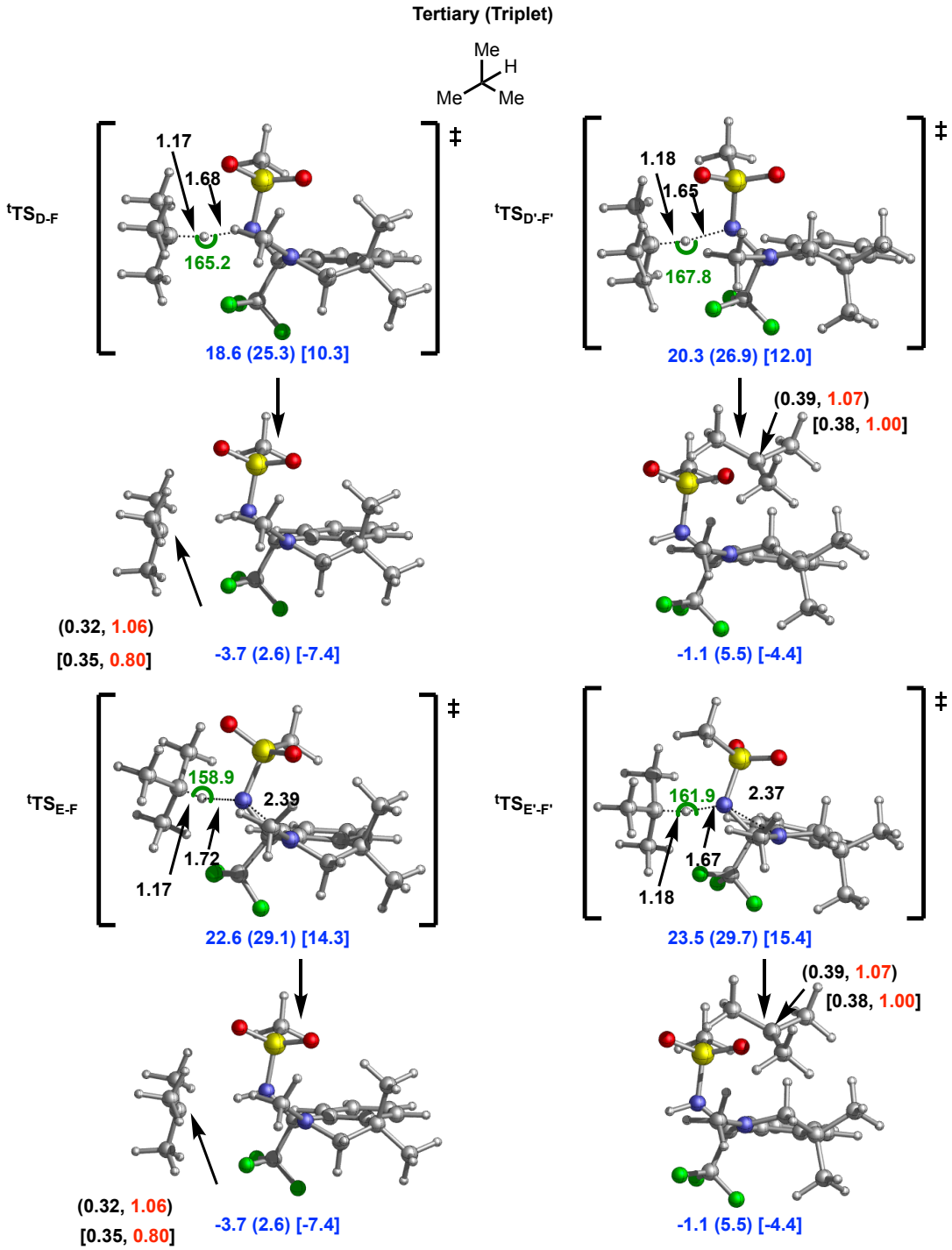


Figure A2.11 Transition states **$TS_{D'-F'}$, $TS_{E'-F'}$, TS_{D-F},** and **$TS_{D'-F'}$** for the tertiary singlet substrate. All singlet transition states with a tertiary substrate proceed through a hydride transfer mechanism to intermediate F. Bond lengths (Å) are given as well as Mulliken charge (black) and spin (red) of the central carbon atom of the substrate. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM),

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory.

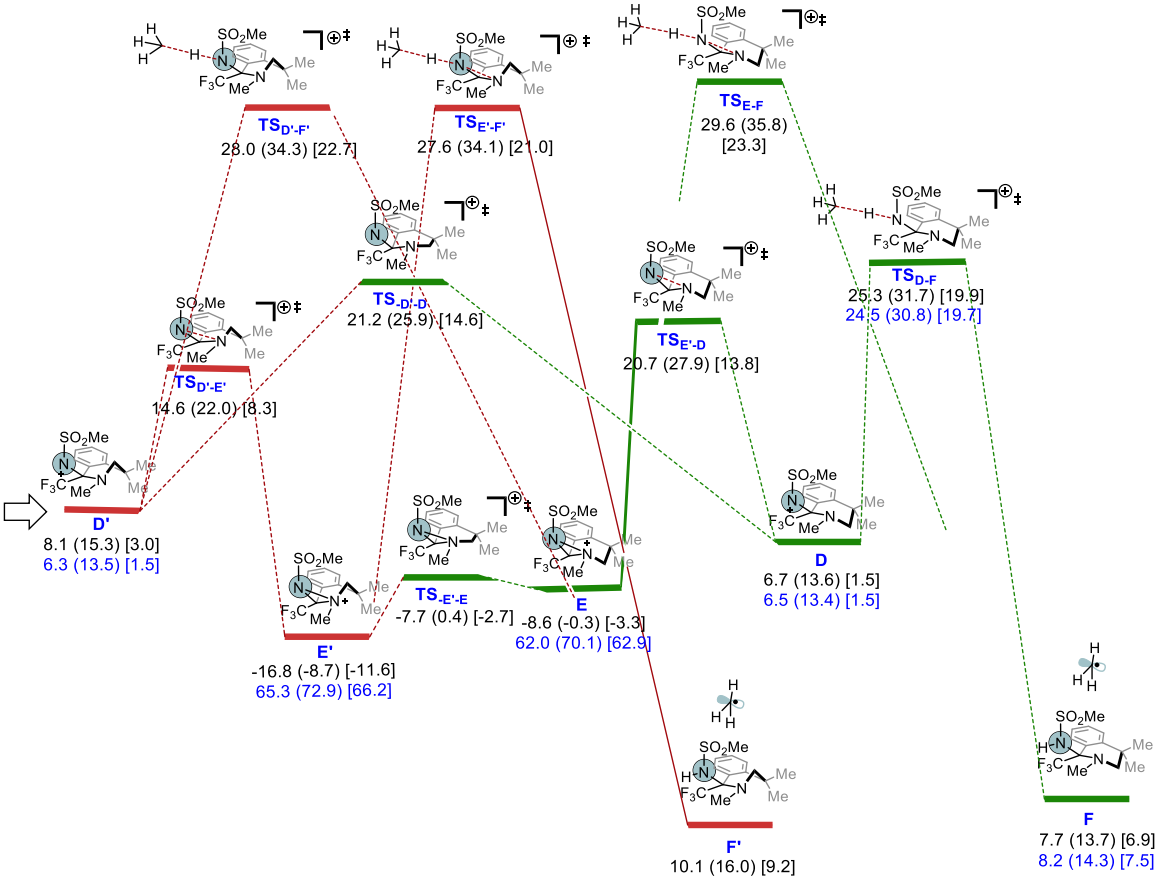


Figure A2.12 Pathways leading to C-H activation via open diaminium species **D** and **D'** and closed diaziridinium species **E** and **E'** which undergo N-H bond formation with the methyl substrate to give F and F' respectively. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory. Singlet energies are given in black and triplet energies are in blue.

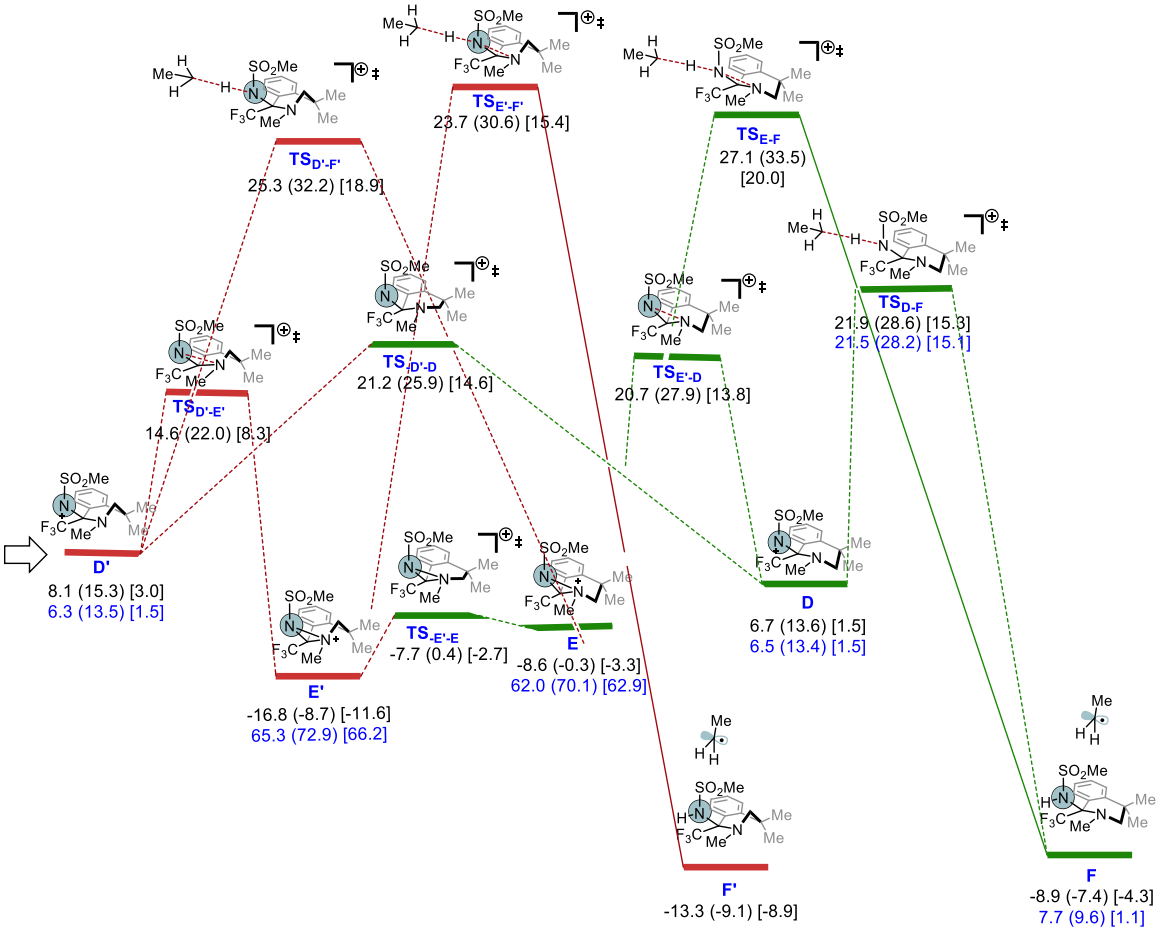


Figure A2.13 Pathways leading to C-H activation via open diaminium species **D** and **D'** and closed diaziridinium species **E** and **E'** which undergo N-H bond formation with the primary substrate to give F and F' respectively. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory. Singlet energies are given in black and triplet energies are in blue.

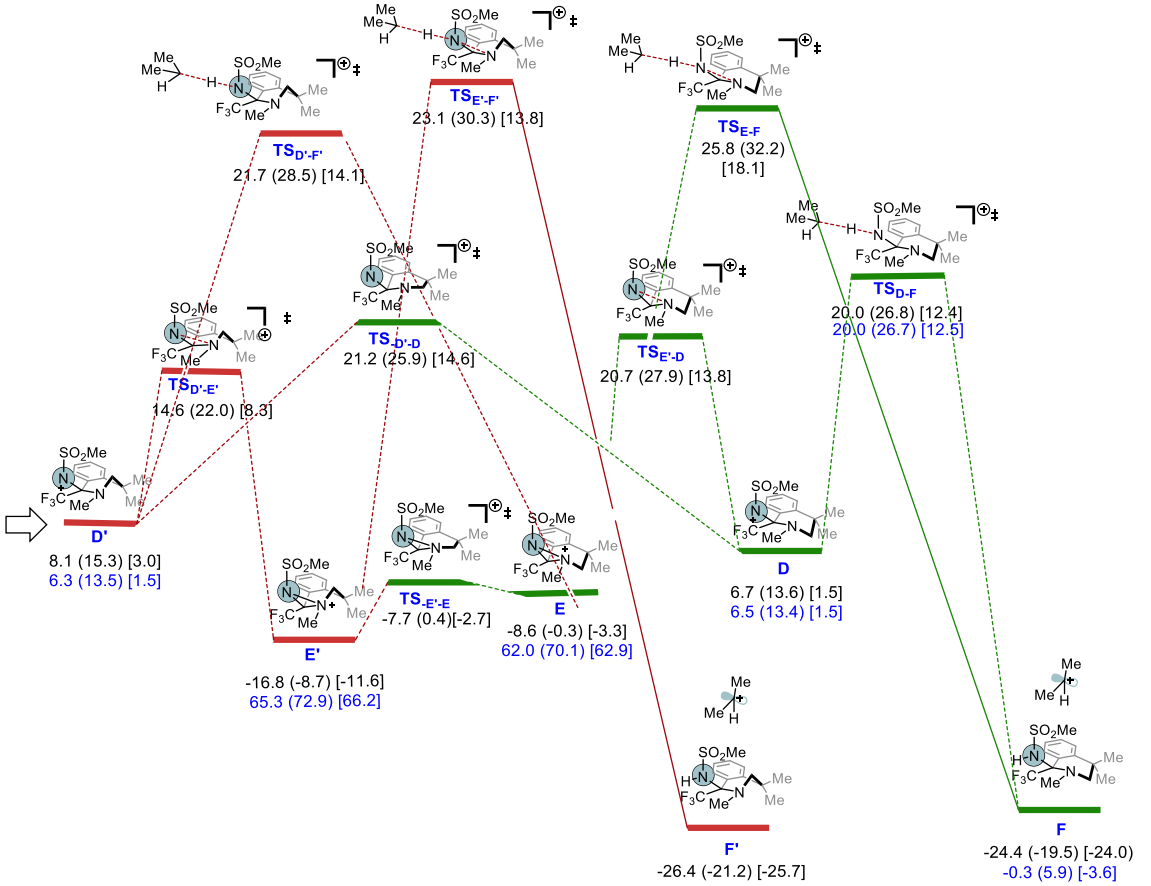


Figure A2.14 Pathways leading to C-H activation via open diaminium species **D** and **D'** and closed diaziridinium species **E** and **E'** which undergo N-H bond formation with the secondary substrate to give **F** and **F'** respectively. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory. Singlet energies are given in black and triplet energies are in blue.

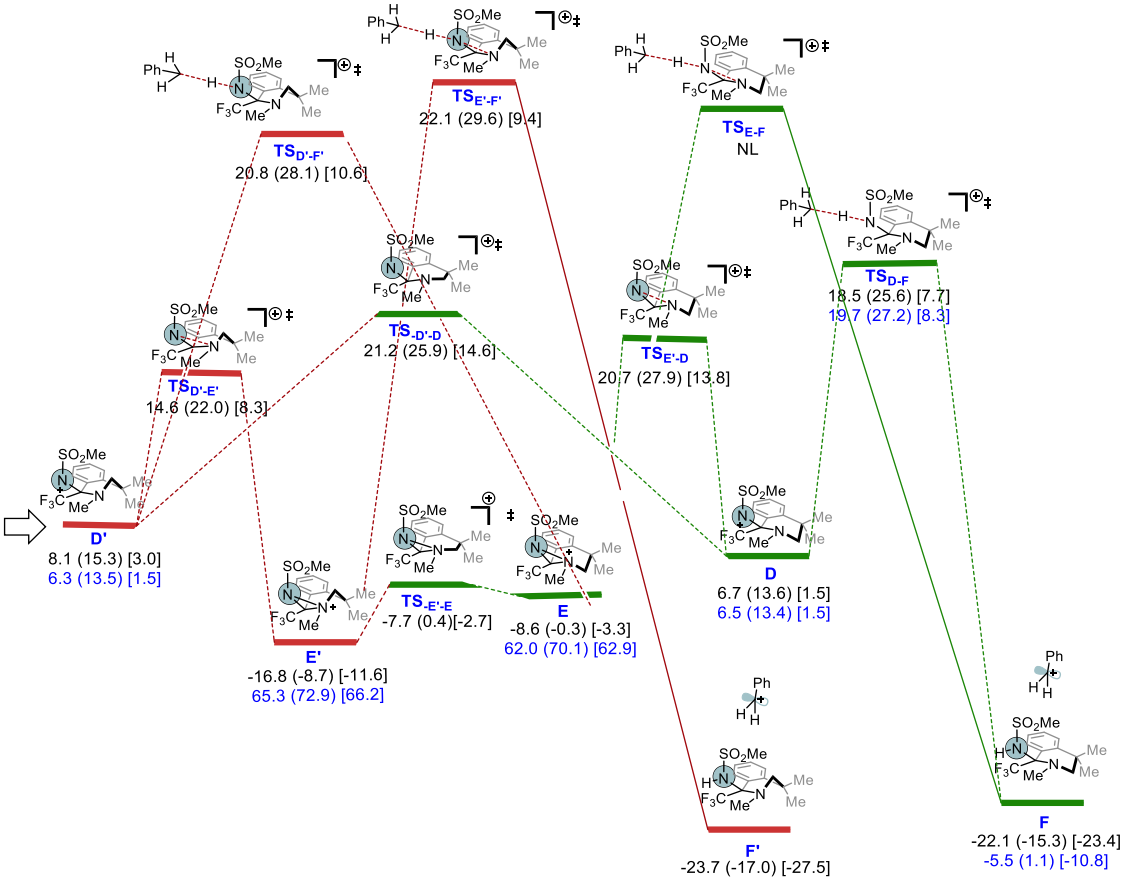


Figure A2.15 Pathways leading to C-H activation via open diaminium species **D** and **D'** and closed diaziridinium species **E** and **E'** which undergo N-H bond formation with the benzylic substrate to give **F** and **F'** respectively. Free energies (kcal/mol) are computed at the UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM), UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (parentheses) and UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) (brackets) levels of theory. Singlet energies are given in black and triplet energies are in blue.

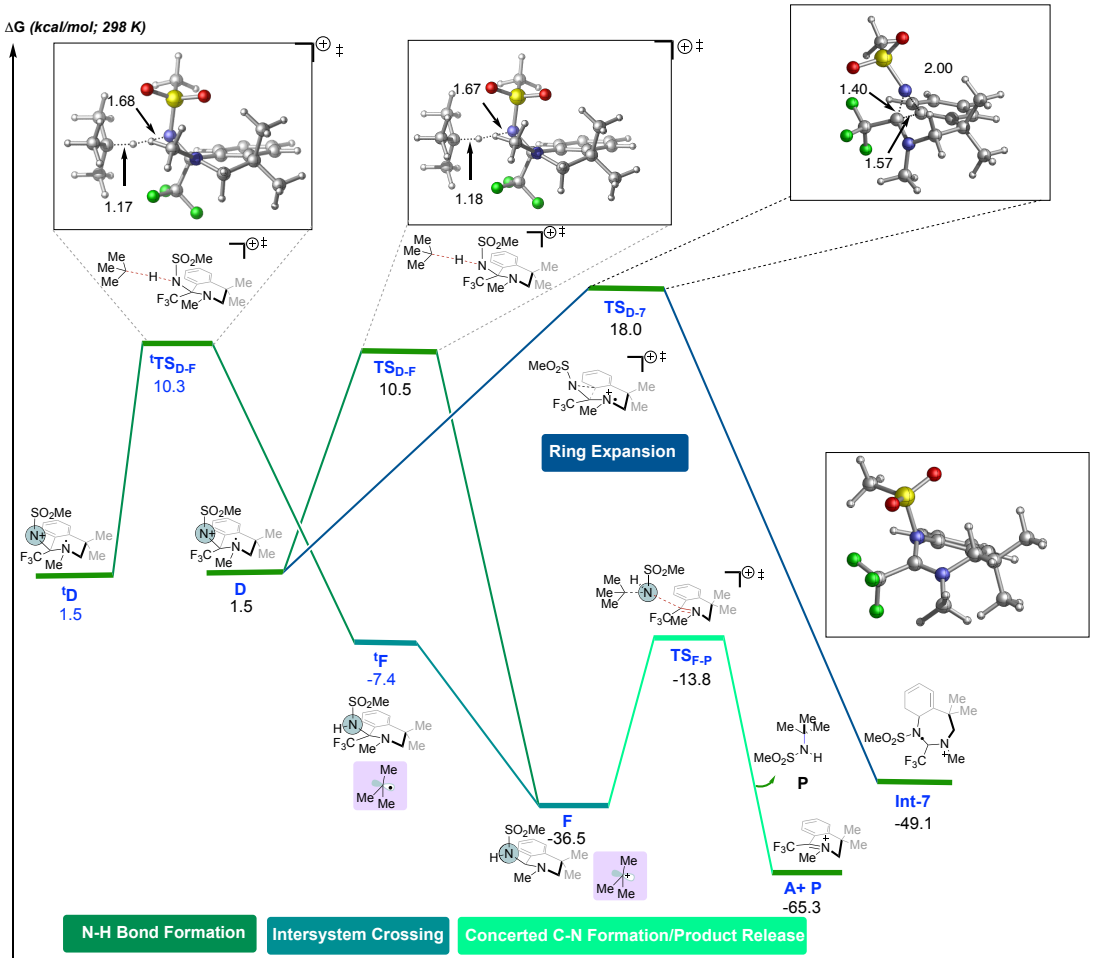


Figure A2.16 Energetics of competing N-H bond formation and ring-expansion to give **F** and **Int-7** respectively. Free energies (kcal/mol) are computed at the UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM) level of theory. Singlet energies are given in black and triplet energies are in blue.

A2.3 Coordinates and Energies

A

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.263263 (Hartree/Particle)
Thermal correction to Energy= 0.278436
Thermal correction to Enthalpy= 0.279380
Thermal correction to Gibbs Free Energy= 0.221725
Sum of electronic and zero-point Energies= -857.963998
Sum of electronic and thermal Energies= -857.948825
Sum of electronic and thermal Enthalpies= -857.947881
Sum of electronic and thermal Free Energies= -858.005536

C	1.596719	-1.359508	0.152726
C	1.582817	0.151736	0.006505
C	0.335034	0.799815	-0.148946
C	2.734164	0.928638	0.053056
H	3.699929	0.456454	0.192382
C	0.269962	2.195969	-0.316784
H	-0.674617	2.69566	-0.490028
C	1.437139	2.944653	-0.30313
H	1.389717	4.017418	-0.450686
C	2.663773	2.313445	-0.099317
H	3.576006	2.90065	-0.07304
C	1.310416	-1.747384	1.614527
H	1.318486	-2.836635	1.719914
H	2.084833	-1.330504	2.263585
H	0.343342	-1.372696	1.964344
C	2.923059	-1.98428	-0.293754
H	3.726201	-1.72816	0.401106
H	2.832678	-3.074317	-0.300449
H	3.206515	-1.651179	-1.296304
C	0.511692	-1.898725	-0.774786
H	0.744202	-1.702856	-1.829518
N	-0.807081	-1.280807	-0.503546
H	0.383143	-2.974102	-0.635347
C	-0.86295	-0.028997	-0.179976
C	-2.245031	0.53684	0.204665
F	-2.145695	1.688164	0.857752
F	-2.882495	-0.317136	1.010918
F	-2.990991	0.728958	-0.886944
C	-1.952406	-2.193883	-0.678801
H	-1.715345	-2.825799	-1.534668
H	-2.869649	-1.649347	-0.876275
H	-2.04957	-2.80874	0.218367

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -858.4509789
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -858.7963764

TS_{A-B}

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -171.37 cm^{-1}
Zero-point correction= 0.353784 (Hartree/Particle)
Thermal correction to Energy= 0.378948
Thermal correction to Enthalpy= 0.379893
Thermal correction to Gibbs Free Energy= 0.299192
Sum of electronic and zero-point Energies= -1552.097395
Sum of electronic and thermal Energies= -1552.072231
Sum of electronic and thermal Enthalpies= -1552.071287
Sum of electronic and thermal Free Energies= -1552.151987

C	0.675159	0.84652	-0.27623
N	1.124659	0.67259	-1.52638
C	0.324858	0.96207	-2.72056
H	-0.718271	0.709649	-2.54079
H	0.403758	2.01069	-3.02162
H	0.705819	0.33301	-3.52582
C	3.391999	-0.232708	-0.83369
C	2.862519	-0.058669	0.57978
C	1.577029	0.451471	0.84318
C	3.653029	-0.467088	1.65702
H	4.644949	-0.863528	1.46744
C	1.112789	0.50713	2.16947
H	0.104549	0.82643	2.38615
C	1.916309	0.102921	3.22346
H	1.536889	0.151881	4.23802
C	3.196989	-0.384918	2.96688
H	3.834589	-0.708758	3.78301
C	-0.126002	2.15019	-0.03244
F	0.782567	3.13183	0.02917
F	-0.839652	2.183759	1.09582
F	-0.972132	2.452729	-1.02344
S	-0.66883	-2.004201	-0.16605
N	-0.936031	-0.353431	-0.05204
I	-2.908631	0.122588	-0.12577
C	-3.325711	-0.274082	1.94383
H	-4.397301	-0.122633	2.06738
H	-3.02333	-1.308782	2.0898
H	-2.738151	0.442718	2.51197
O	0.65796	-2.22421	0.39475
O	-1.8104	-2.711611	0.42118
C	-0.6177	-2.401271	-1.90063
H	-1.5829	-2.158101	-2.3471
H	-0.417849	-3.47121	-1.97758
H	0.18707	-1.8229	-2.35642
C	2.579519	0.628551	-1.78893
C	3.31063	-1.713258	-1.24519
C	4.850269	0.239972	-0.95851
H	2.707789	0.261581	-2.80947
H	2.931688	1.668881	-1.75905
H	4.979858	1.243163	-0.54247
H	5.137529	0.261493	-2.01504
H	5.535369	-0.441547	-0.44971
H	2.27864	-2.064309	-1.27536
H	3.85113	-2.336718	-0.52703
H	3.76887	-1.844388	-2.23084

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1552.7979491
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)

HF = -1553.3771916

B

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.356070 (Hartree/Particle)
Thermal correction to Energy= 0.380634
Thermal correction to Enthalpy= 0.381578
Thermal correction to Gibbs Free Energy= 0.303829
Sum of electronic and zero-point Energies= -1552.115559
Sum of electronic and thermal Energies= -1552.090994
Sum of electronic and thermal Enthalpies= -1552.090050
Sum of electronic and thermal Free Energies= -1552.167799

C	0.35481	-0.17804	0.64722
N	0.985409	0.92765	1.31462
C	0.269579	1.50523	2.45863
H	-0.795771	1.588939	2.24553
H	0.402919	0.91301	3.37349
H	0.670399	2.50558	2.63688
C	3.285789	0.552881	0.39381
C	2.63346	-0.492789	-0.49586
C	1.28359	-0.84846	-0.37418
C	3.39062	-1.088669	-1.51466
H	4.43272	-0.808268	-1.63001
C	0.739621	-1.79436	-1.25452
H	-0.295809	-2.105691	-1.17214
C	1.503271	-2.38076	-2.25215
H	1.054411	-3.10874	-2.91878
C	2.843251	-2.018679	-2.38677
H	3.455941	-2.459939	-3.16598
C	-0.14222	-1.252081	1.68672
F	0.84683	-1.50677	2.54522
F	-0.502809	-2.425421	1.14826
F	-1.1984	-0.818941	2.40038
S	-0.595831	1.769729	-1.1353
N	-0.866791	0.455869	-0.00085
I	-2.55541	-0.602152	-0.42198
C	-3.789941	0.664508	0.79109
H	-4.77729	0.204387	0.78825
H	-3.330891	0.655998	1.77718
H	-3.778931	1.635278	0.30092
O	0.574609	1.49484	-1.94384
O	-1.901961	1.910729	-1.77058
C	-0.331342	3.220719	-0.14191
H	-1.144652	3.302679	0.57808
H	-0.373302	4.039079	-0.86418
H	0.643068	3.151	0.33416
C	2.414459	0.782581	1.62239
C	3.459179	1.863341	-0.39304
C	4.65926	0.084812	0.90143
H	2.719359	1.719571	2.09932
H	2.57397	-0.020069	2.35579
H	4.59685	-0.908378	1.35615
H	5.027949	0.788192	1.65575
H	5.3977	0.052972	0.09702
H	2.496139	2.257951	-0.72204
H	4.072129	1.695781	-1.28391
H	3.960698	2.608641	0.23338

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1552.8196956

UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1553.3856677

$TS_{B\text{-}E}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -428.79 cm^{-1}
Zero-point correction= 0.354413 (Hartree/Particle)
Thermal correction to Energy= 0.379360
Thermal correction to Enthalpy= 0.380304
Thermal correction to Gibbs Free Energy= 0.300614
Sum of electronic and zero-point Energies= -1552.080336
Sum of electronic and thermal Energies= -1552.055388
Sum of electronic and thermal Enthalpies= -1552.054444
Sum of electronic and thermal Free Energies= -1552.134135

C	0.353565	-0.38097	0.711123
N	0.865138	0.778934	1.424106
C	0.323376	1.238659	2.73936
H	-0.758502	1.267861	2.70105
H	0.677965	0.573464	3.528486
H	0.721005	2.240963	2.894145
C	3.259479	0.467961	0.302153
C	2.576809	-0.622357	-0.506027
C	1.241482	-0.992777	-0.339569
C	3.305623	-1.243858	-1.528111
H	4.349003	-0.980898	-1.672458
C	0.640196	-1.911313	-1.211656
H	-0.404152	-2.174436	-1.102321
C	1.376455	-2.499093	-2.229582
H	0.898998	-3.206962	-2.897567
C	2.721605	-2.171054	-2.378686
H	3.314445	-2.630725	-3.161708
C	-0.261676	-1.411105	1.691378
F	0.725639	-1.704894	2.556521
F	-0.646794	-2.539862	1.116581
F	-1.288993	-0.927872	2.389124
S	-0.237826	1.896642	-1.020799
N	-0.422941	0.807582	0.422265
I	-2.80325	-0.474206	-0.55517
C	-3.646372	1.081293	0.66543
H	-4.719132	0.921452	0.698355
H	-3.202298	0.99247	1.652653
H	-3.390623	2.025009	0.188471
O	0.756562	1.364429	-1.924096
O	-1.56836	2.207207	-1.495274
C	0.331375	3.299395	-0.100126
H	-0.38071	3.473811	0.707471
H	0.314429	4.12868	-0.808929
H	1.344502	3.13384	0.259064
C	2.379437	0.969865	1.447683
C	3.660365	1.644517	-0.60857
C	4.541504	-0.082303	0.968265
H	2.566693	2.022304	1.671375
H	2.592981	0.393521	2.356935
H	4.326265	-0.975383	1.562754
H	4.986297	0.677401	1.618447
H	5.282926	-0.339671	0.208623
H	2.80855	2.061444	-1.145985
H	4.383656	1.309849	-1.356988
H	4.136148	2.426442	-0.013156

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1552.7840474
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1553.3683495

E (singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.318648 (Hartree/Particle)
Thermal correction to Energy= 0.339132
Thermal correction to Enthalpy= 0.340077
Thermal correction to Gibbs Free Energy= 0.271359
Sum of electronic and zero-point Energies= -1500.944905
Sum of electronic and thermal Energies= -1500.924421
Sum of electronic and thermal Enthalpies= -1500.923477
Sum of electronic and thermal Free Energies= -1500.992194

H	-2.443597	-2.887949	1.151647
H	1.660972	-1.634196	2.772032
H	1.59585	0.118494	3.148108
H	-0.293819	-2.213519	1.696807
C	1.798662	-0.627257	2.380853
C	-2.446391	-2.060734	0.435128
H	-2.834465	-1.205769	3.011577
H	-1.879159	-2.358489	-0.446689
C	-0.508359	-1.145352	1.753254
H	2.788359	-0.521981	1.955949
H	-3.481215	-1.886774	0.133323
C	-2.796513	-0.398939	2.273032
N	0.772015	-0.475984	1.28859
C	-1.865955	-0.796765	1.103891
O	0.635999	-3.009162	-0.374428
H	-0.525789	-0.851309	2.803334
H	-3.813131	-0.226259	1.915116
H	-2.44066	0.511891	2.763125
N	1.350354	-0.605675	-0.025877
F	2.762066	1.522746	1.216429
S	0.821883	-1.821712	-1.188011
C	0.706144	0.639147	0.308046
C	-1.805943	0.3521	0.110255
O	-0.254434	-1.302639	-2.005291
C	1.72525	1.799664	0.430857
F	1.13734	2.89592	0.90075
H	-3.926334	0.242933	-0.237618
C	-0.636391	1.036738	-0.237869
C	-3.003921	0.751456	-0.495971
H	3.123354	-2.208764	-1.448437
C	2.325284	-1.893391	-2.118611
F	2.214549	2.052038	-0.788207
H	2.145667	-2.628207	-2.905941
C	-0.676091	2.076108	-1.181623
C	-3.045783	1.777722	-1.428746
H	2.508802	-0.905562	-2.542521
C	-1.872763	2.444185	-1.776355
H	0.22295	2.602772	-1.472042
H	-3.990902	2.055014	-1.88332
H	-1.885088	3.246661	-2.50511

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.578579
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0526981

^{t}E (triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.313149 (Hartree/Particle)
Thermal correction to Energy= 0.334592
Thermal correction to Enthalpy= 0.335536
Thermal correction to Gibbs Free Energy= 0.263314
Sum of electronic and zero-point Energies= -1500.829947
Sum of electronic and thermal Energies= -1500.808504
Sum of electronic and thermal Enthalpies= -1500.807560
Sum of electronic and thermal Free Energies= -1500.879782

H	2.696509	1.913841	2.639599
H	-1.918634	0.911931	2.95597
H	-1.579768	-0.848883	3.002058
H	0.201837	1.898122	1.899432
C	-1.886168	-0.01051	2.375884
C	2.697446	1.665855	1.573688
H	2.552568	-0.572094	3.044296
H	2.376062	2.544836	1.007994
C	0.400243	0.827389	1.934723
H	-2.843009	-0.188426	1.90099
H	3.722425	1.41275	1.29025
C	2.329263	-0.789609	1.995475
N	-0.834899	0.180172	1.329403
C	1.766401	0.476795	1.309277
O	0.001853	2.830872	-0.140405
H	0.377883	0.494293	2.973307
H	3.254411	-1.100904	1.50134
H	1.621289	-1.623254	1.95881
N	-1.37218	0.585632	0.053424
F	-2.927126	-1.607026	0.289898
S	-0.868423	1.96905	-0.918486
C	-0.718435	-0.695404	0.064912
C	1.594376	0.217649	-0.16915
O	-0.432281	1.381485	-2.168743
C	-1.675767	-1.893767	-0.059579
F	-1.246883	-2.902575	0.704178
H	3.258302	1.27724	-1.197153
C	0.635375	-0.886891	-0.448476
C	2.743718	0.327537	-1.083754
H	-2.811549	3.009752	-0.10925
C	-2.460258	2.723316	-1.100277
F	-1.703407	-2.300113	-1.330682
H	-2.302368	3.598885	-1.732562
C	1.131046	-2.042841	-1.009633
C	3.165118	-0.788068	-1.717342
H	-3.122935	2.002034	-1.576304
C	2.414624	-2.023889	-1.591252
H	0.546495	-2.95424	-1.074568
H	4.035761	-0.770013	-2.364211
H	2.797306	-2.928103	-2.048346

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.4583375
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.9391911

$TS_{E'-E}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -14.82 cm^{-1}
Zero-point correction= 0.318460 (Hartree/Particle)
Thermal correction to Energy= 0.338125
Thermal correction to Enthalpy= 0.339070
Thermal correction to Gibbs Free Energy= 0.272537
Sum of electronic and zero-point Energies= -1500.944969
Sum of electronic and thermal Energies= -1500.925304
Sum of electronic and thermal Enthalpies= -1500.924360
Sum of electronic and thermal Free Energies= -1500.990893

C	0.710894	0.626973	0.309123
N	0.767056	-0.486792	1.290401
C	1.786347	-0.647812	2.387352
H	2.777798	-0.500526	1.97975
H	1.553279	0.063756	3.178019
H	1.672438	-1.672679	2.738438
C	-1.875013	-0.751371	1.139078
C	-1.798924	0.353858	0.098431
C	-0.622633	1.018433	-0.260437
C	-2.989394	0.746805	-0.526165
H	-3.919306	0.25849	-0.255865
C	-0.642906	2.024847	-1.239445
H	0.265084	2.530962	-1.539625
C	-1.831496	2.383947	-1.855525
H	-1.830743	3.160476	-2.611994
C	-3.013877	1.742413	-1.492323
H	-3.95315	2.015087	-1.961562
C	1.720311	1.795552	0.444097
F	2.246599	2.029537	-0.763079
F	2.731881	1.541662	1.269336
F	1.110441	2.896257	0.873532
S	0.818071	-1.832829	-1.185143
N	1.360995	-0.617316	-0.020165
O	0.731313	-3.042534	-0.387878
O	-0.328083	-1.358664	-1.931723
C	2.269853	-1.811486	-2.196149
H	2.373737	-0.811477	-2.618509
H	2.087233	-2.54824	-2.981133
H	3.120926	-2.087927	-1.575919
C	-0.509696	-1.188168	1.717568
C	-2.546734	-2.008805	0.549537
C	-2.721235	-0.243319	2.327885
H	-0.306665	-2.245026	1.539534
H	-0.507659	-1.018422	2.794114
H	-2.266728	0.643312	2.779967
H	-2.805083	-1.024449	3.089828
H	-3.729432	0.015519	1.997975
H	-2.013544	-2.369702	-0.332694
H	-3.580669	-1.801178	0.268204
H	-2.562126	-2.802678	1.302647

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5785551
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0529197

$TS_{D-D'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -90.06 cm^{-1}
Zero-point correction= 0.313274 (Hartree/Particle)
Thermal correction to Energy= 0.333767
Thermal correction to Enthalpy= 0.334711
Thermal correction to Gibbs Free Energy= 0.265685
Sum of electronic and zero-point Energies= -1500.897160
Sum of electronic and thermal Energies= -1500.876667
Sum of electronic and thermal Enthalpies= -1500.875723
Sum of electronic and thermal Free Energies= -1500.944749

C	0.341339	-0.448717	0.43268
N	0.136294	-1.342387	-0.734562
C	0.984771	-2.503591	-0.917813
H	1.936306	-2.384118	-0.402935
H	0.451881	-3.369829	-0.492867
H	1.11521	-2.683096	-1.986384
C	-2.191439	-0.494727	-1.228846
C	-1.895572	0.616371	-0.236049
C	-0.70704	0.667781	0.505528
C	-2.83586	1.633214	-0.029924
H	-3.769568	1.612566	-0.58082
C	-0.458234	1.722175	1.39571
H	0.471659	1.756031	1.950847
C	-1.400315	2.724029	1.570061
H	-1.199151	3.538103	2.257272
C	-2.59957	2.672041	0.860929
H	-3.34852	3.445274	0.995773
C	0.250117	-1.34818	1.724104
F	-0.858379	-2.089905	1.689553
F	0.228833	-0.592086	2.80988
F	1.296747	-2.173219	1.816848
S	2.571939	0.981332	-0.645345
N	1.664104	0.116135	0.517459
O	1.90544	2.27287	-0.681647
O	3.927825	0.849182	-0.155107
C	2.489121	0.215961	-2.246068
H	3.182423	0.797366	-2.858843
H	1.484315	0.307765	-2.65241
H	2.840772	-0.813216	-2.173549
C	-0.863321	-1.067471	-1.741134
H	-1.006312	-1.985945	-2.316548
H	-0.408798	-0.325766	-2.422314
C	-2.913876	0.031386	-2.481335
C	-3.044165	-1.606336	-0.5928
H	-2.418514	0.917321	-2.888394
H	-3.950866	0.282457	-2.25136
H	-2.934003	-0.746376	-3.250852
H	-2.544497	-2.084121	0.250235
H	-3.280122	-2.369042	-1.341171
H	-3.982682	-1.176058	-0.233205

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5311071
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.01842

TS_{E-D}

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -547.26 cm^{-1}
Zero-point correction= 0.313551 (Hartree/Particle)
Thermal correction to Energy= 0.334555
Thermal correction to Enthalpy= 0.335499
Thermal correction to Gibbs Free Energy= 0.264507
Sum of electronic and zero-point Energies= -1500.896584
Sum of electronic and thermal Energies= -1500.875580
Sum of electronic and thermal Enthalpies= -1500.874636
Sum of electronic and thermal Free Energies= -1500.945628

C	0.658559	-0.624719	0.166629
N	0.354548	-1.324689	-1.084341
C	1.382928	-2.02589	-1.864751
H	2.378848	-1.73804	-1.550701
H	1.216867	-3.09899	-1.719281
H	1.224428	-1.77586	-2.914861
C	-2.113301	-0.697558	-1.064451
C	-1.837761	-0.092948	0.302229
C	-0.564421	-0.081848	0.892229
C	-2.884131	0.546303	0.975809
H	-3.876281	0.546143	0.537749
C	-0.351761	0.611681	2.094279
H	0.640139	0.694611	2.517479
C	-1.40422	1.244312	2.739489
H	-1.22209	1.774472	3.667519
C	-2.6801	1.202903	2.181849
H	-3.51167	1.693313	2.676699
C	1.577198	-1.55714	1.039969
F	1.095547	-2.803249	0.923799
F	1.599828	-1.24726	2.327449
F	2.836558	-1.54922	0.603489
S	1.13618	2.014131	-0.579311
N	1.425439	0.30669	-0.650781
O	-0.25557	2.389451	-0.723561
O	1.86519	2.32811	0.644399
C	2.0559	2.50123	-2.009461
H	3.0736	2.128379	-1.904191
H	2.030321	3.5923	-2.021741
H	1.55728	2.08952	-2.887481
C	-1.014692	-1.689468	-1.423221
C	-2.186251	0.391252	-2.151161
C	-3.424772	-1.504067	-1.077101
H	-1.035272	-1.948158	-2.483241
H	-1.148883	-2.618328	-0.835451
H	-3.477162	-2.193437	-0.230101
H	-3.497652	-2.079277	-2.005321
H	-4.288572	-0.837896	-1.041461
H	-1.222911	0.877372	-2.313721
H	-2.90322	1.162553	-1.858091
H	-2.519981	-0.055967	-3.092411

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5266725
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0185861

D (singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.313210 (Hartree/Particle)
Thermal correction to Energy= 0.334658
Thermal correction to Enthalpy= 0.335602
Thermal correction to Gibbs Free Energy= 0.264298
Sum of electronic and zero-point Energies= -1500.918996
Sum of electronic and thermal Energies= -1500.897548
Sum of electronic and thermal Enthalpies= -1500.896604
Sum of electronic and thermal Free Energies= -1500.967908

C	-0.425322	0.634169	0.37862
N	-0.173833	1.229999	-0.93675
C	-1.254893	1.696728	-1.78108
H	-1.064305	2.748198	-2.02004
H	-1.228492	1.117288	-2.71359
H	-2.218833	1.576376	-1.29028
C	2.112109	0.280403	-1.27544
C	1.82041	-0.537118	-0.02733
C	0.68432	-0.35183	0.77316
C	2.730642	-1.523826	0.36864
H	3.619312	-1.695095	-0.22998
C	0.476221	-1.11331	1.93329
H	-0.408029	-0.953651	2.54
C	1.401172	-2.080338	2.30345
H	1.237483	-2.665799	3.2011
C	2.527193	-2.291387	1.51018
H	3.253074	-3.050166	1.78214
C	-0.527394	1.836789	1.3855
F	0.633295	2.48756	1.46218
F	-0.851193	1.405908	2.59544
F	-1.464675	2.692767	0.96993
C	1.89905	-0.550358	-2.55057
H	2.173639	0.042243	-3.42854
H	2.542091	-1.434457	-2.52269
H	0.864731	-0.882379	-2.64909
C	3.546518	0.834505	-1.25291
H	4.270949	0.031186	-1.40057
H	3.680907	1.549935	-2.06981
H	3.765597	1.335005	-0.30577
S	-2.157429	-1.177944	-0.71012
N	-1.670001	-0.073503	0.51957
O	-3.4223	-0.640046	-1.18627
O	-1.063929	-1.380922	-1.65327
C	-2.408847	-2.627274	0.27387
H	-3.123207	-2.382845	1.05929
H	-1.443396	-2.936453	0.67625
H	-2.809956	-3.380765	-0.40715
C	1.186877	1.523701	-1.30641
H	1.561176	2.254802	-0.57355
H	1.177606	1.984711	-2.29499

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5492833
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0380424

D (triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.313269 (Hartree/Particle)
Thermal correction to Energy= 0.334723
Thermal correction to Enthalpy= 0.335667
Thermal correction to Gibbs Free Energy= 0.263221
Sum of electronic and zero-point Energies= -1500.918203
Sum of electronic and thermal Energies= -1500.896749
Sum of electronic and thermal Enthalpies= -1500.895805
Sum of electronic and thermal Free Energies= -1500.968251

C	-0.430055	0.632393	0.378469
N	-0.177089	1.23042	-0.940793
C	-1.254808	1.735333	-1.766349
H	-1.101325	2.812777	-1.900575
H	-1.17542	1.251521	-2.747887
H	-2.226685	1.541419	-1.317941
C	2.119184	0.294735	-1.258876
C	1.819264	-0.530566	-0.016496
C	0.677133	-0.346972	0.775403
C	2.723389	-1.522649	0.377919
H	3.616247	-1.692833	-0.214865
C	0.459125	-1.115453	1.929172
H	-0.428276	-0.956513	2.531909
C	1.377682	-2.089475	2.298961
H	1.205533	-2.680956	3.191041
C	2.508902	-2.297852	1.513006
H	3.231078	-3.059889	1.785759
C	-0.548261	1.832215	1.385454
F	0.601723	2.50257	1.459301
F	-0.862738	1.398629	2.597254
F	-1.501121	2.671867	0.971478
C	1.934037	-0.536447	-2.538425
H	2.212978	0.061343	-3.411561
H	2.587593	-1.412453	-2.504349
H	0.905233	-0.880558	-2.651783
C	3.54903	0.860101	-1.213151
H	4.281872	0.061933	-1.346387
H	3.692089	1.575368	-2.028772
H	3.747805	1.363715	-0.263156
S	-2.134175	-1.19475	-0.72667
N	-1.687627	-0.069415	0.504373
O	-3.40367	-0.676254	-1.213158
O	-1.028611	-1.375556	-1.660084
C	-2.3711	-2.649256	0.252468
H	-3.092687	-2.416353	1.034922
H	-1.403638	-2.947101	0.658399
H	-2.759479	-3.406101	-0.432354
C	1.18609	1.529031	-1.302051
H	1.545537	2.268778	-0.569461
H	1.181153	1.990921	-2.290666

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5485791
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0369487

$TS_{B\text{-}C'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -130.45 cm^{-1}
Zero-point correction= 0.355685 (Hartree/Particle)
Thermal correction to Energy= 0.379643
Thermal correction to Enthalpy= 0.380587
Thermal correction to Gibbs Free Energy= 0.303527
Sum of electronic and zero-point Energies= -1552.106018
Sum of electronic and thermal Energies= -1552.082061
Sum of electronic and thermal Enthalpies= -1552.081116
Sum of electronic and thermal Free Energies= -1552.158177

C	0.36478	-0.062199	0.5521
N	0.90037	1.10422	1.1586
C	0.188151	1.667311	2.30536
H	-0.889449	1.654801	2.13903
H	0.4152	1.131091	3.2366
H	0.507221	2.705831	2.42766
C	3.33552	0.521109	0.45622
C	2.6516	-0.40846	-0.53015
C	1.28895	-0.7036	-0.48097
C	3.43102	-1.044481	-1.51051
H	4.49471	-0.837611	-1.56012
C	0.740329	-1.609929	-1.39756
H	-0.314121	-1.860549	-1.37187
C	1.519249	-2.22535	-2.36328
H	1.066929	-2.92018	-3.06235
C	2.882999	-1.93736	-2.4188
H	3.514249	-2.409221	-3.16467
C	0.03107	-1.148459	1.6346
F	1.102639	-1.28096	2.42123
F	-0.251161	-2.357099	1.13228
F	-1.00919	-0.804509	2.41812
S	-0.749759	1.736561	-1.24825
N	-0.93243	0.446251	-0.06832
I	-2.59361	-0.696668	-0.30719
C	-3.74922	0.376612	1.14882
H	-4.62371	-0.244647	1.3382
H	-3.10529	0.454152	2.02212
H	-4.004049	1.331932	0.69799
O	0.526041	1.596001	-1.92085
O	-1.990999	1.674382	-2.01003
C	-0.758619	3.243801	-0.30587
H	-0.866438	4.028971	-1.0575
H	0.190261	3.328521	0.21784
H	-1.612929	3.238251	0.36969
C	2.340151	1.37098	1.27752
H	2.607121	1.2778	2.33987
H	2.468901	2.429	1.01751
C	4.272711	1.501869	-0.27321
C	4.17504	-0.342791	1.42039
H	3.722421	2.077789	-1.02389
H	5.10262	0.988789	-0.76353

H 4.703431 2.199129 0.45254
H 3.53854 -1.025851 1.98964
H 4.71481 0.299089 2.12431
H 4.90818 -0.936221 0.86644
UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM)
HF = -1552.8101008
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(DCM)
HF = -1553.3774104

A'

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.263573 (Hartree/Particle)
Thermal correction to Energy= 0.278653
Thermal correction to Enthalpy= 0.279597
Thermal correction to Gibbs Free Energy= 0.222350
Sum of electronic and zero-point Energies= -857.963778
Sum of electronic and thermal Energies= -857.948698
Sum of electronic and thermal Enthalpies= -857.947754
Sum of electronic and thermal Free Energies= -858.005001
C 0.8628 -0.034221 -0.185669
N 0.805829 -1.285581 -0.509609
C 1.951088 -2.197932 -0.685959
H 2.866788 -1.651393 -0.886969
H 2.052647 -2.810942 0.211981
H 1.713057 -2.830862 -1.540599
C -1.596851 -1.358069 0.154061
C -1.5826 0.152771 0.004301
C -0.333589 0.79613 -0.156899
C -2.730689 0.934682 0.055341
H -3.698 0.467473 0.201171
C -0.262448 2.19126 -0.325829
H 0.684682 2.685329 -0.501259
C -1.426057 2.945241 -0.308809
H -1.374166 4.017721 -0.457099
C -2.654558 2.319112 -0.098789
H -3.564227 2.910033 -0.068259
C 2.24094 0.535108 0.207711
F 2.88504 -0.326363 1.000741
F 2.129841 1.673648 0.881531
F 2.984951 0.753437 -0.879719
C -2.924732 -1.984638 -0.285619
H -2.836403 -3.074848 -0.277469
H -3.727942 -1.717017 0.404641
H -3.206412 -1.664068 -1.292809
C -1.306072 -1.741659 1.616401
H -2.086521 -1.333949 2.264121
H -1.300093 -2.830859 1.723071
H -0.344681 -1.35342 1.966771
C -0.516312 -1.8991 -0.778129
H -0.390713 -2.97539 -0.644979
H -0.752822 -1.69733 -1.830649
UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -858.4509828
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -858.7963762

$TS_{A'-C'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -168.26 cm^{-1}
Zero-point correction= 0.353681 (Hartree/Particle)
Thermal correction to Energy= 0.378793
Thermal correction to Enthalpy= 0.379737
Thermal correction to Gibbs Free Energy= 0.299111
Sum of electronic and zero-point Energies= -1552.112741
Sum of electronic and thermal Energies= -1552.087630
Sum of electronic and thermal Enthalpies= -1552.086685
Sum of electronic and thermal Free Energies= -1552.167312
C 0.598811 -0.65746 -0.058969
N 0.990371 -1.223419 1.100501
C 0.108571 -2.10188 1.871981
H -0.932589 -1.83532 1.694531
H 0.268312 -3.15545 1.627411
H 0.320851 -1.9417 2.929331
C 3.368131 -0.508258 0.893691
C 2.89818 0.363151 -0.257779
C 1.56663 0.307021 -0.699759
C 3.78418 1.214162 -0.926309
H 4.81759 1.266992 -0.601389
C 1.14751 1.110771 -1.768979
H 0.11281 1.09078 -2.088859
C 2.040319 1.954301 -2.415369
H 1.698749 2.573721 -3.237659
C 3.368299 2.002072 -1.993539
H 4.076749 2.658082 -2.488999
C 0.075131 -1.69616 -1.084879
F 1.102801 -2.456539 -1.468039
F -0.444939 -1.14002 -2.185639
F -0.862419 -2.51496 -0.581379
S -0.86784 1.66809 1.197911
N -0.93047 0.31035 0.192441
I -2.80593 -0.030201 -0.514499
C -3.587169 -1.061871 1.202791
H -3.238599 -0.475561 2.051901
H -4.670169 -1.026012 1.091461
H -3.202519 -2.077741 1.163621
O -2.07018 1.665369 2.031301
O 0.44138 1.62879 1.834261
C -0.931601 3.10002 0.144691
H -0.048741 3.08809 -0.494419
H -0.920301 3.96308 0.812801
H -1.853951 3.084569 -0.436779
C 2.180581 -0.752169 1.820591
C 4.45768 0.174862 1.730831
C 3.907501 -1.840768 0.344681
H 1.93496 0.148161 2.391351
H 2.442191 -1.549899 2.520851
H 3.128201 -2.409439 -0.168829
H 4.297491 -2.449668 1.167281
H 4.720951 -1.655608 -0.363139
H 4.16156 1.187672 2.020311
H 5.40506 0.228642 1.188851

H	4.6367	-0.407028	2.640721

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1552.8141993
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1553.3891262

C'

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.355154 (Hartree/Particle)
Thermal correction to Energy= 0.380150
Thermal correction to Enthalpy= 0.381094
Thermal correction to Gibbs Free Energy= 0.301992
Sum of electronic and zero-point Energies= -1552.116931
Sum of electronic and thermal Energies= -1552.091935
Sum of electronic and thermal Enthalpies= -1552.090991
Sum of electronic and thermal Free Energies= -1552.170093

C	0.401849	-0.56598	-0.090599
N	0.744919	-1.308871	1.072531
C	-0.359322	-1.75915	1.911031
H	-1.150402	-2.220269	1.321401
H	0.017638	-2.5179	2.598551
H	-0.775441	-0.930899	2.506531
C	3.152149	-0.647303	1.088501
C	2.83527	0.228948	-0.111119
C	1.54399	0.289599	-0.651009
C	3.843941	0.975267	-0.732949
H	4.851761	0.941126	-0.332809
C	1.286891	1.080639	-1.777789
H	0.284911	1.12742	-2.190679
C	2.299862	1.817318	-2.377699
H	2.082122	2.426838	-3.248219
C	3.588681	1.762027	-1.850159
H	4.392402	2.331336	-2.305829
C	0.073139	-1.61247	-1.213979
F	1.201498	-2.186111	-1.625149
F	-0.513971	-1.05506	-2.290109
F	-0.739592	-2.599649	-0.804029
S	-0.738498	1.832211	0.969971
N	-0.83264	0.358871	0.069311
I	-2.73229	-0.142328	-0.440209
C	-3.582041	-0.718717	1.457611
H	-3.05439	-0.115657	2.193851
H	-4.62826	-0.426246	1.372031
H	-3.447742	-1.790577	1.565391
O	-1.986348	1.893192	1.721071
O	0.532231	1.80883	1.666301
C	-0.751167	3.139551	-0.231559
H	0.195873	3.12153	-0.768139
H	-0.863007	4.059611	0.345621
H	-1.603407	2.998081	-0.897409
C	1.873079	-0.860582	1.892431
C	4.16716	0.016486	2.030001
C	3.713818	-1.994913	0.602371
H	1.61949	0.048369	2.450921
H	2.052239	-1.660712	2.618151
H	2.978758	-2.541142	0.006871
H	3.991858	-2.611443	1.464051
H	4.607168	-1.835274	-0.009249
H	3.862591	1.036017	2.286111
H	5.16712	0.050016	1.590651
H	4.237839	-0.565344	2.955001

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1552.8208391
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1553.3903564

$TS_{C'-D'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -84.04 cm^{-1}
Zero-point correction= 0.352848 (Hartree/Particle)
Thermal correction to Energy= 0.377918
Thermal correction to Enthalpy= 0.378862
Thermal correction to Gibbs Free Energy= 0.298827
Sum of electronic and zero-point Energies= -1552.099852
Sum of electronic and thermal Energies= -1552.074782
Sum of electronic and thermal Enthalpies= -1552.073838
Sum of electronic and thermal Free Energies= -1552.153872

C	-0.46758	0.56008	0.024149
N	-1.090731	1.165639	1.185429
C	-0.427871	2.21193	1.955959
H	0.643029	2.20181	1.783099
H	-0.847912	3.181109	1.657699
H	-0.633021	2.044339	3.014099
C	-3.41817	0.456558	0.611649
C	-2.79631	-0.361822	-0.510181
C	-1.41572	-0.352861	-0.747391
C	-3.597169	-1.172712	-1.323161
H	-4.670069	-1.191893	-1.165811
C	-0.858039	-1.178131	-1.730131
H	0.216071	-1.1961	-1.881001
C	-1.666989	-1.987271	-2.515721
H	-1.222578	-2.623441	-3.273031
C	-3.047119	-1.970662	-2.319771
H	-3.693618	-2.591382	-2.931291
C	-0.002171	1.70702	-0.937241
F	-1.025031	2.541149	-1.142781
F	0.399909	1.2525	-2.122131
F	1.007999	2.4303	-0.429161
C	-4.56873	-0.297693	1.296389
H	-4.86592	0.233717	2.206119
H	-5.44746	-0.348023	0.649849
H	-4.271739	-1.315113	1.567179
C	-3.942421	1.802328	0.083519
H	-4.674781	1.628587	-0.710031
H	-4.434711	2.354087	0.890929
H	-3.141261	2.422098	-0.323531
S	0.521961	-1.6393	1.306729
N	0.71176	-0.05094	0.666659
I	2.93385	-0.172378	-0.550121
C	3.554869	1.494272	0.652889
H	4.545209	1.251423	1.029209
H	3.547469	2.377582	0.021939
H	2.819599	1.547042	1.455139
O	-0.857369	-1.826461	1.747689

O	1.078202	-2.617209	0.377789
C	1.567861	-1.515529	2.735479
H	1.520132	-2.490699	3.223129
H	1.17059	-0.732059	3.380349
H	2.587361	-1.299519	2.416519
C	-2.36042	0.682428	1.699619
H	-2.705371	1.428698	2.420429
H	-2.17033	-0.254101	2.239529

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1552.7963065
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1553.3878322

D' (singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.313525 (Hartree/Particle)
Thermal correction to Energy= 0.334920
Thermal correction to Enthalpy= 0.335864
Thermal correction to Gibbs Free Energy= 0.264663
Sum of electronic and zero-point Energies= -1500.916869
Sum of electronic and thermal Energies= -1500.895473
Sum of electronic and thermal Enthalpies= -1500.894529
Sum of electronic and thermal Free Energies= -1500.965730

C	-0.389379	0.505287	0.41214
N	-0.301486	1.10355	-0.943232
C	-1.161453	2.206463	-1.333357
H	-2.10775	2.166921	-0.79946
H	-0.634862	3.141402	-1.086287
H	-1.317804	2.155461	-2.409339
C	2.006831	0.283726	-1.401442
C	1.903133	-0.522124	-0.117766
C	0.772966	-0.450503	0.707981
C	2.941867	-1.374132	0.271724
H	3.835796	-1.436826	-0.338614
C	0.66285	-1.254699	1.850852
H	-0.229839	-1.213134	2.464189
C	1.699632	-2.107192	2.204332
H	1.607994	-2.72755	3.088694
C	2.849758	-2.153925	1.419256
H	3.671366	-2.808102	1.690839
C	-0.409978	1.676017	1.456033
F	-0.292655	1.206468	2.689707
F	-1.549843	2.369557	1.396025
F	0.601906	2.513941	1.216198
S	-2.227715	-1.166883	-0.668321
N	-1.635347	-0.209299	0.626069
O	-2.734972	-0.22629	-1.660811
O	-1.179554	-2.101265	-1.053463
C	-3.550443	-1.998875	0.155128
H	-3.12376	-2.593895	0.962243
H	-4.018269	-2.63427	-0.598836
H	-4.246137	-1.245934	0.524042
C	0.576763	0.521659	-1.926843
C	2.732392	-0.487204	-2.513806
C	2.712564	1.628052	-1.162984
H	0.135882	-0.455146	-2.19764
H	0.567591	1.168894	-2.804748
H	2.197956	2.236706	-0.416588
H	2.77225	2.193628	-2.097907
H	3.729242	1.444732	-0.805348
H	2.327027	-1.495688	-2.633569
H	3.799946	-0.560397	-2.297201
H	2.631148	0.049009	-3.461848

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5469372
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0358978

D' (triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.313442 (Hartree/Particle)
Thermal correction to Energy= 0.334877
Thermal correction to Enthalpy= 0.335821
Thermal correction to Gibbs Free Energy= 0.263462
Sum of electronic and zero-point Energies= -1500.918578
Sum of electronic and thermal Energies= -1500.897144
Sum of electronic and thermal Enthalpies= -1500.896199
Sum of electronic and thermal Free Energies= -1500.968558

C	-0.383362	0.512038	0.399288
N	-0.298052	1.069832	-0.966197
C	-1.118533	2.199222	-1.365889
H	-2.084743	2.160615	-0.86582
H	-0.593336	3.12217	-1.077327
H	-1.237329	2.172649	-2.446642
C	2.000655	0.246992	-1.418751
C	1.913636	-0.518291	-0.109507
C	0.784212	-0.434718	0.716799
C	2.96231	-1.34659	0.302469
H	3.856173	-1.416251	-0.307308
C	0.682632	-1.209457	1.880124
H	-0.210118	-1.161553	2.49259
C	1.729442	-2.040778	2.255456
H	1.644504	-2.638857	3.155676
C	2.879613	-2.095405	1.471642
H	3.70846	-2.733072	1.759945
C	-0.416627	1.699381	1.42249
F	-0.295679	1.254707	2.665041
F	-1.563918	2.379452	1.349287
F	0.587573	2.542979	1.168647
S	-2.237042	-1.181981	-0.642768
N	-1.623729	-0.21492	0.635508
O	-2.717033	-0.252908	-1.659314
O	-1.210824	-2.151659	-0.998795
C	-3.584183	-1.960411	0.193174
H	-3.176426	-2.550882	1.013235
H	-4.067468	-2.59723	-0.549816
H	-4.260042	-1.181461	0.544658
C	0.557789	0.436305	-1.938608
C	2.729831	-0.548896	-2.510439
C	2.683689	1.609822	-1.229501
H	0.130913	-0.560683	-2.142615
H	0.528851	1.033805	-2.849855
H	2.168238	2.23095	-0.493685
H	2.720774	2.149046	-2.181051

H	3.708152	1.456062	-0.880241
H	2.335623	-1.565097	-2.597456
H	3.799048	-0.603102	-2.295906
H	2.618329	-0.042788	-3.47367

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5485886
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0371244

TS$_{D''-E''}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -390.67 cm^{-1}
Zero-point correction= 0.353845 (Hartree/Particle)
Thermal correction to Energy= 0.379052
Thermal correction to Enthalpy= 0.379996
Thermal correction to Gibbs Free Energy= 0.299198
Sum of electronic and zero-point Energies= -1552.092726
Sum of electronic and thermal Energies= -1552.067519
Sum of electronic and thermal Enthalpies= -1552.066575
Sum of electronic and thermal Free Energies= -1552.147372

C	0.46869	-0.20834	0.599289
N	1.044689	0.883921	1.316239
C	0.635938	1.2647	2.673129
H	-0.376401	0.935519	2.881539
H	1.337179	0.826521	3.391899
H	0.677187	2.35296	2.734089
C	3.349289	0.475833	0.409359
C	2.69469	-0.452398	-0.603641
C	1.32378	-0.745859	-0.533471
C	3.436141	-1.017857	-1.648301
H	4.49714	-0.808266	-1.723031
C	0.724191	-1.56443	-1.498731
H	-0.332979	-1.797551	-1.445091
C	1.472742	-2.100569	-2.536291
H	0.993482	-2.727099	-3.279981
C	2.839421	-1.831408	-2.604171
H	3.438972	-2.249297	-3.405931
C	0.025661	-1.38083	1.551719
F	1.048001	-1.666009	2.364609
F	-0.285378	-2.492251	0.887279
F	-1.024799	-1.066141	2.315619
S	-0.685962	2.060839	-0.807311
N	-0.661721	0.689899	0.346179
I	-2.77324	-0.637293	-0.387551
C	-3.754221	0.670646	1.008999
H	-2.987041	0.933337	1.735059
H	-4.090812	1.529986	0.437629
H	-4.56833	0.103995	1.452959
O	-2.102903	2.337998	-0.934631
O	0.160117	3.10033	-0.250651
C	-0.036812	1.51629	-2.369021
H	1.022628	1.282081	-2.262821
H	-0.183613	2.371569	-3.032891
H	-0.614061	0.656379	-2.709331
C	2.293278	1.499802	0.833309
C	4.495218	1.288794	-0.212421
C	3.891	-0.310387	1.613229
H	2.074038	2.170892	0.000749
H	2.657738	2.119022	1.656399
H	3.10294	-0.841468	2.149029
H	4.386069	0.373834	2.309889
H	4.624921	-1.047806	1.275999
H	4.188438	1.765783	-1.148041
H	5.364589	0.657365	-0.408821
H	4.812078	2.067684	0.487819

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1552.7884546
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1553.3827679

TS$_{D'-E'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -339.95 cm^{-1}
Zero-point correction= 0.313388 (Hartree/Particle)
Thermal correction to Energy= 0.334213
Thermal correction to Enthalpy= 0.335157
Thermal correction to Gibbs Free Energy= 0.265604
Sum of electronic and zero-point Energies= -1500.907502
Sum of electronic and thermal Energies= -1500.886677
Sum of electronic and thermal Enthalpies= -1500.885733
Sum of electronic and thermal Free Energies= -1500.955287

C	0.18396	-0.09629	0.17906
N	-0.04192	-1.49813	-0.18599
C	0.84693	-2.60962	0.15111
H	0.90563	-3.25936	-0.72261
H	1.8308	-2.2616	0.45343
H	0.36984	-3.15693	0.97523
C	-2.48741	-1.19605	-0.43396
C	-2.27927	0.3065	-0.32832
C	-1.00115	0.81688	-0.08673
C	-3.32397	1.21972	-0.49582
H	-4.32988	0.858	-0.6788
C	-0.74869	2.19134	-0.0748
H	0.26267	2.56384	0.06525
C	-1.80059	3.08113	-0.2522
H	-1.61165	4.14875	-0.2421
C	-3.09166	2.59127	-0.44638
H	-3.91891	3.28029	-0.58019
C	0.63351	0.0879	1.67289
F	-0.45326	0.2221	2.43536
F	1.36522	1.19583	1.77546
F	1.33177	-0.929	2.17127
S	2.80332	0.28961	-0.71651
N	1.10449	0.02934	-0.93258
O	2.88171	1.73687	-0.60044
O	3.30999	-0.56818	0.34291
C	3.39292	-0.24543	-2.29481
H	3.19526	-1.31284	-2.39204
H	4.466	-0.04519	-2.29318
H	2.88374	0.33706	-3.0616
C	-1.19663	-1.79261	-1.02882
C	-3.61467	-1.56147	-1.40736
C	-2.7717	-1.81388	0.94476
H	-0.99994	-1.36269	-2.02053

H -1.25355 -2.87895 -1.12047
H -1.97191 -1.61126 1.66372
H -2.89596 -2.89814 0.85834
H -3.69406 -1.39171 1.35204
H -3.49056 -1.06268 -2.3726
H -4.58485 -1.28188 -0.9905
H -3.63036 -2.64307 -1.56947
UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5374467
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0284128

E' (singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.318664 (Hartree/Particle)
Thermal correction to Energy= 0.338991
Thermal correction to Enthalpy= 0.339935
Thermal correction to Gibbs Free Energy= 0.271840
Sum of electronic and zero-point Energies= -1500.958479
Sum of electronic and thermal Energies= -1500.938152
Sum of electronic and thermal Enthalpies= -1500.937208
Sum of electronic and thermal Free Energies= -1501.005303
C -0.39812 0.680541 0.311249
N -0.558204 0.735638 -1.157259
C -1.131009 1.925047 -1.858363
H -1.870733 2.404486 -1.226183
H -0.305454 2.595806 -2.095256
H -1.598284 1.544422 -2.765684
C 1.886876 0.171294 -1.427979
C 1.871579 -0.363335 -0.001846
C 0.760944 -0.125632 0.822692
C 2.925787 -1.111505 0.524365
H 3.80191 -1.309996 -0.082055
C 0.682095 -0.663612 2.111255
H -0.202594 -0.507219 2.718064
C 1.738585 -1.417227 2.608074
H 1.678039 -1.836791 3.605904
C 2.865379 -1.62782 1.816701
H 3.696966 -2.210277 2.199176
C -0.719022 1.992055 1.079523
F -0.439589 1.865931 2.370816
F -1.999886 2.337031 0.970341
F 0.028412 2.987012 0.585288
S -1.82613 -1.674245 -0.199046
N -1.543757 0.072394 -0.315215
O -0.722137 -2.440546 -0.744823
O -2.182828 -1.784476 1.19938
C -3.247223 -1.780514 -1.246919
H -4.00741 -1.109486 -0.84982
H -3.569728 -2.822509 -1.198999
H -2.949549 -1.513986 -2.261447
C 0.476287 0.009324 -2.00172
C 2.798019 -0.649186 -2.351715
C 2.341604 1.640403 -1.445429
H 0.193495 -1.039198 -2.056934
H 0.392593 0.461787 -2.990181
H 1.713944 2.283285 -0.822788
H 2.338202 2.029043 -2.468949
H 3.360133 1.707976 -1.054734
H 2.572622 -1.717838 -2.293274
H 3.847723 -0.496634 -2.091895
H 2.66854 -0.319761 -3.386668
UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5923617
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0663585

E' (triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.312900 (Hartree/Particle)
Thermal correction to Energy= 0.334260
Thermal correction to Enthalpy= 0.335204
Thermal correction to Gibbs Free Energy= 0.263765
Sum of electronic and zero-point Energies= -1500.825388
Sum of electronic and thermal Energies= -1500.804028
Sum of electronic and thermal Enthalpies= -1500.803083
Sum of electronic and thermal Free Energies= -1500.874522
C -0.531617 0.636862 0.305935
N -0.592238 0.696206 -1.175977
C -1.337484 1.779992 -1.88863
H -2.198373 2.081187 -1.300863
H -0.645875 2.607533 -2.044626
H -1.65981 1.35139 -2.836741
C 1.932646 0.544106 -1.288416
C 1.928953 -0.116123 0.067104
C 0.696846 0.087944 0.906973
C 2.946702 -0.835971 0.582889
H 3.849288 -0.99198 0.00214
C 0.617769 -0.541917 2.23892
H -0.297479 -0.465506 2.81212
C 1.662207 -1.250497 2.700255
H 1.601595 -1.736321 3.668165
C 2.88887 -1.399016 1.910332
H 3.739023 -1.927403 2.318454
C -1.191193 1.823341 1.064956
F -0.93502 1.750337 2.366326
F -2.511518 1.861453 0.90497
F -0.681023 2.974999 0.607837
S -1.394295 -1.931198 -0.346034
N -1.5027 -0.171883 -0.441338
O -0.066315 -2.399082 -0.701374
O -1.916579 -2.149728 0.986373
C -2.579146 -2.360274 -1.587814
H -3.521981 -1.88041 -1.329151
H -2.662792 -3.44827 -1.548877
H -2.203383 -2.036412 -2.558741
C 0.603152 0.205379 -1.97653
C 3.033873 0.009709 -2.208637
C 2.092324 2.069404 -1.134239
H 0.499364 -0.866864 -2.124657
H 0.518318 0.716203 -2.935789
H 1.347574 2.512569 -0.466824
H 2.01945 2.560653 -2.110136

H	3.07585	2.285504	-0.71067
H	2.97574	-1.077409	-2.3143
H	4.018185	0.271625	-1.81325
H	2.946388	0.464573	-3.199278

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.4542787
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.9344043

$TS_{D'-D}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -90.06 cm^{-1}
Zero-point correction= 0.313274 (Hartree/Particle)
Thermal correction to Energy= 0.333767
Thermal correction to Enthalpy= 0.334711
Thermal correction to Gibbs Free Energy= 0.265685
Sum of electronic and zero-point Energies= -1500.897160
Sum of electronic and thermal Energies= -1500.876667
Sum of electronic and thermal Enthalpies= -1500.875723
Sum of electronic and thermal Free Energies= -1500.944749

C	0.341339	-0.448717	0.43268
N	0.136294	-1.342387	-0.734562
C	0.984771	-2.503591	-0.917813
H	1.936306	-2.384118	-0.402935
H	0.451881	-3.369829	-0.492867
H	1.11521	-2.683096	-1.986384
C	-2.191439	-0.494727	-1.228846
C	-1.895572	0.616371	-0.236049
C	-0.70704	0.667781	0.505528
C	-2.83586	1.633214	-0.029924
H	-3.769568	1.612566	-0.58082
C	-0.458234	1.722175	1.39571
H	0.471659	1.756031	1.950847
C	-1.400315	2.724029	1.570061
H	-1.199151	3.538103	2.257272
C	-2.59957	2.672041	0.860929
H	-3.34852	3.445274	0.995773
C	0.250117	-1.34818	1.724104
F	-0.858379	-2.089905	1.689553
F	0.228833	-0.592086	2.80988
F	1.296747	-2.173219	1.816848
S	2.571939	0.981332	-0.645345
N	1.664104	0.116135	0.517459
O	1.90544	2.27287	-0.681647
O	3.927825	0.849182	-0.155107
C	2.489121	0.215961	-2.246068
H	3.182423	0.797366	-2.858843
H	1.484315	0.307765	-2.65241
H	2.840772	-0.813216	-2.173549
C	-0.863321	-1.067471	-1.741134
H	-1.006312	-1.985945	-2.316548
H	-0.408798	-0.325766	-2.422314
C	-2.913876	0.031386	-2.481335
C	-3.044165	-1.606336	-0.5928
H	-2.418514	0.917321	-2.888394
H	-3.950866	0.282457	-2.25136
H	-2.934003	-0.746376	-3.250852
H	-2.544497	-2.084121	0.250235
H	-3.280122	-2.369042	-1.341171
H	-3.982682	-1.176058	-0.233205

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5311071
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.01842

TS_{D-F}

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -518.94 cm^{-1}
Zero-point correction= 0.443189 (Hartree/Particle)
Thermal correction to Energy= 0.470804
Thermal correction to Enthalpy= 0.471748
Thermal correction to Gibbs Free Energy= 0.387816
Sum of electronic and zero-point Energies= -1659.162640
Sum of electronic and thermal Energies= -1659.135025
Sum of electronic and thermal Enthalpies= -1659.134081
Sum of electronic and thermal Free Energies= -1659.218013

C	-0.12551	-0.441959	0.142456
N	-0.46479	-0.898382	-1.223484
C	0.508045	-0.914519	-2.293352
H	0.521084	-1.920799	-2.723263
H	0.172458	-0.209633	-3.066212
H	1.49403	-0.628239	-1.934062
C	-2.933253	-0.557915	-1.07227
C	-2.638475	0.112833	0.259918
C	-1.362453	0.15895	0.835513
C	-3.682931	0.733368	0.956799
H	-4.680812	0.728453	0.530482
C	-1.146291	0.777462	2.073472
H	-0.148324	0.800452	2.497118
C	-2.203577	1.370056	2.75091
H	-2.030779	1.844957	3.710254
C	-3.475696	1.357048	2.181586
H	-4.308722	1.828572	2.691958
C	0.332354	-1.739827	0.89852
F	-0.705486	-2.543352	1.134229
F	0.898048	-1.435893	2.057266
F	1.212606	-2.417827	0.150293
C	-3.136061	0.485189	-2.182876
H	-3.3982	-0.016157	-3.119776
H	-3.959509	1.151833	-1.911567
H	-2.241479	1.091106	-2.335322
C	-4.171297	-1.464893	-0.983698
H	-5.080673	-0.86764	-0.892361
H	-4.26208	-2.058894	-1.898264
H	-4.109137	-2.142496	-0.127555
S	0.943663	1.855543	-0.773274
N	0.955838	0.4953	0.252744
O	2.128563	1.794837	-1.618495
O	-0.369298	1.925708	-1.412337
C	1.111631	3.165865	0.408025
H	2.038977	3.006127	0.95792
H	0.241756	3.142679	1.064916
H	1.148532	4.090646	-0.17034
H	3.836751	-0.100407	-1.928226

H	4.077977	1.729656	-0.178512
C	4.062591	-0.846626	-1.161093
H	5.147336	-1.015419	-1.163551
C	4.245256	0.977721	0.5955
H	3.582614	-1.795661	-1.421789
H	2.48342	-0.165723	0.16516
C	3.641656	-0.367021	0.217752
H	5.328495	0.855341	0.722176
H	3.842327	1.336111	1.548531
C	3.86894	-1.40536	1.306042
H	3.424114	-2.371452	1.059979
H	4.951146	-1.554112	1.415545
H	3.480345	-1.068809	2.270866
C	-1.758366	-1.493964	-1.450607
H	-1.81116	-2.395734	-0.822984
H	-1.816448	-1.791032	-2.49857

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1659.9598753
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.5571041

$^{t}TS_{D\text{-}F}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -511.38 cm^{-1}
Zero-point correction= 0.443141 (Hartree/Particle)
Thermal correction to Energy= 0.470818
Thermal correction to Enthalpy= 0.471762
Thermal correction to Gibbs Free Energy= 0.386600
Sum of electronic and zero-point Energies= -1659.161960
Sum of electronic and thermal Energies= -1659.134283
Sum of electronic and thermal Enthalpies= -1659.133338
Sum of electronic and thermal Free Energies= -1659.218501

C	-0.13065	-0.447844	0.142579
N	-0.464971	-0.887315	-1.232412
C	0.526786	-0.939434	-2.283371
H	0.553899	-1.962286	-2.674155
H	0.194161	-0.270191	-3.088132
H	1.50571	-0.63485	-1.921332
C	-2.937904	-0.542353	-1.075394
C	-2.641303	0.110582	0.265978
C	-1.365364	0.14146	0.842339
C	-3.682891	0.729269	0.967991
H	-4.680518	0.734976	0.540981
C	-1.147254	0.745699	2.087371
H	-0.149456	0.759908	2.511872
C	-2.20165	1.337241	2.770573
H	-2.026877	1.801095	3.734954
C	-3.473281	1.337591	2.200402
H	-4.304201	1.807401	2.715775
C	0.337213	-1.749813	0.882467
F	-0.695816	-2.564777	1.101696
F	0.897231	-1.458556	2.047255
F	1.225589	-2.411408	0.128322
C	-3.1544	0.516482	-2.168668
H	-3.423469	0.027649	-3.110249
H	-3.977466	1.176574	-1.880943
H	-2.262606	1.126403	-2.320748
C	-4.171711	-1.456333	-0.991982
H	-5.0827	-0.864674	-0.882745
H	-4.267621	-2.035638	-1.915472
H	-4.099242	-2.147662	-0.147609
S	0.934012	1.858987	-0.769252
N	0.952245	0.495525	0.255556
O	2.114945	1.793894	-1.62001
O	-0.381737	1.934145	-1.401455
C	1.111202	3.166986	0.41311
H	2.042887	3.007545	0.955573
H	0.246493	3.141338	1.076795
H	1.142313	4.093048	-0.16361
H	3.848794	-0.088183	-1.926408
H	4.074204	1.746023	-0.177017
C	4.07899	-0.830889	-1.157099
H	5.165273	-0.989203	-1.155361
C	4.24518	0.995268	0.597545
H	3.608642	-1.784632	-1.417856
H	2.491697	-0.159306	0.163596
C	3.648288	-0.352454	0.219536
H	5.32902	0.878827	0.724445
H	3.840068	1.352004	1.550262
C	3.876728	-1.389091	1.309509
H	3.435095	-2.356629	1.062988
H	4.959001	-1.53474	1.422213
H	3.483884	-1.052895	2.272761
C	-1.764061	-1.465719	-1.476716
H	-1.813892	-2.385752	-0.873795
H	-1.820411	-1.738937	-2.531494

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1659.9592091
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.5561593

F (singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.447369 (Hartree/Particle)
Thermal correction to Energy= 0.475368
Thermal correction to Enthalpy= 0.476312
Thermal correction to Gibbs Free Energy= 0.389541
Sum of electronic and zero-point Energies= -1659.247407
Sum of electronic and thermal Energies= -1659.219408
Sum of electronic and thermal Enthalpies= -1659.218464
Sum of electronic and thermal Free Energies= -1659.305235

C	0.074993	-0.784173	0.533727
N	1.283068	-1.410779	0.998883
C	1.483713	-1.541124	2.438111
H	0.941545	-2.392663	2.874124
H	2.552847	-1.679733	2.614147
H	1.185982	-0.63025	2.95865
C	2.108879	-2.212575	-1.182546
C	0.963126	-1.417318	-1.792464
C	0.012158	-0.758925	-0.999547
C	0.881143	-1.270787	-3.185337
H	1.620582	-1.757719	-3.813058
C	-0.989784	0.012633	-1.60709
H	-1.696015	0.552779	-0.986634

C	-1.064776	0.132057	-2.987336
H	-1.845595	0.735916	-3.437457
C	-0.117497	-0.513198	-3.783049
H	-0.154001	-0.421156	-4.863798
C	-1.206442	-1.499572	1.088572
F	-1.154103	-2.811988	0.845846
F	-2.360293	-1.043583	0.577733
F	-1.304879	-1.339872	2.426101
C	3.379175	-1.343501	-1.178198
H	4.233254	-1.935822	-0.83206
H	3.603076	-0.976051	-2.184628
H	3.260184	-0.488549	-0.504611
C	2.374098	-3.514527	-1.950396
H	2.804298	-3.325161	-2.937002
H	3.093072	-4.124292	-1.392937
H	1.455179	-4.095023	-2.077837
S	1.142165	1.757011	0.943391
N	-0.085071	0.59866	1.045827
O	0.514162	2.920848	1.582587
O	2.419514	1.30394	1.478235
C	1.339233	2.091144	-0.78842
H	0.376778	2.376793	-1.210512
H	1.749784	1.212814	-1.286926
H	2.048621	2.920543	-0.820437
H	-1.20221	3.110296	3.210192
H	-1.518357	3.440556	0.503186
C	-2.259223	2.819997	3.241258
H	-2.769551	3.640808	3.773324
C	-2.423411	3.884556	0.967287
H	-2.422515	1.887246	3.777779
H	-0.387131	0.616964	2.021876
C	-2.814691	2.829731	1.889069
H	-2.084603	4.792834	1.466963
H	-3.151748	4.062844	0.176425
C	-3.771492	1.811272	1.469013
H	-3.609893	0.848202	1.9543
H	-4.732178	2.200799	1.860475
H	-3.875255	1.735065	0.386521
C	1.737617	-2.579165	0.251757
H	1.00227`	-3.397785	0.25738
H	2.633596	-2.949219	0.76044

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.0522688
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.63369

F (triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.445814 (Hartree/Particle)
Thermal correction to Energy= 0.475013
Thermal correction to Enthalpy= 0.475957
Thermal correction to Gibbs Free Energy= 0.385678
Sum of electronic and zero-point Energies= -1659.193833
Sum of electronic and thermal Energies= -1659.164634
Sum of electronic and thermal Enthalpies= -1659.163690
Sum of electronic and thermal Free Energies= -1659.253969

C	-0.137211	-0.384785	0.045699
N	0.781878	-1.178635	0.908635
C	1.189738	-0.73406	2.220677
H	1.044076	-1.562399	2.919479
H	2.26257	-0.497987	2.173376
H	0.633092	0.147112	2.530795
C	1.975728	-2.378246	-0.908996
C	1.184399	-1.498468	-1.86451
C	0.217649	-0.583297	-1.430792
C	1.444633	-1.568678	-3.239251
H	2.204999	-2.252117	-3.602262
C	-0.488042	0.205521	-2.3468
H	-1.233748	0.909063	-1.989826
C	-0.227774	0.103756	-3.70676
H	-0.780245	0.717224	-4.409836
C	0.752666	-0.78208	-4.151885
H	0.976647	-0.863041	-5.210206
C	-1.567264	-0.961541	0.345274
F	-1.705871	-2.189421	-0.148071
F	-2.507073	-0.184275	-0.180827
F	-1.76053	-1.018491	1.670041
C	3.378181	-1.798603	-0.669277
H	3.943774	-2.451953	0.002488
H	3.91533	-1.739975	-1.620171
H	3.331792	-0.794268	-0.243453
C	2.087697	-3.822838	-1.419045
H	2.758467	-3.876192	-2.278918
H	2.510077	-4.46125	-0.637139
H	1.111624	-4.220665	-1.710259
S	1.118439	2.026025	0.340917
N	-0.199872	0.990726	0.427973
O	1.041423	2.843628	1.543002
O	2.279313	1.177003	0.095666
C	0.833447	3.060022	-1.070521
H	-0.135775	3.544186	-0.945871
H	0.866161	2.439055	-1.965186
H	1.640592	3.79453	-1.071706
H	-0.591055	2.27477	3.436848
H	-1.335961	3.738735	1.582984
C	-1.612213	1.913442	3.601265
H	-2.028305	2.500923	4.436891
C	-2.363307	3.361652	1.616996
H	-1.57799	0.870686	3.935785
H	-0.92759	1.291051	1.094078
C	-2.462811	2.07332	2.377653
H	-2.975138	4.139593	2.103037
H	-2.743145	3.255941	0.594128
C	-3.787015	1.375664	2.357092
H	-4.506665	1.916173	2.99405
H	-4.21272	1.343103	1.349473
H	-3.718271	0.354942	2.743996
C	1.215582	-2.470446	0.440095
H	0.318175	-3.08759	0.293883
H	1.840743	-2.924345	1.210093

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1659.9943374
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.5834907

TS_{F-P}

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = - 238.76 cm^{-1}
Zero-point correction= 0.454350 (Hartree/Particle)

Thermal correction to Energy= 0.480340
Thermal correction to Enthalpy= 0.481284
Thermal correction to Gibbs Free Energy= 0.402416
Sum of electronic and zero-point Energies= -1659.221419
Sum of electronic and thermal Energies= -1659.195430
Sum of electronic and thermal Enthalpies= -1659.194486
Sum of electronic and thermal Free Energies= -1659.273354

C	0.05457	0.79792	-0.05885
N	0.32257	0.81036	-1.39806
C	-0.64275	1.29627	-2.37837
H	-0.57086	0.65443	-3.26
H	-1.65164	1.228581	-1.98581
H	-0.445509	2.33482	-2.66482
C	2.69391	-0.018601	-1.24265
C	2.39791	-0.153781	0.24327
C	1.16509	0.224029	0.80385
C	3.365009	-0.714972	1.08614
H	4.314389	-1.028302	0.66463
C	0.9593	0.082539	2.18705
H	0.03544	0.40361	2.656
C	1.932679	-0.473411	3.00423
H	1.744589	-0.582821	4.06627
C	3.141509	-0.886202	2.44655
H	3.910739	-1.328942	3.07029
C	-0.335639	2.19137	0.54058
F	0.819741	2.836209	0.75746
F	-0.984389	2.12613	1.71226
F	-1.036049	2.96122	-0.28904
C	2.562509	-1.383951	-1.94201
H	2.922699	-1.298142	-2.9722
H	3.168299	-2.141672	-1.43453
H	1.522709	-1.718511	-1.97682
C	4.10741	0.536448	-1.48182
H	4.87487	-0.205432	-1.24974
H	4.21768	0.799008	-2.539
H	4.29122	1.431588	-0.88081
S	-1.060141	-2.01096	-0.28353
N	-1.40192	-0.28619	0.30117
O	-2.186742	-2.812879	0.15306
O	-0.775851	-1.84221	-1.69228
C	0.329848	-2.67084	0.61584
H	0.180029	-2.50697	1.68242
H	1.268839	-2.266801	0.25575
H	0.242718	-3.73515	0.38215
H	-3.632191	-1.693119	-1.15468
C	-3.526561	-0.612299	-1.20231
H	-4.5204	-0.187328	-1.35772
H	-2.91925	-0.353469	-2.07083
H	-1.3222	-0.3409	1.32467
C	-2.9906	0.004781	0.09777
C	-3.33094	1.495871	0.07232
H	-3.006339	2.007501	-0.83086
H	-4.42304	1.530902	0.07877
H	-2.995029	2.034921	0.95379
C	1.71431	0.974509	-1.84892
H	2.034541	2.005659	-1.63839
H	1.70162	0.848839	-2.93485
C	-3.659361	-0.580419	1.34899
H	-3.461151	-1.640289	1.48733
H	-3.34864	-0.026109	2.24123
H	-4.738621	-0.446638	1.24012

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)

HF = -1660.0305537

UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)

HF = -1660.610503

A + P

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)

Zero-point correction= 0.452697 (Hartree/Particle)
Thermal correction to Energy= 0.480768
Thermal correction to Enthalpy= 0.481712
Thermal correction to Gibbs Free Energy= 0.393150
Sum of electronic and zero-point Energies= -1659.292145
Sum of electronic and thermal Energies= -1659.264073
Sum of electronic and thermal Enthalpies= -1659.263129
Sum of electronic and thermal Free Energies= -1659.351692

C	1.78556	0.93511	-0.261
N	0.86607	0.35272	-0.95858
C	-0.37018	0.98845	-1.45892
H	-0.56837	0.53396	-2.42976
H	-1.19652	0.773891	-0.77822
H	-0.2263	2.05808	-1.58549
C	1.948429	-1.86543	-0.49788
C	3.21268	-1.072281	-0.22626
C	3.09138	0.323479	-0.05114
C	4.466839	-1.654361	-0.07953
H	4.583269	-2.726301	-0.19153
C	4.2221	1.114199	0.22476
H	4.144101	2.190529	0.31707
C	5.46726	0.513899	0.33976
H	6.34186	1.123028	0.53651
C	5.58541	-0.868841	0.20052
H	6.55717	-1.340702	0.30235
C	1.479991	2.32358	0.33176
F	1.764511	3.2819	-0.55446
F	2.195461	2.53627	1.43323
F	0.195561	2.43141	0.67862
C	1.227549	-2.13273	0.83613
H	0.306069	-2.69286	0.65717
H	1.881499	-2.71151	1.49402
H	0.96731	-1.20356	1.35332
C	2.220999	-3.19674	-1.20646
H	2.740949	-3.89151	-0.54287
H	1.272389	-3.6622	-1.48909
H	2.823049	-3.055481	-2.10881
S	-2.75593	-1.062379	0.90905
N	-3.31561	0.444081	0.45084
O	-3.829451	-2.012369	1.21251
O	-1.773801	-1.484299	-0.09785
C	-1.89749	-0.655279	2.4125
H	-2.62032	-0.335229	3.16334
H	-1.16173	0.120631	2.20039
H	-1.408551	-1.578079	2.72943
H	-4.16921	-1.419759	-1.48463
C	-4.09294	-0.366359	-1.76813
H	-4.82864	-0.173798	-2.5533
H	-3.09466	-0.186109	-2.17501
H	-3.58352	0.964041	1.28817
C	-4.3904	0.562072	-0.59062
C	-4.33429	2.020882	-1.04829
H	-3.363659	2.248721	-1.49803

H	-5.116679	2.203372	-1.79026
H	-4.498089	2.701782	-0.20676
C	1.07774	-1.03349	-1.4378
H	1.52481	-0.95141	-2.43723
H	0.080319	-1.4715	-1.51998
C	-5.76515	0.247492	0.00823
H	-5.81332	-0.787008	0.35475
H	-5.97832	0.911952	0.85245
H	-6.53994	0.402702	-0.74826

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.0988859
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.6832705

$TS_{D'-F'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -557.67 cm^{-1}
Zero-point correction= 0.443212 (Hartree/Particle)
Thermal correction to Energy= 0.470706
Thermal correction to Enthalpy= 0.471651
Thermal correction to Gibbs Free Energy= 0.388241
Sum of electronic and zero-point Energies= -1659.158718
Sum of electronic and thermal Energies= -1659.131223
Sum of electronic and thermal Enthalpies= -1659.130279
Sum of electronic and thermal Free Energies= -1659.213688

C	-0.16473	-0.33798	0.077389
N	-0.4647	-0.67195	-1.344081
C	0.598321	-1.08001	-2.243781
H	0.423311	-2.13145	-2.507111
H	0.52333	-0.47751	-3.154561
H	1.574781	-0.96047	-1.784231
C	-2.97841	-0.486071	-1.064721
C	-2.67942	0.154529	0.282299
C	-1.37887	0.26794	0.791169
C	-3.72851	0.648639	1.066729
H	-4.7471	0.568509	0.703199
C	-1.14028	0.87489	2.031059
H	-0.12535	0.95592	2.403119
C	-2.19802	1.363779	2.785899
H	-2.00498	1.831849	3.744769
C	-3.49923	1.242539	2.302469
H	-4.33631	1.615059	2.883309
C	0.193271	-1.68908	0.788709
F	-0.885289	-2.46275	0.892429
F	0.661941	-1.45173	2.006899
F	1.117991	-2.37616	0.106499
C	-4.0858	0.273839	-1.817501
H	-4.13828	-0.081531	-2.851271
H	-5.06186	0.091779	-1.364001
H	-3.89535	1.350679	-1.826031
C	-3.412709	-1.954701	-0.904211
H	-4.267439	-2.012791	-0.224901
H	-3.718119	-2.355331	-1.875771
H	-2.615689	-2.583411	-0.506231
S	1.12213	1.85948	-0.804611
N	0.97756	0.52916	0.249199
O	2.24327	1.612531	-1.701931
O	-0.19628	2.11228	-1.384141
C	1.519669	3.15478	0.337039
H	2.43862	2.886611	0.856479
H	0.681619	3.26343	1.025599
H	1.655929	4.05473	-0.265521
H	3.87628	-0.460569	-1.804511
H	4.21245	1.501471	-0.205541
C	4.021991	-1.146709	-0.964761
H	5.091731	-1.387019	-0.909761
C	4.30876	0.801301	0.627769
H	3.487331	-2.082259	-1.157511
H	2.45712	-0.218679	0.234399
C	3.59535	-0.512689	0.347999
H	5.37692	0.596151	0.773379
H	3.93805	1.264611	1.547789
C	3.683241	-1.461139	1.533459
H	3.176831	-2.409699	1.345609
H	4.742891	-1.678569	1.720929
H	3.270291	-1.009369	2.439529
C	-1.74366	-0.391271	-1.960441
H	-1.826449	-1.045041	-2.834641
H	-1.62815	0.6425	-2.331961

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1659.9562253
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.5527567

$^{t}TS_{D'-F'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -505.00 cm^{-1}
Zero-point correction= 0.443263 (Hartree/Particle)
Thermal correction to Energy= 0.470768
Thermal correction to Enthalpy= 0.471712
Thermal correction to Gibbs Free Energy= 0.387120
Sum of electronic and zero-point Energies= -1659.159705
Sum of electronic and thermal Energies= -1659.132201
Sum of electronic and thermal Enthalpies= -1659.131257
Sum of electronic and thermal Free Energies= -1659.215849

C	-0.172189	-0.34698	0.069549
N	-0.468289	-0.640641	-1.354771
C	0.586602	-1.05858	-2.259871
H	0.387983	-2.10081	-2.542801
H	0.527651	-0.43845	-3.159921
H	1.564092	-0.969859	-1.796341
C	-2.975329	-0.450373	-1.084281
C	-2.685149	0.145767	0.284739
C	-1.38522	0.242249	0.798829
C	-3.73544	0.617956	1.080399
H	-4.75334	0.550045	0.712439
C	-1.14784	0.815199	2.054629
H	-0.13334	0.88678	2.429759
C	-2.206671	1.283878	2.821059
H	-2.014731	1.726148	3.792319
C	-3.50727	1.176427	2.333009
H	-4.344801	1.533406	2.922919
C	0.193442	-1.70705	0.758359
F	-0.883387	-2.484341	0.855319

F	0.667152	-1.48687	1.978169
F	1.116833	-2.383779	0.063879
C	-4.08971	0.321146	-1.813131
H	-4.136379	0.000256	-2.858341
H	-5.064149	0.112115	-1.367631
H	-3.912351	1.399856	-1.784911
C	-3.386257	-1.930223	-0.979351
H	-4.241707	-2.027244	-0.305421
H	-3.681827	-2.300714	-1.965821
H	-2.579887	-2.559723	-0.601201
S	1.120969	1.883011	-0.762571
N	0.97284	0.523541	0.255149
O	2.210159	1.635182	-1.698521
O	-0.205701	2.1908	-1.292921
C	1.581578	3.132121	0.406419
H	2.507758	2.829832	0.892399
H	0.765318	3.239361	1.120779
H	1.722097	4.046322	-0.173371
H	3.837831	-0.462446	-1.823081
H	4.222969	1.492564	-0.220811
C	3.990642	-1.151986	-0.987191
H	5.059282	-1.400375	-0.950021
C	4.332	0.784134	0.604199
H	3.446333	-2.083047	-1.173251
H	2.454031	-0.208148	0.239109
C	3.592501	-0.517137	0.333989
H	5.40075	0.561505	0.715739
H	3.99683	1.244564	1.538929
C	3.683212	-1.470327	1.515439
H	3.162943	-2.411917	1.330819
H	4.742402	-1.701026	1.689129
H	3.286612	-1.016357	2.427659
C	-1.735879	-0.304592	-1.967531
H	-1.815798	-0.903662	-2.879821
H	-1.61312	0.749828	-2.271141

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1659.9571336
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.5540027

F' (singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.447988 (Hartree/Particle)
Thermal correction to Energy= 0.476605
Thermal correction to Enthalpy= 0.477550
Thermal correction to Gibbs Free Energy= 0.390717
Sum of electronic and zero-point Energies= -1659.258719
Sum of electronic and thermal Energies= -1659.230102
Sum of electronic and thermal Enthalpies= -1659.229158
Sum of electronic and thermal Free Energies= -1659.315990

C	-1.14132	-0.75321	0.21436
N	-1.79765	-0.73115	-1.0632
C	-1.917149	-2.00229	-1.77871
H	-2.75446	-1.92118	-2.47598
H	-1.004719	-2.2288	-2.34822
H	-2.116249	-2.82383	-1.09528
C	-1.724111	1.73971	-1.34979
C	-0.952671	1.79557	-0.04026
C	-0.60063	0.620201	0.64086
C	-0.556851	3.025381	0.50465
H	-0.829432	3.944121	-0.00436
C	0.17405	0.696351	1.80723
H	0.47602	-0.208829	2.32271
C	0.568959	1.923551	2.32599
H	1.164979	1.961291	3.23209
C	0.184719	3.098081	1.67846
H	0.474978	4.064681	2.0776
C	-2.23291	-1.14218	1.26711
F	-3.11792	-0.15625	1.41894
F	-1.69638	-1.39046	2.4816
F	-2.910449	-2.24424	0.92284
C	-1.212831	2.79045	-2.3468
H	-1.661931	2.60758	-3.32855
H	-1.489712	3.80406	-2.04619
H	-0.123881	2.745031	-2.45283
C	-3.223961	1.96739	-1.10133
H	-3.386141	2.92838	-0.60297
H	-3.757701	1.982999	-2.05786
H	-3.647061	1.17621	-0.47989
S	1.35375	-1.780909	-0.3518
N	-0.14464	-1.861459	0.3618
O	1.18509	-1.168879	-1.66678
O	2.35003	-1.165118	0.54068
C	1.761911	-3.497709	-0.52528
H	1.003861	-3.962609	-1.15455
H	1.800651	-3.954269	0.46399
H	2.744731	-3.525028	-0.99905
H	4.06153	-0.447448	-1.77266
H	2.133199	1.000112	-1.59234
C	4.56236	-0.006578	-0.91131
H	5.3645	0.658243	-1.27895
C	2.590759	1.586012	-0.79457
H	5.04197	-0.753447	-0.27714
H	-0.058639	-2.209199	1.3171
C	3.695169	0.886532	-0.14128
H	3.084249	2.463162	-1.25429
H	1.860549	1.970281	-0.07985
C	4.030369	1.213292	1.24592
H	5.065389	0.985363	1.50056
H	3.746499	2.236432	1.50238
H	3.37607	0.547532	1.83415
C	-1.476	0.36627	-1.96996
H	-2.13369	0.2507	-2.83828
H	-0.43693	0.300841	-2.32605

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = - 1660.0615641
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.6430458

F' (triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.445644 (Hartree/Particle)
Thermal correction to Energy= 0.475212
Thermal correction to Enthalpy= 0.476156
Thermal correction to Gibbs Free Energy= 0.383215

Sum of electronic and zero-point Energies= -1659.187406
Sum of electronic and thermal Energies= -1659.157838
Sum of electronic and thermal Enthalpies= -1659.156894
Sum of electronic and thermal Free Energies= -1659.249834

C	0.873581	-0.545781	0.67942
N	-0.327569	0.2406	1.10447
C	-1.314299	-0.33286	2.00023
H	-1.328599	0.27988	2.91059
H	-2.290419	-0.247199	1.50789
H	-1.09243	-1.36659	2.24145
C	0.425832	2.384019	-0.01004
C	1.501912	1.543848	-0.6802
C	1.663441	0.179088	-0.40526
C	2.364252	2.130768	-1.61477
H	2.260523	3.185268	-1.84552
C	2.649781	-0.568332	-1.06279
H	2.76351	-1.623222	-0.83651
C	3.487911	0.032197	-1.99131
H	4.246341	-0.557053	-2.49465
C	3.347842	1.392907	-2.26116
H	3.999272	1.877947	-2.98032
C	1.78045	-0.694352	1.94993
F	2.112151	0.498738	2.43202
F	2.8883	-1.362873	1.65478
F	1.14352	-1.370511	2.917
C	-0.222477	3.368039	-1.00043
H	-1.111927	3.81512	-0.54451
H	0.459674	4.184759	-1.24367
H	-0.517577	2.86631	-1.92674
C	0.989683	3.181829	1.17881
H	1.815193	3.812378	0.83764
H	0.209863	3.830049	1.59019
H	1.359553	2.536198	1.97555
S	-0.592841	-2.22397	-0.92334
N	0.50772	-1.888991	0.31643
O	-1.400101	-3.3217	-0.41768
O	-1.2089	-0.95117	-1.28064
C	0.390299	-2.799691	-2.28037
H	0.986389	-3.643951	-1.9342
H	1.01126	-1.975841	-2.63071
H	-0.318511	-3.10972	-3.05012
H	-3.028169	0.692921	-2.05031
H	-3.77312	-1.359878	-0.8272
C	-3.707768	1.315632	-1.45738
H	-4.613108	1.474052	-2.06751
C	-4.44324	-0.778298	-0.18627
H	-3.251578	2.302111	-1.31362
H	0.463419	-2.591101	1.05301
C	-4.048329	0.664882	-0.1538
H	-5.46472	-0.896077	-0.58636
H	-4.44601	-1.225028	0.81474
C	-4.613788	1.525322	0.93285
H	-4.082587	2.480262	1.01387
H	-5.671798	1.767063	0.73361
H	-4.584568	1.024872	1.90723
C	-0.709238	1.46584	0.44138
H	-1.421548	1.98111	1.09438
H	-1.272738	1.11205	-0.44171

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1659.9873336
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.5761865

$TS_{F'-P}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -228.06 cm^{-1}
Zero-point correction= 0.452703 (Hartree/Particle)
Thermal correction to Energy= 0.478865
Thermal correction to Enthalpy= 0.479809
Thermal correction to Gibbs Free Energy= 0.401073
Sum of electronic and zero-point Energies= -1659.226702
Sum of electronic and thermal Energies= -1659.200539
Sum of electronic and thermal Enthalpies= -1659.199595
Sum of electronic and thermal Free Energies= -1659.278331

C	0.097912	0.014449	-0.940478
N	1.054883	-0.478425	-0.048373
C	1.227526	0.120166	1.274225
H	2.223049	0.567404	1.348908
H	0.496217	0.904212	1.444169
H	1.105918	-0.63912	2.05223
C	1.939008	-2.270451	-1.523274
C	1.028036	-1.70206	-2.601009
C	0.175315	-0.617625	-2.340515
C	1.012296	-2.264334	-3.88356
H	1.669279	-3.098689	-4.103634
C	-0.680189	-0.148536	-3.347776
H	-1.381226	0.661063	-3.167924
C	-0.676667	-0.715685	-4.615298
H	-1.341382	-0.328724	-5.379521
C	0.180267	-1.779989	-4.885813
H	0.197463	-2.234075	-5.870948
C	-1.332394	-0.347998	-0.416265
F	-1.618541	-1.613449	-0.730821
F	-2.280379	0.428812	-0.979184
F	-1.45861	-0.254647	0.908565
C	3.27406	-2.771093	-2.09214
H	3.954231	-3.001406	-1.266019
H	3.147757	-3.687975	-2.672553
H	3.751761	-2.020126	-2.729838
C	1.22364	-3.431043	-0.809366
H	0.936003	-4.201073	-1.531366
H	1.897287	-3.882916	-0.07364
H	0.32419	-3.087167	-0.293464
S	1.686809	2.250176	-1.695153
N	0.114658	1.621936	-1.111413
O	1.389148	3.609443	-2.117084
O	2.614462	1.996457	-0.610047
C	2.222603	1.398356	-3.167434
H	1.43488	1.441074	-3.91885
H	2.529028	0.380647	-2.945985
H	3.079174	2.007311	-3.469856
H	1.139539	4.327665	0.044136
C	0.524226	3.757642	0.734346
H	0.093582	4.455181	1.464107
H	1.130039	3.041834	1.291928
H	-0.538716	1.827017	-1.874668
C	-0.667542	3.115234	0.090445
C	-1.605754	2.489614	1.072955
H	-1.119362	1.9061	1.851443
H	-2.047378	3.365695	1.567341
H	-2.425429	1.943617	0.616316
C	2.253388	-1.154658	-0.531662

H 2.72717 -1.597261 0.350257
H 2.978757 -0.44238 -0.95286
C -1.370771 3.870181 -0.999973
H -0.697765 4.243613 -1.767887
H -2.189259 3.28945 -1.433441
H -1.822895 4.735956 -0.499177
UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.0355797
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.6155228

A' + P

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.452828 (Hartree/Particle)
Thermal correction to Energy= 0.480802
Thermal correction to Enthalpy= 0.481746
Thermal correction to Gibbs Free Energy= 0.394562
Sum of electronic and zero-point Energies= -1659.301802
Sum of electronic and thermal Energies= -1659.273828
Sum of electronic and thermal Enthalpies= -1659.272884
Sum of electronic and thermal Free Energies= -1659.360067
C -0.546382 -1.559925 0.204459
N 0.499963 -1.270113 0.90617
C 0.535977 -0.73126 2.275681
H 1.26661 0.077236 2.269115
H -0.426157 -0.343687 2.58946
H 0.863876 -1.533378 2.941349
C 1.905154 -2.828406 -0.413858
C 0.78394 -2.821394 -1.439198
C -0.421341 -2.15011 -1.127813
C 0.891327 -3.465451 -2.668577
H 1.798161 -4.004536 -2.918222
C -1.451408 -2.06484 -2.082283
H -2.339889 -1.482175 -1.884055
C -1.307369 -2.686447 -3.313044
H -2.09793 -2.607004 -4.050471
C -0.146111 -3.405225 -3.596873
H -0.037265 -3.90421 -4.55432
C -1.908013 -1.409736 0.915117
F -2.924197 -1.853453 0.188013
F -2.163357 -0.140886 1.249327
F -1.879149 -2.135318 2.042484
C 3.293165 -2.920134 -1.05849
H 4.062085 -2.777824 -0.293566
H 3.453789 -3.904691 -1.5033
H 3.425849 -2.159469 -1.833151
C 1.713362 -3.996853 0.569584
H 1.760325 -4.944976 0.027609
H 2.508002 -3.987758 1.322435
H 0.747665 -3.953573 1.083146
S -0.350954 1.90288 -0.581587
N -1.491267 2.866434 0.123097
O 0.739813 1.564548 0.340551
O -1.095291 0.791494 -1.189576
C 0.335362 2.887403 -1.890275
H 0.824341 3.757796 -1.454391
H -0.477612 3.178727 -2.553848
H 1.06064 2.255406 -2.404568
H -0.118867 2.302028 2.49947
C -1.028272 2.901739 2.578385
H -0.936704 3.563257 3.445015
H -1.881625 2.236327 2.746226
H -2.363806 2.342104 0.174002
C -1.241124 3.735552 1.31089
C -2.507684 4.584033 1.446226
H -3.386671 3.952378 1.612368
H -2.407604 5.255525 2.303141
H -2.669254 5.182076 0.545567
C 1.835115 -1.486798 0.309972
H 2.557483 -1.444086 1.126454
H 2.013692 -0.643326 -0.368828
C -0.039853 4.642737 1.046976
H 0.887208 4.069762 0.952006
H -0.196545 5.241194 0.14437
H 0.078776 5.326396 1.891659
UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.1084991
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1660.6912353

Methyl $TS_{D\text{-}F}$ (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -951.40 cm^{-1}
Zero-point correction= 0.356427 (Hartree/Particle)
Thermal correction to Energy= 0.380320
Thermal correction to Enthalpy= 0.381265
Thermal correction to Gibbs Free Energy= 0.305145
Sum of electronic and zero-point Energies= -1541.349696
Sum of electronic and thermal Energies= -1541.325803
Sum of electronic and thermal Enthalpies= -1541.324859
Sum of electronic and thermal Free Energies= -1541.400978
C 0.349884 -0.521453 0.271807
N 0.045172 -1.12453 -1.048161
C 1.044154 -1.338727 -2.070408
H 1.075595 -2.412898 -2.286116
H 0.717359 -0.81101 -2.974953
H 2.021401 -0.978763 -1.761278
C -2.352229 -0.489224 -1.166328
C -2.07601 0.329962 0.084678
C -0.850694 0.307216 0.763346
C -3.082248 1.160028 0.59479
H -4.036308 1.213919 0.080738
C -0.655071 1.056164 1.930305
H 0.301979 1.019661 2.439687
C -1.6766 1.855321 2.426154
H -1.519548 2.431198 3.331416
C -2.891093 1.916853 1.744656
H -3.692822 2.549052 2.111146
C 0.592303 -1.740992 1.238199
F -0.553659 -2.357845 1.525479
F 1.147028 -1.337164 2.373282
F 1.405441 -2.633934 0.659143
S 1.758409 1.555011 -0.770324
N 1.533747 0.282534 0.339278

O	3.079417	1.372934	-1.35338
O	0.587555	1.600535	-1.643188
C	1.770515	2.973456	0.294197
H	2.554952	2.827997	1.036558
H	0.786371	3.06313	0.753958
H	1.986152	3.828954	-0.348582
H	3.835403	-1.509325	1.392378
C	3.829989	-1.039394	0.410071
C	-1.290296	-1.616735	-1.275341
H	-1.504236	-2.370376	-0.505662
H	-1.321316	-2.08788	-2.258397
H	2.753001	-0.472945	0.35738
H	3.8543	-1.751283	-0.413459
H	4.540135	-0.222268	0.301373
C	-2.303987	0.388606	-2.425885
H	-1.326768	0.857145	-2.55486
H	-2.537658	-0.213912	-3.309264
H	-3.053582	1.181074	-2.346236
C	-3.708263	-1.207367	-1.083998
H	-4.528017	-0.491339	-1.170704
H	-3.805134	-1.915232	-1.912804
H	-3.815426	-1.750642	-0.141008

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1542.0327264
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1542.5584777

Methyl $TS_{D\text{-}F}$ (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -856.99 cm^{-1}
Zero-point correction= 0.356376 (Hartree/Particle)
Thermal correction to Energy= 0.380380
Thermal correction to Enthalpy= 0.381324
Thermal correction to Gibbs Free Energy= 0.303247
Sum of electronic and zero-point Energies= -1541.349133
Sum of electronic and thermal Energies= -1541.325129
Sum of electronic and thermal Enthalpies= -1541.324185
Sum of electronic and thermal Free Energies= -1541.402262

C	0.343733	-0.522207	0.271715
N	0.043048	-1.117132	-1.05492
C	1.0549	-1.356914	-2.057621
H	1.084701	-2.4355	-2.253193
H	0.740726	-0.846242	-2.976501
H	2.02928	-0.995436	-1.741335
C	-2.356864	-0.481937	-1.166136
C	-2.08083	0.330411	0.090127
C	-0.855227	0.301754	0.767611
C	-3.08432	1.161465	0.602633
H	-4.038976	1.219949	0.089561
C	-0.656477	1.047285	1.936223
H	0.301084	1.006525	2.445085
C	-1.675531	1.847749	2.435328
H	-1.515956	2.420455	3.342373
C	-2.890402	1.913644	1.755426
H	-3.690631	2.546272	2.124832
C	0.591014	-1.747463	1.228962
F	-0.554742	-2.367133	1.513246
F	1.148693	-1.354225	2.366101
F	1.402469	-2.636546	0.640336
S	1.757717	1.555438	-0.773108
N	1.530673	0.283081	0.337651
O	3.071958	1.361217	-1.366826
O	0.580915	1.615659	-1.636399
C	1.790874	2.968984	0.295472
H	2.577438	2.813739	1.033626
H	0.809847	3.066027	0.760836
H	2.0112	3.825474	-0.344577
H	3.827587	-1.549208	1.375493
C	3.846468	-1.012135	0.428346
C	-1.293789	-1.603552	-1.290049
H	-1.502288	-2.369454	-0.529614
H	-1.323644	-2.063883	-2.278567
H	2.764088	-0.469363	0.366769
H	3.924621	-1.663926	-0.440523
H	4.541719	-0.175219	0.4055
C	-2.316036	0.406679	-2.418508
H	-1.338671	0.874612	-2.54955
H	-2.556013	-0.188282	-3.305372
H	-3.064485	1.198892	-2.326673
C	-3.710536	-1.204683	-1.084845
H	-4.532548	-0.49044	-1.164347
H	-3.807948	-1.907787	-1.917834
H	-3.813266	-1.75421	-0.144855

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1542.0321851
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1542.5577151

Methyl F (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.359197 (Hartree/Particle)
Thermal correction to Energy= 0.384788
Thermal correction to Enthalpy= 0.385733
Thermal correction to Gibbs Free Energy= 0.304972
Sum of electronic and zero-point Energies= -1541.374820
Sum of electronic and thermal Energies= -1541.349229
Sum of electronic and thermal Enthalpies= -1541.348285
Sum of electronic and thermal Free Energies= -1541.429045

C	0.333804	-0.465363	0.334374
N	0.094137	-1.236179	-0.918476
C	1.131632	-1.487459	-1.891405
H	1.139175	-2.560003	-2.107265
H	0.86306	-0.947181	-2.810201
H	2.103916	-1.153951	-1.536665
C	-2.320703	-0.721427	-1.163623
C	-2.131006	0.212585	0.021676
C	-0.918139	0.331491	0.712211
C	-3.198113	1.020156	0.435496
H	-4.142552	0.966145	-0.095669
C	-0.79451	1.200986	1.802345
H	0.153456	1.278056	2.324839
C	-1.872605	1.976692	2.207102

H	-1.767979	2.646726	3.053242
C	-3.077361	1.891801	1.51067
H	-3.924483	2.501343	1.806607
C	0.641579	-1.550715	1.427278
F	-0.432971	-2.28859	1.694757
F	1.055546	-0.983257	2.5534
F	1.611401	-2.364501	0.986426
S	1.667266	1.632176	-0.809412
N	1.509896	0.349022	0.27747
O	3.044174	1.553388	-1.273635
O	0.559237	1.516826	-1.750959
C	1.467126	3.101994	0.159334
H	2.190492	3.070845	0.97377
H	0.441373	3.138931	0.524307
H	1.672213	3.933305	-0.517481
H	4.557026	-1.084287	1.221461
C	4.460109	-1.210167	0.150659
C	-1.211676	-1.806281	-1.131272
H	-1.417489	-2.487077	-0.294503
H	-1.19287	-2.374571	-2.06176
H	2.412309	-0.107472	0.440027
H	4.328529	-2.206121	-0.250087
H	4.73924	-0.400087	-0.50979
C	-2.24756	0.053182	-2.488287
H	-1.287374	0.558548	-2.60859
H	-2.407841	-0.628065	-3.329919
H	-3.035074	0.811912	-2.509476
C	-3.648524	-1.489355	-1.081569
H	-4.491563	-0.820909	-1.267493
H	-3.67523	-2.267522	-1.850409
H	-3.780204	-1.956595	-0.101743

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1542.0612702
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1542.578951

Methyl ^{t}F (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.359977 (Hartree/Particle)
Thermal correction to Energy= 0.385100
Thermal correction to Enthalpy= 0.386044
Thermal correction to Gibbs Free Energy= 0.305861
Sum of electronic and zero-point Energies= -1541.374177
Sum of electronic and thermal Energies= -1541.349055
Sum of electronic and thermal Enthalpies= -1541.348110
Sum of electronic and thermal Free Energies= -1541.428293

C	0.3299	-0.459711	0.343456
N	0.100424	-1.2416	-0.904144
C	1.14346	-1.491568	-1.871842
H	1.152652	-2.563826	-2.088892
H	0.879534	-0.950967	-2.792089
H	2.113675	-1.15721	-1.511364
C	-2.313401	-0.733304	-1.170039
C	-2.134814	0.208106	0.010201
C	-0.92658	0.336867	0.706464
C	-3.207721	1.013574	0.41253
H	-4.149235	0.951643	-0.123075
C	-0.812553	1.215316	1.790193
H	0.132015	1.299723	2.317859
C	-1.896286	1.989049	2.183853
H	-1.799391	2.665645	3.025831
C	-3.097045	1.89306	1.482332
H	-3.949135	2.499844	1.769796
C	0.63556	-1.534224	1.447791
F	-0.43489	-2.280054	1.71015
F	1.033186	-0.954177	2.573493
F	1.617688	-2.341644	1.021925
S	1.670247	1.629121	-0.809835
N	1.504344	0.356606	0.287611
O	3.042918	1.529184	-1.283125
O	0.553045	1.519107	-1.74093
C	1.496703	3.107423	0.152322
H	2.231843	3.073752	0.956282
H	0.476781	3.156023	0.532372
H	1.699518	3.933182	-0.532036
H	4.566273	-1.149209	1.20088
C	4.468496	-1.230114	0.125729
C	-1.202585	-1.816438	-1.120873
H	-1.413982	-2.489557	-0.27937
H	-1.176705	-2.392705	-2.046378
H	2.405886	-0.094472	0.463627
H	4.327433	-2.207492	-0.316016
H	4.753029	-0.395374	-0.500885
C	-2.230395	0.032317	-2.499134
H	-1.268074	0.534159	-2.617559
H	-2.387955	-0.654046	-3.337213
H	-3.015623	0.793281	-2.52974
C	-3.64033	-1.503386	-1.094923
H	-4.482676	-0.837738	-1.294477
H	-3.658335	-2.287831	-1.857826
H	-3.780864	-1.963046	-0.112685

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1542.0611
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1542.5788687

Primary TS$_{D\text{-}F}$ (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -629.57 cm^{-1}
Zero-point correction= 0.386401 (Hartree/Particle)
Thermal correction to Energy= 0.411355
Thermal correction to Enthalpy= 0.412299
Thermal correction to Gibbs Free Energy= 0.333675
Sum of electronic and zero-point Energies= -1580.619554
Sum of electronic and thermal Energies= -1580.594601
Sum of electronic and thermal Enthalpies= -1580.593657
Sum of electronic and thermal Free Energies= -1580.672281

C	0.195171	-0.391529	0.348358
N	0.041412	-1.123763	-0.928715
C	1.116074	-1.27445	-1.882425
H	1.271925	-2.346888	-2.045088
H	0.793383	-0.820717	-2.828571
H	2.028848	-0.797636	-1.5343
C	-2.409289	-0.832759	-1.197192

C	-2.311131	0.100397	-0.000512
C	-1.130367	0.294781	0.728695
C	-3.445016	0.815781	0.404354
H	-4.370718	0.699504	-0.149677
C	-1.09626	1.146093	1.840365
H	-0.17022	1.278597	2.389234
C	-2.240497	1.828647	2.231314
H	-2.208847	2.48397	3.094623
C	-3.416328	1.671418	1.499384
H	-4.313984	2.210084	1.783671
C	0.563261	-1.492242	1.412634
F	-0.492592	-2.255125	1.695253
F	0.991149	-0.935442	2.537041
F	1.529309	-2.288305	0.934708
S	1.387278	1.754485	-0.815445
N	1.245517	0.579352	0.407993
O	2.739943	1.654885	-1.345314
O	0.251711	1.606302	-1.723591
C	1.220728	3.250902	0.120605
H	1.992126	3.250479	0.890298
H	0.218425	3.274201	0.548747
H	1.36758	4.067417	-0.588535
H	4.339309	-0.580987	-1.320159
C	4.359619	-1.146701	-0.384658
H	5.408608	-1.377209	-0.163118
H	3.841724	-2.099832	-0.523822
C	3.778105	-0.347445	0.756145
C	-1.2024	-1.808838	-1.172421
H	-1.353398	-2.525528	-0.353947
H	-1.117719	-2.351435	-2.114766
H	2.65455	-0.050623	0.537527
H	4.240363	0.633023	0.890553
H	3.715853	-0.889721	1.702443
C	-2.409742	-0.044753	-2.515874
H	-1.498468	0.543672	-2.635478
H	-2.512231	-0.731953	-3.361576
H	-3.261671	0.641081	-2.529578
C	-3.660237	-1.722089	-1.12233
H	-4.561789	-1.132439	-1.300295
H	-3.615795	-2.491457	-1.899158
H	-3.746979	-2.2094	-0.147288

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1581.342143
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1581.8919929

Primary $TS_{D\text{-}F}$ (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -632.40 cm^{-1}
Zero-point correction= 0.386271 (Hartree/Particle)
Thermal correction to Energy= 0.411337
Thermal correction to Enthalpy= 0.412281
Thermal correction to Gibbs Free Energy= 0.332274
Sum of electronic and zero-point Energies= -1580.618945
Sum of electronic and thermal Energies= -1580.593879
Sum of electronic and thermal Enthalpies= -1580.592934
Sum of electronic and thermal Free Energies= -1580.672942

C	0.19209	-0.39825	0.336771
N	0.046134	-1.088424	-0.967016
C	1.153916	-1.279071	-1.874917
H	1.299306	-2.358168	-2.005684
H	0.869485	-0.847109	-2.842466
H	2.06179	-0.809749	-1.50452
C	-2.420724	-0.798227	-1.206718
C	-2.315078	0.098316	0.017131
C	-1.130047	0.270159	0.743301
C	-3.445627	0.804567	0.445723
H	-4.374653	0.706005	-0.106582
C	-1.089461	1.092718	1.877043
H	-0.159885	1.212363	2.423018
C	-2.230217	1.766332	2.292455
H	-2.193291	2.399136	3.172251
C	-3.410122	1.630139	1.563448
H	-4.305478	2.162471	1.866755
C	0.56834	-1.527604	1.365197
F	-0.483109	-2.310519	1.610431
F	0.981492	-1.004967	2.511448
F	1.54665	-2.29863	0.870788
S	1.374356	1.763778	-0.80338
N	1.243127	0.578621	0.414903
O	2.728643	1.67905	-1.331971
O	0.240579	1.608145	-1.712888
C	1.192145	3.253273	0.141604
H	1.966221	3.257973	0.908893
H	0.191016	3.261271	0.573634
H	1.326415	4.07534	-0.563804
H	4.390729	-0.511838	-1.287261
C	4.409357	-1.088264	-0.358305
H	5.459916	-1.294975	-0.121262
H	3.918513	-2.052286	-0.51874
C	3.78777	-0.317978	0.782114
C	-1.202077	-1.752193	-1.253462
H	-1.332555	-2.529004	-0.485035
H	-1.115944	-2.233776	-2.228711
H	2.665883	-0.041542	0.546699
H	4.230366	0.667983	0.941701
H	3.720064	-0.875743	1.71924
C	-2.471608	0.036597	-2.495852
H	-1.569761	0.638376	-2.621058
H	-2.591029	-0.621534	-3.362382
H	-3.331861	0.71103	-2.460072
C	-3.65553	-1.710842	-1.130747
H	-4.571323	-1.132014	-1.267118
H	-3.61704	-2.454462	-1.932907
H	-3.709245	-2.230108	-0.169554

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1581.3414236
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1581.8909172

Primary F (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.388637 (Hartree/Particle)
Thermal correction to Energy= 0.415204
Thermal correction to Enthalpy= 0.416148
Thermal correction to Gibbs Free Energy= 0.332609
Sum of electronic and zero-point Energies= -1580.646223

Sum of electronic and thermal Energies= -1580.619656
Sum of electronic and thermal Enthalpies= -1580.618712
Sum of electronic and thermal Free Energies= -1580.702251

C	0.167121	-0.40845	0.316974
N	-0.049992	-1.216797	-0.916018
C	0.988618	-1.440068	-1.893844
H	1.068479	-2.519167	-2.059813
H	0.671931	-0.963118	-2.831406
H	1.937266	-1.021444	-1.5679
C	-2.499205	-0.859343	-1.113002
C	-2.346112	0.098868	0.057812
C	-1.127364	0.306603	0.715643
C	-3.454479	0.838966	0.489511
H	-4.405873	0.715794	-0.01717
C	-1.034614	1.197913	1.791302
H	-0.080327	1.347191	2.286261
C	-2.151768	1.904428	2.215616
H	-2.071015	2.591435	3.050683
C	-3.365527	1.72986	1.551836
H	-4.243883	2.285262	1.862971
C	0.58035	-1.453537	1.414452
F	-0.436672	-2.248815	1.733943
F	1.001663	-0.840313	2.514429
F	1.581594	-2.215901	0.951194
S	1.356498	1.740236	-0.892561
N	1.282347	0.477923	0.212513
O	2.741464	1.758906	-1.339621
O	0.271333	1.514173	-1.841611
C	1.029203	3.217296	0.03083
H	1.739487	3.264478	0.856226
H	-0.00188	3.183512	0.381407
H	1.180217	4.044499	-0.664778
H	4.306549	-0.411748	-1.264382
C	4.574608	-1.044452	-0.412184
H	5.652847	-1.247537	-0.497114
H	4.067904	-2.010427	-0.503597
C	4.262469	-0.374615	0.882044
C	-1.322558	-1.869421	-1.091452
H	-1.46448	-2.550856	-0.241425
H	-1.287379	-2.449275	-2.014304
H	2.215296	0.147943	0.495698
H	4.445795	0.68948	0.993268
H	4.182151	-0.959356	1.792019
C	-2.500014	-0.096153	-2.446457
H	-1.575606	0.466926	-2.589323
H	-2.631874	-0.795114	-3.278468
H	-3.33425	0.611056	-2.460021
C	-3.77387	-1.708791	-0.99717
H	-4.661008	-1.097176	-1.1734
H	-3.765699	-2.49584	-1.757367
H	-3.857888	-2.172165	-0.010246

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1581.3520985
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1581.9144623

Primary ^{t}F (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.389365 (Hartree/Particle)
Thermal correction to Energy= 0.415570
Thermal correction to Enthalpy= 0.416515
Thermal correction to Gibbs Free Energy= 0.332990
Sum of electronic and zero-point Energies= -1580.645550
Sum of electronic and thermal Energies= -1580.619344
Sum of electronic and thermal Enthalpies= -1580.618400
Sum of electronic and thermal Free Energies= -1580.701924

C	0.160279	-0.405708	0.335348
N	-0.03979	-1.229292	-0.890116
C	1.011666	-1.459411	-1.85318
H	1.077406	-2.537391	-2.030014
H	0.717972	-0.96711	-2.791
H	1.962454	-1.059612	-1.508335
C	-2.486287	-0.871246	-1.12651
C	-2.347459	0.103305	0.032177
C	-1.137683	0.318595	0.703765
C	-3.460006	0.851699	0.437704
H	-4.405044	0.722998	-0.079677
C	-1.058045	1.224345	1.767928
H	-0.110297	1.378807	2.273818
C	-2.17977	1.938428	2.167264
H	-2.10934	2.63627	2.994388
C	-3.384161	1.75689	1.489054
H	-4.265792	2.318102	1.780145
C	0.552651	-1.436932	1.45417
F	-0.474517	-2.220219	1.773321
F	0.965028	-0.810351	2.549915
F	1.553414	-2.213682	1.014573
S	1.362844	1.723777	-0.887452
N	1.280096	0.476393	0.236697
O	2.737662	1.707605	-1.364956
O	0.252972	1.510473	-1.810412
C	1.090456	3.215136	0.031063
H	1.824946	3.254487	0.83565
H	0.069373	3.204227	0.41127
H	1.237618	4.033663	-0.675615
H	4.320182	-0.400317	-1.295495
C	4.619337	-1.024646	-0.447402
H	5.70832	-1.163288	-0.527379
H	4.170381	-2.017389	-0.551295
C	4.262606	-0.385757	0.851002
C	-1.310619	-1.881893	-1.075371
H	-1.465362	-2.551563	-0.217993
H	-1.264212	-2.474182	-1.989917
H	2.211876	0.131278	0.50651
H	4.40032	0.68423	0.976064
H	4.203259	-0.98351	1.754239
C	-2.470544	-0.129634	-2.471763
H	-1.540921	0.424278	-2.617153
H	-2.601202	-0.841611	-3.292897
H	-3.299467	0.583302	-2.503422
C	-3.762371	-1.71918	-1.014849
H	-4.647005	-1.111346	-1.215955
H	-3.742161	-2.519485	-1.761104
H	-3.861658	-2.165305	-0.021397

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1581.3717666
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1581.9139708

Secondary $TS_{D\text{-}F}$ (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -507.24 cm^{-1}
Zero-point correction= 0.415223 (Hartree/Particle)
Thermal correction to Energy= 0.441514
Thermal correction to Enthalpy= 0.442458
Thermal correction to Gibbs Free Energy= 0.361096
Sum of electronic and zero-point Energies= -1619.890467
Sum of electronic and thermal Energies= -1619.864176
Sum of electronic and thermal Enthalpies= -1619.863232
Sum of electronic and thermal Free Energies= -1619.944594

C	0.065488	-0.399281	0.179047
N	-0.194182	-0.885625	-1.193134
C	0.798781	-0.820494	-2.2409
H	0.933704	-1.831022	-2.640592
H	0.404456	-0.178214	-3.039592
H	1.738828	-0.419591	-1.870185
C	-2.676072	-0.698256	-1.148094
C	-2.480678	-0.003272	0.190155
C	-1.234886	0.122004	0.819086
C	-3.589512	0.555575	0.838081
H	-4.566291	0.488394	0.370176
C	-1.109942	0.755912	2.062039
H	-0.134624	0.840447	2.528527
C	-2.22909	1.286124	2.689891
H	-2.126596	1.773739	3.652941
C	-3.47238	1.195425	2.066448
H	-4.353156	1.61831	2.537802
C	0.593073	-1.655043	0.964218
F	-0.383138	-2.541936	1.158462
F	1.079958	-1.302093	2.144875
F	1.562298	-2.257469	0.262102
S	1.035102	1.975854	-0.691109
N	1.075326	0.607137	0.32387
O	2.297671	2.022646	-1.415278
O	-0.215453	1.9431	-1.447583
C	0.98393	3.279403	0.508665
H	1.862701	3.181393	1.14574
H	0.057722	3.183073	1.075611
H	1.006653	4.21153	-0.058711
H	3.964886	-0.16571	-1.926328
C	4.214661	-0.765116	-1.0466
H	5.305295	-0.880083	-1.024386
H	3.783708	-1.766252	-1.153423
C	3.759854	-0.096891	0.234536
C	-1.433576	-1.573591	-1.453672
H	-1.460646	-2.456827	-0.800032
H	-1.430539	-1.899542	-2.494464
H	2.597222	0.035083	0.202898
H	4.07782	0.950257	0.278527
C	4.102888	-0.844414	1.507358
H	3.673014	-0.362298	2.388772
H	3.761836	-1.882543	1.470539
H	5.192967	-0.856487	1.629516
C	-2.876017	0.323959	-2.277793
H	-3.751461	0.942189	-2.059829
H	-2.012185	0.982267	-2.384115
H	-3.053801	-0.196535	-3.22402
C	-3.865518	-1.670731	-1.11092
H	-4.808962	-1.123434	-1.062384
H	-3.883792	-2.270796	-2.025912
H	-3.804227	-2.341967	-0.249815

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1620.6510513
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1621.2248201

Secondary $TS_{D\text{-}F}$ (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -535.19 cm^{-1}
Zero-point correction= 0.415435 (Hartree/Particle)
Thermal correction to Energy= 0.441643
Thermal correction to Enthalpy= 0.442588
Thermal correction to Gibbs Free Energy= 0.360254
Sum of electronic and zero-point Energies= -1619.889460
Sum of electronic and thermal Energies= -1619.863251
Sum of electronic and thermal Enthalpies= -1619.862307
Sum of electronic and thermal Free Energies= -1619.944641

C	0.059309	-0.403749	0.172585
N	-0.196901	-0.859491	-1.213337
C	0.819265	-0.823147	-2.240063
H	0.948844	-1.840897	-2.624772
H	0.445232	-0.189679	-3.055399
H	1.758231	-0.431065	-1.857891
C	-2.685186	-0.673981	-1.153431
C	-2.484691	-0.005153	0.197862
C	-1.236413	0.104533	0.823881
C	-3.589695	0.547238	0.856512
H	-4.568532	0.489559	0.391026
C	-1.106344	0.719815	2.076017
H	-0.129398	0.79533	2.541064
C	-2.22163	1.245395	2.714968
H	-2.114017	1.718118	3.684982
C	-3.466956	1.167837	2.09456
H	-4.345384	1.585425	2.575227
C	0.59061	-1.672381	0.932754
F	-0.382362	-2.570455	1.095692
F	1.064282	-1.344786	2.126214
F	1.570463	-2.253261	0.226548
S	1.03174	1.981555	-0.67639
N	1.075103	0.602549	0.328186
O	2.289963	2.026993	-1.408313
O	-0.224644	1.960873	-1.423125
C	0.996695	3.275086	0.535546
H	1.880377	3.167787	1.16454
H	0.074231	3.177544	1.108539
H	1.018608	4.212165	-0.023913
H	3.999083	-0.120679	-1.910333
C	4.249432	-0.728643	-1.03662
H	5.341609	-0.825228	-1.00262
H	3.836983	-1.735222	-1.163872
C	3.767557	-0.088359	0.249294
C	-1.442365	-1.529928	-1.495182
H	-1.459516	-2.438033	-0.873931
H	-1.441015	-1.822171	-2.546313
H	2.606589	0.032718	0.202946
H	4.07809	0.959906	0.318285
C	4.098571	-0.857791	1.512514

H	3.652202	-0.39627	2.396823
H	3.765477	-1.897506	1.449933
H	5.186859	-0.864462	1.650447
C	-2.909098	0.372238	-2.256175
H	-3.784882	0.979456	-2.010639
H	-2.049784	1.036985	-2.359352
H	-3.097333	-0.127682	-3.211461
C	-3.865821	-1.657789	-1.123343
H	-4.813415	-1.12069	-1.049336
H	-3.890886	-2.237189	-2.0516
H	-3.786964	-2.348243	-0.278742

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1620.6502666
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1621.2237289

Secondary F (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.419046 (Hartree/Particle)
Thermal correction to Energy= 0.446508
Thermal correction to Enthalpy= 0.447452
Thermal correction to Gibbs Free Energy= 0.361790
Sum of electronic and zero-point Energies= -1619.958006
Sum of electronic and thermal Energies= -1619.930544
Sum of electronic and thermal Enthalpies= -1619.929600
Sum of electronic and thermal Free Energies= -1620.015262

C	-0.233462	-0.312257	0.655007
N	-1.057382	-1.488097	0.569147
C	-0.528632	-2.747687	1.082307
H	-0.641452	-2.849907	2.171107
H	-1.072912	-3.560127	0.595247
H	0.524548	-2.863327	0.825757
C	-3.140602	-0.390407	-0.164683
C	-2.304562	0.875033	-0.296173
C	-0.955842	0.917303	0.086257
C	-2.865312	2.021993	-0.877663
H	-3.902552	2.000403	-1.196253
C	-0.211472	2.090183	-0.109153
H	0.840218	2.104553	0.153497
C	-0.788212	3.220193	-0.671373
H	-0.194562	4.116603	-0.816243
C	-2.127022	3.183633	-1.062223
H	-2.591462	4.054753	-1.513143
C	0.205138	-0.006287	2.128807
F	-0.861452	0.082283	2.928077
F	0.908148	1.128543	2.270307
F	0.991328	-0.991697	2.610317
S	1.199788	-1.066607	-1.612823
N	1.067228	-0.476707	-0.036543
O	2.653998	-1.042567	-1.823553
O	0.512988	-2.333617	-1.826743
C	0.447268	0.168453	-2.640823
H	0.917938	1.130603	-2.444463
H	-0.625172	0.200003	-2.447363
H	0.645978	-0.171767	-3.659073
H	4.705808	-1.187097	-0.525883
C	5.226628	-0.278577	-0.210253
H	5.860388	-0.019777	-1.089643
H	5.868778	-0.387837	0.661467
C	4.344598	0.854953	-0.177313
C	-2.476712	-1.309337	0.857217
H	-2.658002	-0.939507	1.877787
H	-2.939152	-2.299287	0.788397
H	1.739798	-1.014157	0.514137
H	3.560158	0.882223	-0.935843
C	4.410858	1.923373	0.783327
H	3.604618	1.600523	1.483647
H	5.339758	1.967663	1.349897
H	4.069698	2.881993	0.389187
C	-3.199202	-1.099647	-1.529443
H	-3.564742	-0.420707	-2.306273
H	-2.208662	-1.468377	-1.815373
H	-3.880442	-1.955807	-1.474633
C	-4.563592	-0.088797	0.324267
H	-5.156662	0.422983	-0.437763
H	-5.073832	-1.029597	0.556827
H	-4.550882	0.528863	1.227557

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1620.725406
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1621.2834074

Secondary ^{t}F (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.418073 (Hartree/Particle)
Thermal correction to Energy= 0.445702
Thermal correction to Enthalpy= 0.446646
Thermal correction to Gibbs Free Energy= 0.359687
Sum of electronic and zero-point Energies= -1619.918586
Sum of electronic and thermal Energies= -1619.890957
Sum of electronic and thermal Enthalpies= -1619.890013
Sum of electronic and thermal Free Energies= -1619.976972

C	0.037649	-0.403452	0.124327
N	-0.282419	-0.943836	-1.227362
C	0.648784	-0.869482	-2.32849
H	0.723711	-1.86424	-2.777045
H	0.230754	-0.176432	-3.072205
H	1.620731	-0.511445	-1.997664
C	-2.756081	-0.751616	-1.071578
C	-2.511971	-0.056369	0.258391
C	-1.234129	0.106379	0.807526
C	-3.596811	0.48656	0.958996
H	-4.595935	0.395647	0.545617
C	-1.057085	0.759467	2.033066
H	-0.058397	0.878383	2.441299
C	-2.149347	1.271937	2.719532
H	-2.002826	1.774094	3.669517
C	-3.424913	1.142457	2.171575
H	-4.286773	1.549959	2.68957
C	0.63542	-1.6242	0.911431
F	-0.292163	-2.548836	1.144819
F	1.148696	-1.232998	2.071892
F	1.616281	-2.186601	0.190139
S	0.958392	2.038334	-0.701153

N	1.084197	0.56818	0.097894
O	2.269376	2.254359	-1.294934
O	-0.231182	1.941585	-1.540945
C	0.692256	3.257447	0.556515
H	1.502722	3.178603	1.281679
H	-0.281299	3.078943	1.01224
H	0.715277	4.222384	0.046959
H	3.916976	0.199446	-1.782042
C	4.344355	-0.529275	-1.086472
H	5.41831	-0.606415	-1.319431
H	3.914363	-1.518697	-1.285282
C	4.141354	-0.123074	0.336702
C	-1.531229	-1.639021	-1.411706
H	-1.528318	-2.505557	-0.734938
H	-1.57916	-1.991289	-2.442997
H	2.061665	0.262085	0.218919
H	4.17653	0.941534	0.56329
C	4.470423	-1.077688	1.436259
H	4.082281	-0.741228	2.401093
H	4.075137	-2.077599	1.227527
H	5.561576	-1.184102	1.542736
C	-2.971202	0.279095	-2.190375
H	-3.841859	0.896961	-1.952715
H	-2.10722	0.937755	-2.301125
H	-3.162749	-0.230969	-3.139752
C	-3.953287	-1.711355	-1.006026
H	-4.890186	-1.155222	-0.935235
H	-3.999269	-2.310426	-1.920693
H	-3.878739	-2.384423	-0.147255

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1620.6828566
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1621.2488583

Benzylic $TS_{D\text{-}F}$ (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -568.31 cm^{-1}
Zero-point correction= 0.440114 (Hartree/Particle)
Thermal correction to Energy= 0.468572
Thermal correction to Enthalpy= 0.469516
Thermal correction to Gibbs Free Energy= 0.379473
Sum of electronic and zero-point Energies= -1772.244569
Sum of electronic and thermal Energies= -1772.216112
Sum of electronic and thermal Enthalpies= -1772.215168
Sum of electronic and thermal Free Energies= -1772.305210

C	-0.464901	-0.170374	-0.313552
N	-1.201334	0.06172	-1.572784
C	-0.74954	0.998667	-2.577888
H	-0.62166	0.447454	-3.516011
H	-1.540381	1.747006	-2.716737
H	0.17801	1.483508	-2.282785
C	-3.437962	-0.713906	-0.794597
C	-2.80104	-0.782515	0.584405
C	-1.436158	-0.565579	0.815109
C	-3.603365	-1.076094	1.694033
H	-4.666925	-1.236779	1.550847
C	-0.891162	-0.668937	2.102024
H	0.168519	-0.495765	2.254669
C	-1.70775	-0.978099	3.181536
H	-1.280572	-1.058728	4.174836
C	-3.07304	-1.16896	2.975728
H	-3.725912	-1.396137	3.811726
C	0.520023	-1.358874	-0.620161
F	-0.150143	-2.502817	-0.774087
F	1.390498	-1.511901	0.366286
F	1.190574	-1.121129	-1.753888
C	-4.243632	0.582673	-0.969098
H	-4.733293	0.587877	-1.947848
H	-5.020086	0.636043	-0.200621
H	-3.610522	1.466404	-0.876453
C	-4.344484	-1.927663	-1.055637
H	-5.250405	-1.869924	-0.449012
H	-4.654958	-1.94046	-2.104997
H	-3.829327	-2.865241	-0.828717
S	-0.319632	2.466887	0.253709
N	0.352541	0.907886	0.151334
O	0.542629	3.348939	-0.521685
O	-1.742467	2.398339	-0.078448
C	-0.119297	2.807283	1.983164
H	0.938238	2.702503	2.224653
H	-0.736283	2.104852	2.543803
H	-0.459231	3.834701	2.126495
C	-2.327056	-0.786609	-1.873569
H	-1.951661	-1.818884	-1.917596
H	-2.713972	-0.505712	-2.854002
H	2.861927	1.18434	-2.223464
H	4.003776	-0.966416	-2.141422
C	4.25962	-0.799555	-1.098646
C	2.881184	1.302656	-1.138036
H	5.439726	-2.589062	-0.94011
C	5.063823	-1.712002	-0.423216
C	3.775602	0.346475	-0.44666
H	3.044906	2.345247	-0.855521
H	1.817707	1.103658	-0.757337
C	5.385396	-1.500367	0.919495
C	4.1097	0.548944	0.904353
C	4.90667	-0.365889	1.582006
H	6.008942	-2.214604	1.447609
H	3.734745	1.431928	1.416139
H	5.158901	-0.198509	2.624174

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1773.0637702
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1773.6947035

Benzylic $^{t}TS_{D\text{-}F}$ (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -633.43 cm^{-1}
Zero-point correction= 0.440091 (Hartree/Particle)
Thermal correction to Energy= 0.468567
Thermal correction to Enthalpy= 0.469511
Thermal correction to Gibbs Free Energy= 0.380101
Sum of electronic and zero-point Energies= -1772.243267
Sum of electronic and thermal Energies= -1772.214791
Sum of electronic and thermal Enthalpies= -1772.213847

Sum of electronic and thermal Free Energies= -1772.303257

C	-0.84419	-0.4454	0.42437
N	-1.08479	-1.17823	-0.83954
C	-0.00682	-1.63874	-1.68542
H	-0.13404	-2.71558	-1.83895
H	-0.10912	-1.13724	-2.65833
H	0.96514	-1.41618	-1.25137
C	-3.41044	-0.38499	-1.23782
C	-3.17072	0.54735	-0.0604
C	-2.00748	0.51718	0.71982
C	-4.14245	1.50028	0.26486
H	-5.04936	1.55704	-0.32834
C	-1.83785	1.39006	1.80183
H	-0.92864	1.34753	2.39212
C	-2.82528	2.31662	2.11194
H	-2.6895	2.98941	2.95156
C	-3.97766	2.37755	1.33094
H	-4.75231	3.10402	1.55268
C	-0.77161	-1.55361	1.54013
F	-1.98548	-2.04531	1.79729
F	-0.27231	-1.05916	2.6646
F	0.00305	-2.57049	1.13985
C	-3.20247	0.34989	-2.57108
H	-3.41663	-0.32399	-3.4066
H	-3.89221	1.19665	-2.63197
H	-2.18459	0.73245	-2.66513
C	-4.81871	-0.99844	-1.1968
H	-5.57487	-0.2431	-1.4202
H	-4.90559	-1.78122	-1.95671
H	-5.03552	-1.43311	-0.21694
S	0.80642	1.33617	-0.75721
N	0.39204	0.27778	0.50102
O	2.06034	0.85635	-1.32442
O	-0.34415	1.50483	-1.64422
C	1.09806	2.83017	0.1517
H	1.86798	2.62359	0.89514
H	0.15953	3.1392	0.61284
H	1.44063	3.56579	-0.57851
C	-2.43349	-1.58273	-1.14695
H	-2.7639	-2.24287	-0.33089
H	-2.41713	-2.15083	-2.07815
H	2.70677	-1.34254	2.11646
H	4.12498	0.74303	1.95561
C	4.53131	0.35566	1.02454
C	2.72778	-1.38408	1.02394
H	6.08964	1.83066	0.90664
C	5.63165	0.96669	0.43585
C	3.93088	-0.76645	0.42648
H	2.54155	-2.40077	0.67188
H	1.81827	-0.75929	0.71911
C	6.15074	0.46599	-0.76235
C	4.46362	-1.25931	-0.77698
C	5.56634	-0.65192	-1.36461
H	7.00971	0.94353	-1.22293
H	4.0029	-2.124	-1.24766
H	5.97256	-1.04405	-2.29143

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1773.0619177
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1773.6944137

Benzylic F (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.447840 (Hartree/Particle)
Thermal correction to Energy= 0.476502
Thermal correction to Enthalpy= 0.477446
Thermal correction to Gibbs Free Energy= 0.386458
Sum of electronic and zero-point Energies= -1772.308513
Sum of electronic and thermal Energies= -1772.279851
Sum of electronic and thermal Enthalpies= -1772.278907
Sum of electronic and thermal Free Energies= -1772.369895

C	2.038389	-0.478658	-0.413367
N	1.337749	0.192242	-1.488897
C	2.087559	0.467182	-2.714077
H	2.187149	-0.412988	-3.365497
H	1.551859	1.245592	-3.262587
H	3.079919	0.856102	-2.483487
C	-0.954521	-0.148888	-0.594397
C	-0.280631	-0.660578	0.670413
C	1.111019	-0.767818	0.773613
C	-1.054041	-0.942028	1.806003
H	-2.135071	-0.852017	1.749793
C	1.696029	-1.132928	1.993103
H	2.776479	-1.181888	2.071753
C	0.914579	-1.411598	3.106273
H	1.386289	-1.691118	4.042683
C	-0.473741	-1.320008	3.009983
H	-1.099351	-1.533488	3.871083
C	2.677869	-1.834638	-0.871517
F	1.757899	-2.626918	-1.435537
F	3.246539	-2.527898	0.123073
F	3.646619	-1.630768	-1.789047
C	-1.285411	1.339903	-0.391917
H	-1.81672	1.727343	-1.271437
H	-1.91887	1.474023	0.492143
H	-0.36833	1.915852	-0.245537
C	-2.235091	-0.927257	-0.922657
H	-3.015481	-0.757337	-0.174987
H	-2.626861	-0.596787	-1.891917
H	-2.045521	-2.003897	-0.976437
S	3.01291	1.905902	0.469243
N	3.210969	0.287172	0.040653
O	3.4038	2.761222	-0.651027
O	1.69024	2.069872	1.057573
C	4.23926	2.060781	1.743713
H	5.21183	1.794751	1.329323
H	3.959549	1.398201	2.562223
H	4.22774	3.105311	2.058503
C	-0.005691	-0.302658	-1.781107
H	0.001829	-1.347118	-2.128267
H	-0.388591	0.303032	-2.609947
H	-4.52312	2.777873	-1.857847
H	-5.536841	0.629753	-2.395417
C	-5.536061	0.362603	-1.342817
C	-4.53197	2.509463	-0.804697
H	-6.387061	-1.584376	-1.622867
C	-6.002931	-0.858656	-0.916347
C	-5.028831	1.304133	-0.384737
H	-4.13268	3.231533	-0.097157
H	4.000139	0.219861	-0.602237
C	-5.975211	-1.161156	0.456423
C	-5.015021	0.966763	1.011773
C	-5.485001	-0.258977	1.419543

H -6.344031 -2.127756 0.786853
H -4.62624 1.686493 1.726103
H -5.480731 -0.535657 2.467093
UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1773.1359115
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1773.7512552

Benzylic ^{t}F (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Zero-point correction= 0.443599 (Hartree/Particle)
Thermal correction to Energy= 0.472629
Thermal correction to Enthalpy= 0.473573
Thermal correction to Gibbs Free Energy= 0.381812
Sum of electronic and zero-point Energies= -1772.281652
Sum of electronic and thermal Energies= -1772.252622
Sum of electronic and thermal Enthalpies= -1772.251678
Sum of electronic and thermal Free Energies= -1772.343438
C -0.70756 -0.61464 0.09331
N -1.25236 -1.39867 -1.05091
C -0.40308 -2.03002 -2.03423
H -0.71365 -3.07495 -2.12592
H -0.57607 -1.52602 -2.99517
H 0.64674 -1.95505 -1.76256
C -3.4714 -0.28203 -1.17555
C -2.93377 0.66444 -0.11324
C -1.6687 0.51688 0.46844
C -3.71237 1.75707 0.28991
H -4.68708 1.91062 -0.16116
C -1.21853 1.41086 1.4472
H -0.23339 1.27944 1.88395
C -2.01698 2.474 1.84675
H -1.66088 3.16111 2.60631
C -3.26678 2.65192 1.25485
H -3.89628 3.48584 1.54655
C -0.60382 -1.64457 1.27378
F -1.80888 -2.01017 1.70337
F 0.068 -1.12393 2.29526
F 0.04394 -2.74206 0.86008
C -3.34167 0.33844 -2.5754
H -3.7591 -0.34053 -3.32558
H -3.90525 1.27504 -2.61248
H -2.30145 0.5575 -2.8238
C -4.93465 -0.66729 -0.90974
H -5.59652 0.18095 -1.09537
H -5.23637 -1.4701 -1.58945
H -5.07706 -1.00494 0.12054
S 1.00296 0.94042 -1.36344
N 0.62651 -0.15143 -0.13296
O 2.27774 0.48358 -1.89058
O -0.17819 1.00352 -2.21946
C 1.23354 2.50671 -0.56809
H 1.98797 2.37745 0.2087
H 0.27693 2.83635 -0.16463
H 1.58648 3.18427 -1.34762
C -2.67615 -1.61159 -1.12098
H -2.97123 -2.15779 -0.21409
H -2.88868 -2.22997 -1.99388
H 2.51858 -2.08524 2.01029
H 3.01128 0.33893 2.2708
C 3.69138 0.2965 1.42271
C 3.12885 -2.08806 1.11419
H 4.26982 2.35511 1.58412
C 4.39694 1.42599 1.03594
C 3.84914 -0.93361 0.72668
H 3.24564 -3.02278 0.578
H 1.4112 -0.77159 0.08715
C 5.27739 1.37283 -0.05148
C 4.74797 -0.96296 -0.37331
C 5.44902 0.17074 -0.7487
H 5.82777 2.25918 -0.34927
H 4.87917 -1.89364 -0.91842
H 6.13312 0.12725 -1.59032
UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1773.1051692
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1773.7264968

Truncated TS$_{D\text{-}F}$ (Singlet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -1390.43 cm^{-1}
Zero-point correction= 0.384101 (Hartree/Particle)
Thermal correction to Energy= 0.406212
Thermal correction to Enthalpy= 0.407156
Thermal correction to Gibbs Free Energy= 0.335307
Sum of electronic and zero-point Energies= -957.120720
Sum of electronic and thermal Energies= -957.098609
Sum of electronic and thermal Enthalpies= -957.097665
Sum of electronic and thermal Free Energies= -957.16951
H 3.793033 -1.541714 -0.066105
H 3.420974 -0.977221 -1.705528
H 2.714425 -0.149523 -0.311363
C 3.006669 -1.128066 -0.704952
H 1.849663 -0.143867 2.282269
H 1.141389 1.648969 0.841574
H 0.932799 1.353762 -0.899372
C 0.422966 1.690613 0.011481
H 0.125144 2.72796 -0.13518
C 0.800427 -0.470251 2.305182
H -0.545778 3.694261 2.024373
H -0.634843 1.953405 3.848669
C 1.815114 -2.0943 -0.771925
H 1.933611 -2.497477 1.389439
H 0.143143 0.36872 2.513526
H 2.760043 -3.384316 -2.223273
H 0.708022 -1.237108 3.084077
H 3.005633 -3.897317 -0.545529
C 2.278412 -3.475991 -1.245824
N 0.469679 -1.078562 1.041941
C 1.181656 -2.266296 0.63284
C 0.745351 -1.56372 -1.687144
C -1.608988 3.526654 1.827253
C -1.681687 1.734546 3.614382
N -0.780084 0.88976 0.203588

H	-2.296727	2.330352	4.302645
H	-2.1768	4.24167	2.437765
C	-0.344656	-0.920064	-1.276846
C	-0.603646	-0.524884	0.173271
C	-2.039293	2.11783	2.191696
H	-1.81876	3.750022	0.776502
H	-1.405336	1.400858	1.378038
H	-1.886893	0.680602	3.823054
H	1.436403	-4.167862	-1.337408
H	0.447404	-3.082594	0.577569
C	-1.916247	-1.199732	0.659824
F	-2.111251	-0.970719	1.967233
C	-3.486526	1.838424	1.829469
H	-4.131666	2.54105	2.374064
F	-1.864587	-2.525669	0.491102
F	-2.960116	-0.731419	-0.013485
H	-3.661809	1.982672	0.759136
H	-3.789753	0.825188	2.102923
H	0.878845	-1.736034	-2.753688
H	-1.100388	-0.555872	-1.963992

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -957 .7564987
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -958.192104

Truncated $^{t}TS_{D\text{-}F}$ (Triplet)

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -1338.42 cm^{-1}
Zero-point correction= 0.384233 (Hartree/Particle)
Thermal correction to Energy= 0.406231
Thermal correction to Enthalpy= 0.407175
Thermal correction to Gibbs Free Energy= 0.334823
Sum of electronic and zero-point Energies= -957.120601
Sum of electronic and thermal Energies= -957.098603
Sum of electronic and thermal Enthalpies= -957.097659
Sum of electronic and thermal Free Energies= -957.170011

C	-0.491865	-0.680055	0.07879
N	0.577196	-1.249212	0.940715
C	0.845784	-0.705579	2.248062
H	0.743977	-1.515804	2.980433
H	1.888143	-0.35954	2.278823
H	0.163418	0.108878	2.473916
C	1.927318	-2.215522	-0.909015
C	0.839975	-1.688938	-1.807313
C	-0.252387	-1.065477	-1.373629
C	-1.816987	-1.323696	0.566324
F	-1.786874	-2.65029	0.394013
F	-2.851582	-0.834803	-0.107164
F	-2.011754	-1.096311	1.874263
C	3.111288	-1.238913	-0.856418
H	3.918417	-1.656101	-0.246352
H	3.497316	-1.066037	-1.864861
H	2.820928	-0.271446	-0.435818
C	2.397424	-3.588019	-1.404554
H	2.866406	-3.480295	-2.386456
H	3.136658	-4.011155	-0.717972
H	1.560572	-4.286329	-1.49478
C	0.591913	1.524955	-0.034766
N	-0.627225	0.746181	0.137427
H	-0.544272	1.838835	3.724442
H	-0.457026	3.591472	1.912183
C	-1.596424	1.639953	3.4956
H	-2.197082	2.259648	4.175524
C	-1.514632	3.415386	1.693939
H	-1.825366	0.594202	3.720317
H	-1.297331	1.28187	1.274576
C	-1.945195	2.008664	2.066522
H	-2.098907	4.13453	2.283788
H	-1.703124	3.625354	0.636317
C	-3.389753	1.725103	1.696893
H	-3.69337	0.712914	1.973657
H	-4.039323	2.429396	2.23413
H	-3.558964	1.863617	0.624824
C	1.325712	-2.406878	0.501154
H	0.609089	-3.242122	0.463018
H	2.094515	-2.622591	1.245444
H	0.96776	-1.842533	-2.877294
H	-1.019598	-0.702232	-2.048789
H	0.314964	2.574971	-0.120636
H	1.07554	1.228474	-0.973523
H	1.322009	1.423755	0.780167

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -957.7565991
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -958.1984075

$TS_{D'\text{-}E'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -339.95 cm^{-1}
Zero-point correction= 0.313388 (Hartree/Particle)
Thermal correction to Energy= 0.334213
Thermal correction to Enthalpy= 0.335157
Thermal correction to Gibbs Free Energy= 0.265604
Sum of electronic and zero-point Energies= -1500.907502
Sum of electronic and thermal Energies= -1500.886677
Sum of electronic and thermal Enthalpies= -1500.885733
Sum of electronic and thermal Free Energies= -1500.955287

C	0.183960	-0.096290	0.179060
N	-0.041920	-1.498130	-0.185990
C	0.846930	-2.609620	0.151110
H	0.905630	-3.259360	-0.722610
H	1.830800	-2.261600	0.453430
H	0.369840	-3.156930	0.975230
C	-2.487410	-1.196050	-0.433960
C	-2.279270	0.306500	-0.328320
C	-1.001150	0.816880	-0.086730
C	-3.323970	1.219720	-0.495820
H	-4.329880	0.858000	-0.678800
C	-0.748690	2.191340	-0.074800
H	0.262670	2.563840	0.065250
C	-1.800590	3.081130	-0.252200
H	-1.611650	4.148750	-0.242100
C	-3.091660	2.591270	-0.446380
H	-3.918910	3.280290	-0.580190

C	0.633510	0.087900	1.672890
F	-0.453260	0.222100	2.435360
F	1.365220	1.195830	1.775460
F	1.331770	-0.929000	2.171270
S	2.803320	0.289610	-0.716510
N	1.104490	0.029340	-0.932580
O	2.881710	1.736870	-0.600440
O	3.309990	-0.568180	0.342910
C	3.392920	-0.245430	-2.294810
H	3.195260	-1.312840	-2.392040
H	4.466000	-0.045190	-2.293180
H	2.883740	0.337060	-3.061600
C	-1.196630	-1.792610	-1.028820
C	-3.614670	-1.561470	-1.407360
C	-2.771700	-1.813880	0.944760
H	-0.999940	-1.362690	-2.020530
H	-1.253550	-2.878950	-1.120470
H	-1.971910	-1.611260	1.663720
H	-2.895960	-2.898140	0.858340
H	-3.694060	-1.391710	1.352040
H	-3.490560	-1.062680	-2.372600
H	-4.584850	-1.281880	-0.990500
H	-3.630360	-2.643070	-1.569470

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5374467
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0284128

$TS_{E\text{-}D}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -547.26 cm^{-1}
Zero-point correction= 0.313551 (Hartree/Particle)
Thermal correction to Energy= 0.334555
Thermal correction to Enthalpy= 0.335499
Thermal correction to Gibbs Free Energy= 0.264507
Sum of electronic and zero-point Energies= -1500.896584
Sum of electronic and thermal Energies= -1500.875580
Sum of electronic and thermal Enthalpies= -1500.874636
Sum of electronic and thermal Free Energies= -1500.945628

C	0.658559	-0.624719	0.166629
N	0.354548	-1.324689	-1.084341
C	1.382928	-2.025890	-1.864751
H	2.378848	-1.738040	-1.550701
H	1.216867	-3.098990	-1.719281
H	1.224428	-1.775860	-2.914861
C	-2.113301	-0.697558	-1.064451
C	-1.837761	-0.092948	0.302229
C	-0.564421	-0.081848	0.892229
C	-2.884131	0.546303	0.975809
H	-3.876281	0.546143	0.537749
C	-0.351761	0.611681	2.094279
H	0.640139	0.694611	2.517479
C	-1.404220	1.244312	2.739489
H	-1.222090	1.774472	3.667519
C	-2.680100	1.202903	2.181849
H	-3.511670	1.693313	2.676699
C	1.577198	-1.557140	1.039969
F	1.095547	-2.803249	0.923799
F	1.599828	-1.247260	2.327449
F	2.836558	-1.549220	0.603489
S	1.136180	2.014131	-0.579311
N	1.425439	0.306690	-0.650781
O	-0.255570	2.389451	-0.723561
O	1.865190	2.328110	0.644399
C	2.055900	2.501230	-2.009461
H	3.073600	2.128379	-1.904191
H	2.030321	3.592300	-2.021741
H	1.557280	2.089520	-2.887481
C	-1.014692	-1.689468	-1.423221
C	-2.186251	0.391252	-2.151161
C	-3.424772	-1.504067	-1.077101
H	-1.035272	-1.948158	-2.483241
H	-1.148883	-2.618328	-0.835451
H	-3.477162	-2.193437	-0.230101
H	-3.497652	-2.079277	-2.005321
H	-4.288572	-0.837896	-1.041461
H	-1.222911	0.877372	-2.313721
H	-2.903220	1.162553	-1.858091
H	-2.519981	-0.055967	-3.092411

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5266725
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0185861

$^{R}TS_{D'\text{-}E'}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -288.14 cm^{-1}
Zero-point correction= 0.313645 (Hartree/Particle)
Thermal correction to Energy= 0.334464
Thermal correction to Enthalpy= 0.335408
Thermal correction to Gibbs Free Energy= 0.266024
Sum of electronic and zero-point Energies= -1500.881170
Sum of electronic and thermal Energies= -1500.860351
Sum of electronic and thermal Enthalpies= -1500.859407
Sum of electronic and thermal Free Energies= -1500.928791

C	0.224429	-0.318422	0.333125
N	-0.126941	-1.712033	0.142518
C	0.936776	-2.727872	0.122622
H	1.024046	-3.153048	-0.881161
H	1.893656	-2.309737	0.425192
H	0.643548	-3.515992	0.822691
C	-2.519923	-1.239883	-0.410794
C	-2.164371	0.231954	-0.421809
C	-0.876018	0.673860	-0.032608
C	-3.109537	1.211680	-0.698013
H	-4.122059	0.923266	-0.957489
C	-0.540675	2.054381	0.001201
H	0.465578	2.366826	0.257614
C	-1.504461	2.997626	-0.295732
H	-1.259511	4.052580	-0.265005
C	-2.788772	2.573552	-0.644399
H	-3.553097	3.306048	-0.883012
C	0.713393	-0.088543	1.796511
F	-0.364800	0.001452	2.580406

F	1.402972	1.049378	1.900401
F	1.469079	-1.076882	2.265759
S	2.629867	0.527408	-0.769215
N	0.983258	-0.036483	-0.813635
O	2.634724	1.953747	-0.500032
O	3.288842	-0.405816	0.135974
C	3.087175	0.208883	-2.447259
H	2.961679	-0.857385	-2.635615
H	4.133703	0.506063	-2.534418
H	2.450233	0.816866	-3.089268
C	-1.265083	-2.058124	-0.692510
C	-3.551178	-1.589723	-1.492311
C	-3.080421	-1.611888	0.979100
H	-0.973004	-1.958048	-1.751002
H	-1.456485	-3.121682	-0.514003
H	-2.331724	-1.464989	1.761978
H	-3.387953	-2.661908	0.978130
H	-3.951804	-0.994885	1.213367
H	-3.249718	-1.210748	-2.472863
H	-4.535295	-1.184986	-1.246372
H	-3.654918	-2.677023	-1.556042

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5089767
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0140872

$^{R}TS_{E\text{-}D}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -208.48 cm^{-1}
Zero-point correction= 0.312483 (Hartree/Particle)
Thermal correction to Energy= 0.333246
Thermal correction to Enthalpy= 0.334190
Thermal correction to Gibbs Free Energy= 0.264619
Sum of electronic and zero-point Energies= -1500.870067
Sum of electronic and thermal Energies= -1500.849304
Sum of electronic and thermal Enthalpies= -1500.848360
Sum of electronic and thermal Free Energies= -1500.917931

C	0.678282	0.603091	-0.178577
N	0.354009	1.224063	1.090852
C	1.322479	1.344445	2.173431
H	2.317138	1.089726	1.801852
H	1.259573	2.368435	2.549005
H	1.066422	0.662507	2.994813
C	-2.147173	0.787870	1.016655
C	-1.858115	0.088107	-0.288802
C	-0.580663	0.014593	-0.869260
C	-2.917542	-0.503856	-0.991392
H	-3.917666	-0.456939	-0.574797
C	-0.359685	-0.679818	-2.068158
H	0.639509	-0.766448	-2.476871
C	-1.426126	-1.259749	-2.733083
H	-1.257275	-1.775608	-3.671598
C	-2.709115	-1.179813	-2.184433
H	-3.546416	-1.654264	-2.685200
C	1.393443	1.661037	-1.068813
F	0.515388	2.575043	-1.487130
F	1.962743	1.084678	-2.123065
F	2.345380	2.290032	-0.372977
S	1.180622	-1.972042	0.642438
N	1.602674	-0.394644	0.178015
O	-0.156112	-2.108938	1.196342
O	1.520399	-2.713659	-0.569184
C	2.396546	-2.252793	1.894775
H	3.376419	-2.029902	1.474762
H	2.309218	-3.308876	2.159245
H	2.165255	-1.626361	2.756999
C	-0.953877	1.759243	1.297765
C	-2.269507	-0.173743	2.211455
C	-3.407472	1.659123	0.929848
H	-1.022698	2.119691	2.323646
H	-1.058377	2.585107	0.574818
H	-3.415539	2.268669	0.022698
H	-3.461104	2.318188	1.801132
H	-4.303000	1.034145	0.943325
H	-1.328065	-0.675651	2.432490
H	-3.018000	-0.938034	1.980348
H	-2.603241	0.382684	3.091719

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1501.5001673
UB3LYP-D3/6-311+G(d,p)-SDD(I)-CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
HF = -1502.0040163

$TS_{E'\text{-}E}$

UM06-2X/6-31+G(d,p)-LANL2DZ(I)-CPCM(dichloromethane)
Imaginary frequency = -14.82 cm^{-1}
Zero-point correction= 0.318460 (Hartree/Particle)
Thermal correction to Energy= 0.338125
Thermal correction to Enthalpy= 0.339070
Thermal correction to Gibbs Free Energy= 0.272537
Sum of electronic and zero-point Energies= -1500.944969
Sum of electronic and thermal Energies= -1500.925304
Sum of electronic and thermal Enthalpies= -1500.924360
Sum of electronic and thermal Free Energies= -1500.990893

C	0.710894	0.626973	0.309123
N	0.767056	-0.486792	1.290401
C	1.786347	-0.647812	2.387352
H	2.777798	-0.500526	1.979750
H	1.553279	0.063756	3.178019
H	1.672438	-1.672679	2.738438
C	-1.875013	-0.751371	1.139078
C	-1.798924	0.353858	0.098431
C	-0.622633	1.018433	-0.260437
C	-2.989394	0.746805	-0.526165
H	-3.919306	0.258490	-0.255865
C	-0.642906	2.024847	-1.239445
H	0.265084	2.530962	-1.539625
C	-1.831496	2.383947	-1.855525
H	-1.830743	3.160476	-2.611994
C	-3.013877	1.742413	-1.492323
H	-3.953150	2.015087	-1.961562
C	1.720311	1.795552	0.444097
F	2.246599	2.029537	-0.763079
F	2.731881	1.541662	1.269336
F	1.110441	2.896257	0.873532

S	0.818071	-1.832829	-1.185143
N	1.360995	-0.617316	-0.020165
O	0.731313	-3.042534	-0.387878
O	-0.328083	-1.358664	-1.931723
C	2.269853	-1.811486	-2.196149
H	2.373737	-0.811477	-2.618509
H	2.087233	-2.548240	-2.981133
H	3.120926	-2.087927	-1.575919
C	-0.509696	-1.188168	1.717568
C	-2.546734	-2.008805	0.549537
C	-2.721235	-0.243319	2.327885
H	-0.306665	-2.245026	1.539534
H	-0.507659	-1.018422	2.794114
H	-2.266728	0.643312	2.779967
H	-2.805083	-1.024449	3.089828
H	-3.729432	0.015519	1.997975
H	-2.013544	-2.369702	-0.332694
H	-3.580669	-1.801178	0.268204
H	-2.562126	-2.802678	1.302647

UM06-2X/6-311+G(d,p)-LANL2DZ(I)-
SMD(DCM)//UM06-2X/6-31+G(d,p)-LANL2DZ(I)-
CPCM(dichloromethane)
HF = -1501.5785551
UB3LYP-D3/6-311+G(d,p)-SDD(I)-
CPCM(DCM)///UM06-2X/6-31+G(d,p)-LANL2DZ(I)-
CPCM(dichloromethane)
HF = -1502.

Appendix 3: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 3 (The Role of the Trichloroacetimidate to Enable Iridium-Catalyzed Regio- and Enantioselective Allylic Fluorination)

A3.1 Methods

All optimizations of intermediates and transition states were calculated without constraints using restricted M06/6-31G(d,p)-LANL2DZ(Ir) level of the theory in implicit solvent (diethyl ether) using CPCM as solvation model as implemented in Gaussian09.[226] Frequency calculations, at the same level of theory, were used to obtain thermal corrections (at 298K) and to characterize optimized structures as transition states (only a single imaginary frequency) or intermediate (if no imaginary frequencies were found). Single point energy calculations in implicit solvent using B3LYP-D3/6-311+G(d,p)-SDD(Ir) were also performed on all structures (see below).[227] For comparison, singlet point energies were also computed using the ORCA suite of programs base on version 4.1.1 using DLPNO-CCSD(T)/def2TZVPP calculations with NormalPNO settings and SlowConv keyword as implemented in ORCA.[228] Solvation, entropy, and thermal corrections were obtained from M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM (diethyl ether) level calculations. This protocol is denoted as DLPNO-CCSD(T) + CPCM (diethyl ether)//6-31G(d,p)-LANL2DZ(Ir)/def2TZVPP. All 3-D structures were generated using CYLview.[229]

A3.2 Supplementary Figures

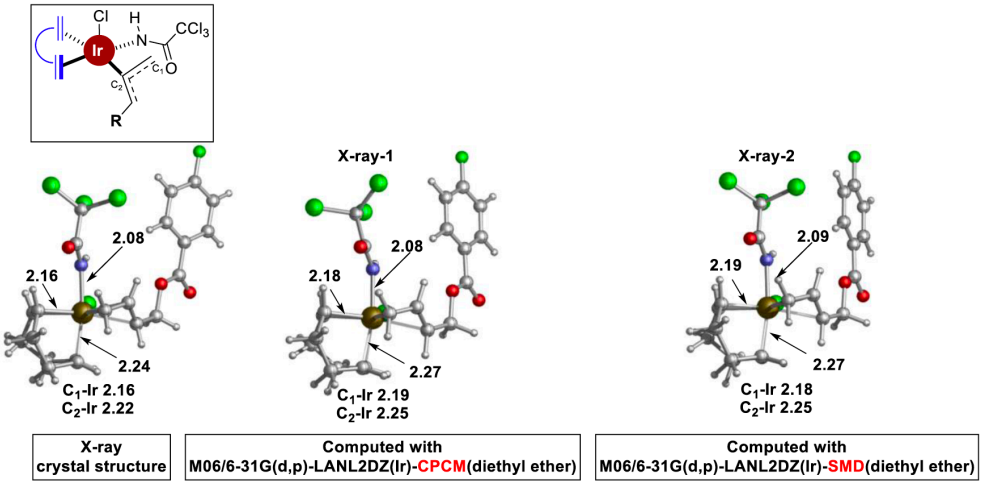


Figure A3.1 Comparison between x-ray crystal structure (experimental, left) and computed structures with M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) (X-ray-1, middle) and M06/6-31G(d,p)-LANL2DZ(Ir)-SMD(diethyl ether) (X-ray-2, right). Key bond lengths are given. The resulting geometry from both solvation models are very similar to the experimental structure, showing that the method used for the computations is suitable to represent the experimental system.

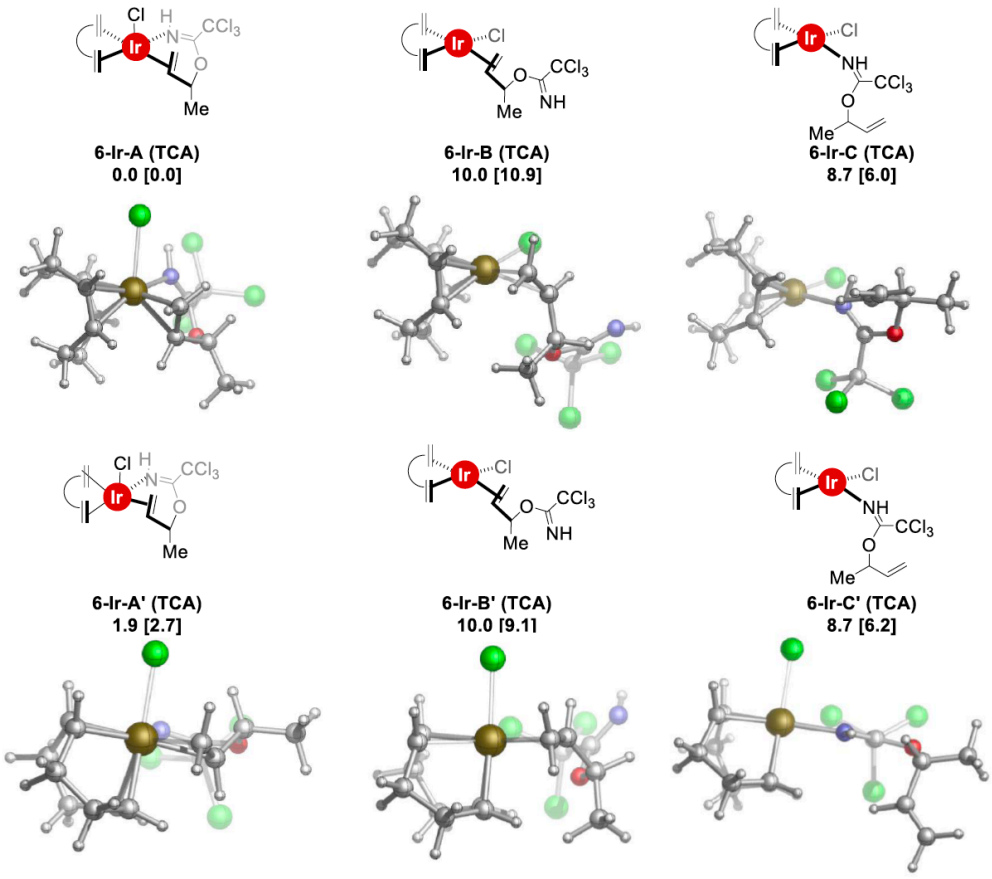


Figure A3.2 Conformers of various modes of iridium coordination with achiral COD ligand to allylic trichloroacetimidates. Free energies (kcal/mol) were computed using M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and, in brackets, B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether). Energetic preference for bidentate coordination shown in **6-Ir-A** observed with trichloroacetimidate substrate.

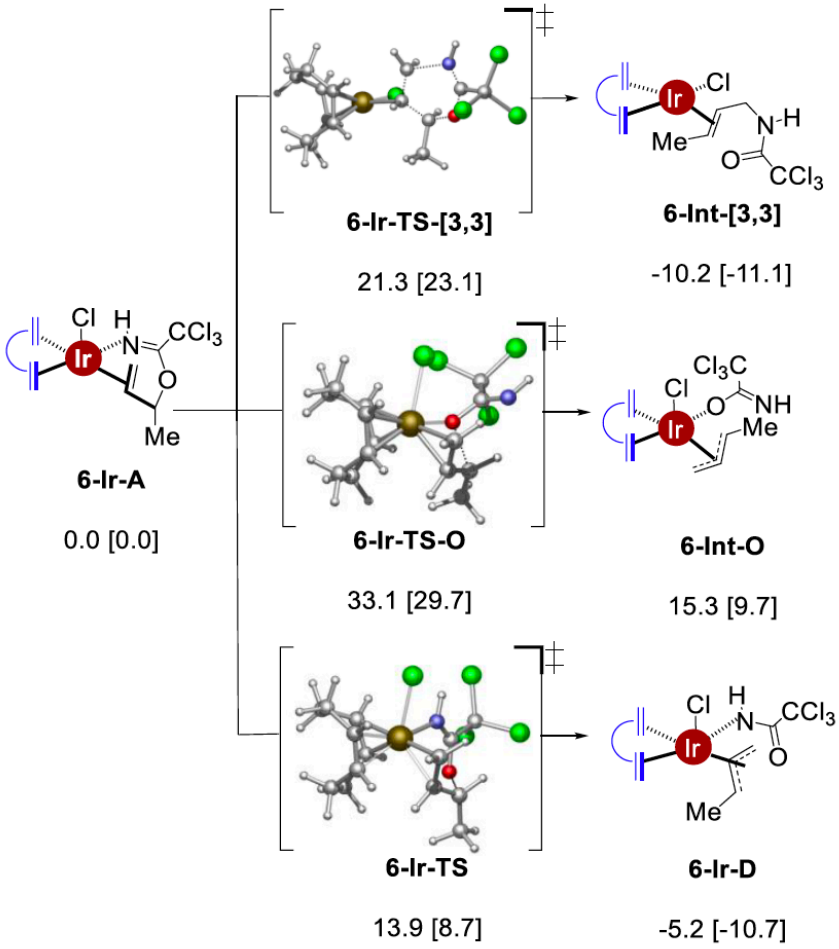
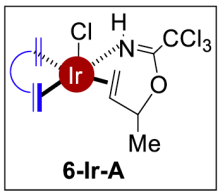
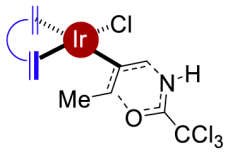


Figure A3.3 Three distinct pathways for C-O bond breaking including a [3,3]-sigmatropic rearrangement (top), a 5-member π-O-chelation (middle), and the lowest 7-member π-N-chelation pathway (bottom) for the trichloroacetimidate substrate using the achiral COD ligand. Free energies (kcal/mol) were computed using M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and, in brackets, B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) level of theory. All three transition states were compared to the starting material, **6-Ir-A**, to determine the distortion energy while the separated Ir(Cl)COD and trichloroacetimidate components of each TS were compared to the interacting components as a complex to determine the interaction energy. The distortion energy is greater than the interaction energy for all three transition states. The lowest energy transition state (**6-Ir-TS-N**) has a greater interaction energy between the Ir(Cl)COD and the trichloroacetimidate fragments, making it a more favorable transition state. The iridium-nitrogen bond in **6-Ir-TS-N** may contribute to this favorable interaction through strong metal-to-ligand back bonding.



6-Ir-A

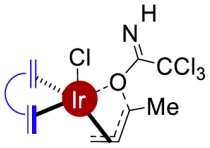


6-Ir-TS-[3,3]

E (distortion) = 66.6 kcal/mol

E (interaction) = 40.9 kcal/mol

E (distortion) - E (interaction) = 25.7 kcal/mol

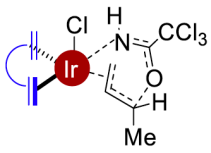


6-Ir-TS-O

E (distortion) = 94.1 kcal/mol

E (interaction) = 62.4 kcal/mol

E (distortion) - E (interaction) = 31.7 kcal/mol



6-Ir-TS-N

E (distortion) = 107.7 kcal/mol

E (interaction) = 96.7 kcal/mol

E (distortion) - E (interaction) = 11.0 kcal/mol

Figure A3.4 Interaction-distortion analysis of the ionization transition states (**6-Ir-TS-[3,3], 6-Ir-TS-O, 6-Ir-TS-N**) for the COD ligand calculated using B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(Et_2O)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(Et_2O) level of theory. All three transition states were compared to the starting material, **6-Ir-A**, to determine the distortion energy while the separated Ir(Cl)COD and trichloroacetimidate components of each TS were compared to the interacting components as a complex to determine the interaction energy. The distortion energy is greater than the interaction energy for all three transition states. The lowest energy transition state (**6-Ir-TS-N**) has a greater interaction energy between the Ir(Cl)COD and the trichloroacetimidate fragments, making it a more favorable transition state. It is hypothesized that the iridium-nitrogen bond in **6-Ir-TS-N** contributes to this favorable interaction from strong metal-to-ligand back bonding.

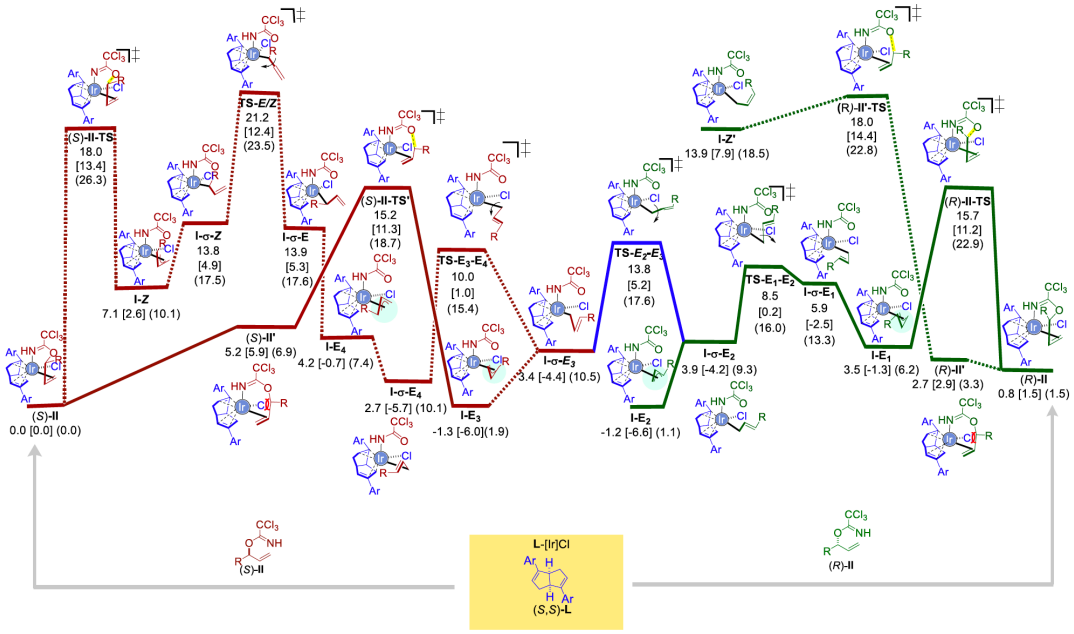


Figure A3.5 Energetics of all competing pathways for the formation of the π-allyliridium intermediates from both (*S*)- and *(R)*-allylic trichloroacetimidate (R = Me) using the chiral *(S,S)*-diene (L) ligated iridium catalyst (L = bicyclo[3.3.0]octadiene). Lowest energy pathway is denoted with solid lines. Free energies (kcal/mol) were computed at the M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and, in brackets, B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and in parenthesis, DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)// M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) levels of theory.

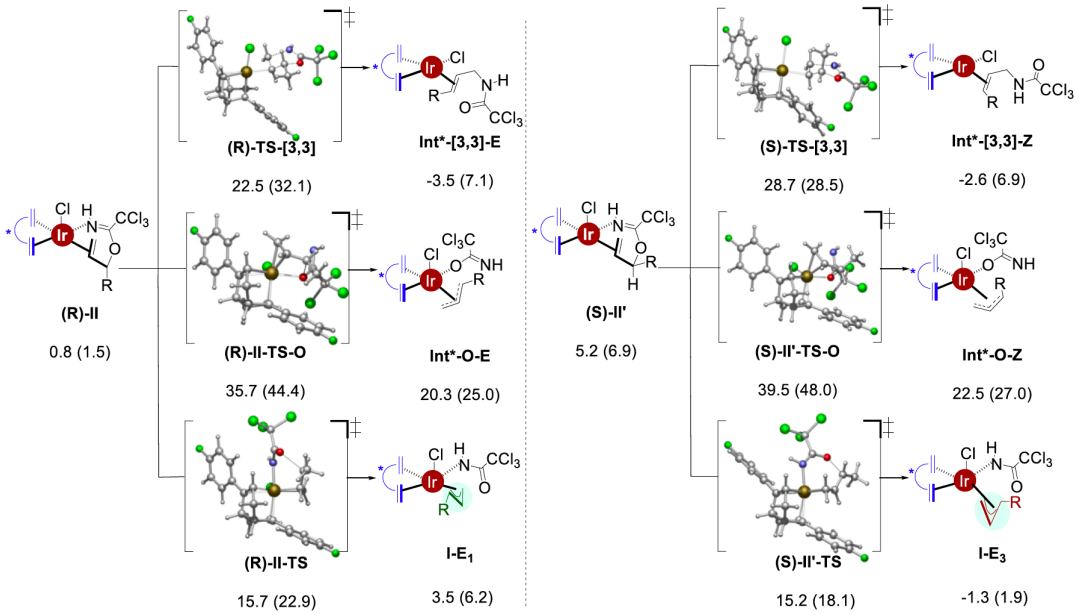


Figure A3.6 Three distinct pathways for C-O bond breaking including a [3,3]-sigmatropic rearrangement (top), a 5-member π-O-chelation (middle), and the lowest 7-member π-N-chelation pathway (bottom) for the *(R)*- and *(S)*- trichloroacetimidate substrates using chiral *(S,S)*-diene ligand. Free energies (kcal/mol) were computed using M06/6-31G(d,p) LANL2DZ(Ir)-CPCM(diethyl ether) and, in parenthesis, DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)// M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether).

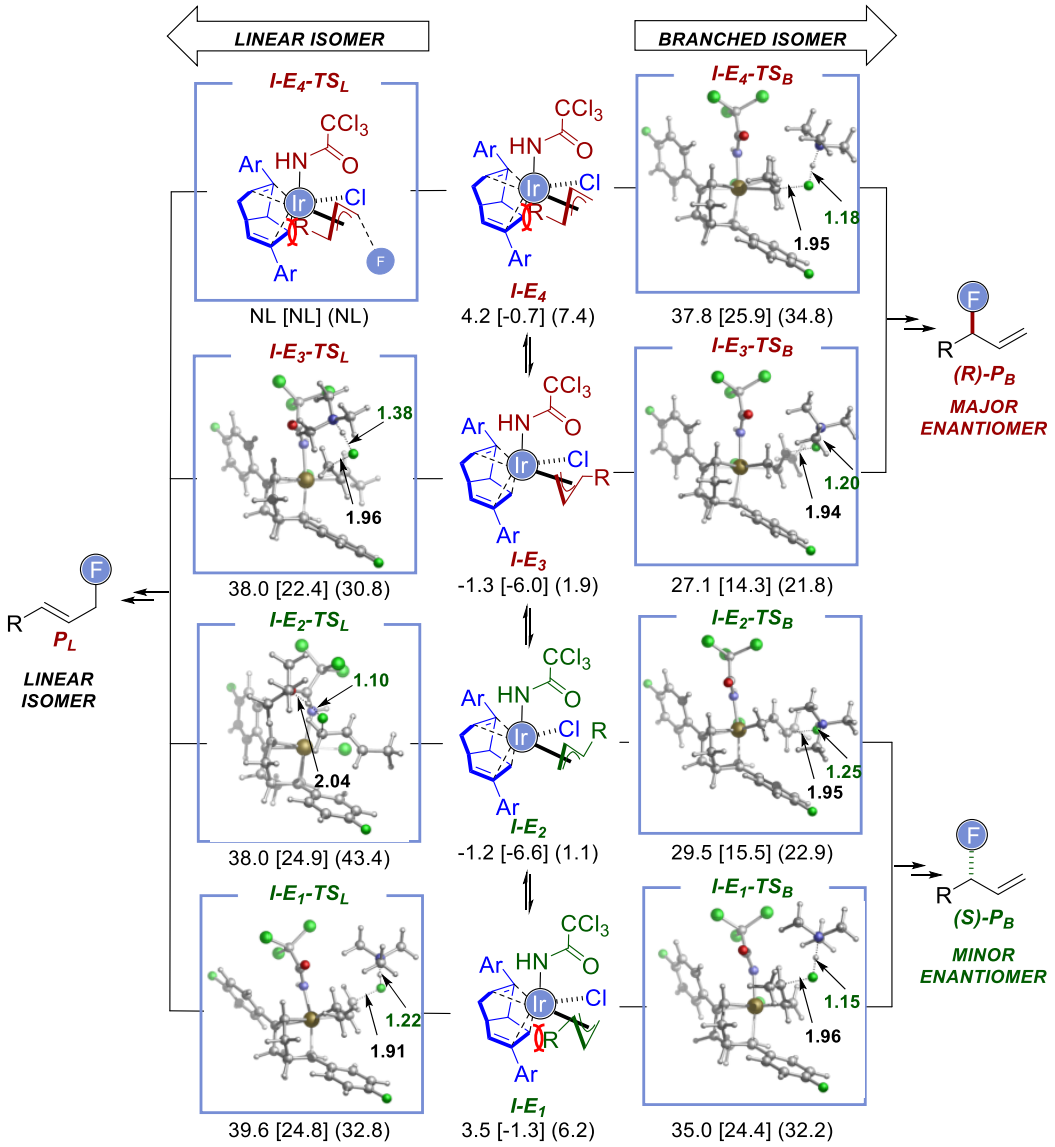


Figure A3.7 Relative energetics for allylic fluorination of π-allyl-iridium intermediates and regioselectivity. Key bond distances (C-F and F-H) are shown in black and green respectively. Free energies (kcal/mol) were computed at the M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and, in brackets, B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and in parenthesis, DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether) level of theory.

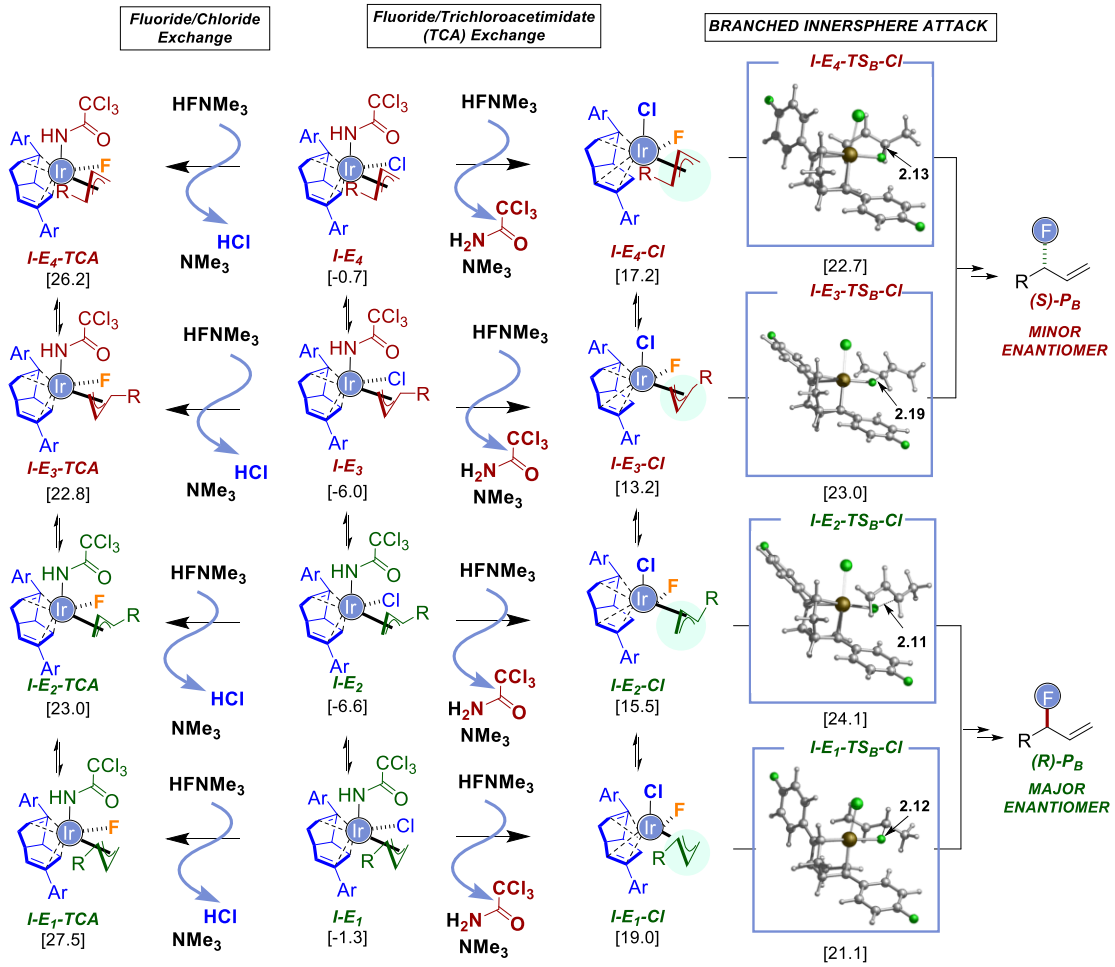


Figure A3.8 Relative energetics for inner-sphere allylic fluorination of π-allyl-iridium intermediates. Free energies (kcal/mol) were computed at the B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) level of theory with respect to Me_3N•3HF complex.

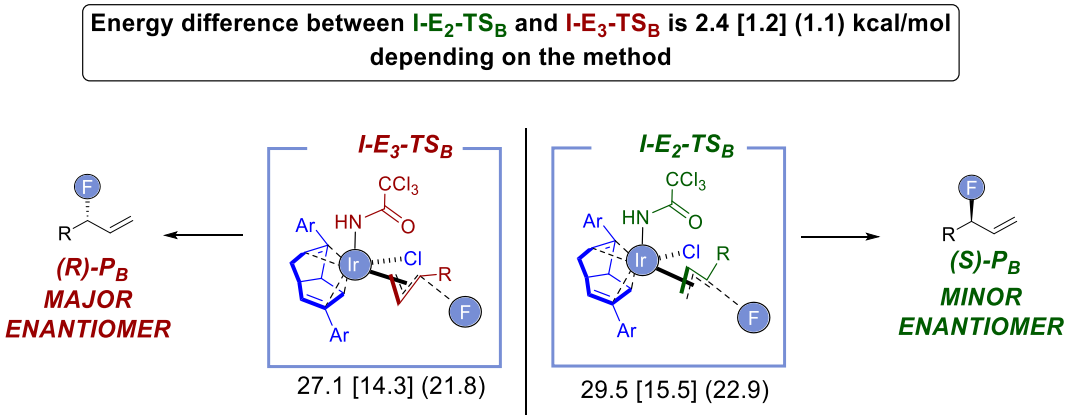


Figure A3.9 Lowest energy diastereomeric transition states leading to major and minor branched-selective allylic fluorides with relative energies of fluoride addition. Free energies (kcal/mol) were computed at the M06/6-31G(d,p)-LANL2DZ(Ir)-

CPCM(diethyl ether) and, in brackets, B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) and in parenthesis, DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether) levels of theory.

Investigation of Fluoride Source

In this system, the experimental source of fluoride is $3HF{\bullet}NEt_3$ but the exact source of fluoride in the C-F bond formation step is not known. Fortunately, the X-ray structure of $3HF{\bullet}NEt_3$ is known[230] which allows for the calibration of the computational methods. As shown in **Figure A3.10**, the computed structure is able to capture the bonding in the complex, that is that the amine deprotonates one of the H-F to form an ionic $Et_3NH^+ \bullet\bullet F(2HF)^-$ complex as evident from the N-H bond. However, the overall geometry of the ionic complex is more distorted from a V-shaped to a bend-like structure. This discrepancy is likely due to the difference between solid-state geometry (X-ray) and solution-phase geometry (computed) in which the HF bonded is likely to be more disordered. To reduce computational cost associated with conformations of the ethyl groups, the model was truncated to the $Me_3NH^+ \bullet\bullet F(2HF)^-$ complex which, again, is able to capture the anionic features of the complex although the complex about the $F(2HF)^-$ bonding becomes more linear due to less steric interactions with the Me_3NH^+ moiety vs. and Et_3NH^+ group. Further, as shown in **Figure A3.10**, C-F bond formation directly from the $Me_3NH^+ \bullet\bullet F$ complex plus two dissociated HF molecules. As such, the computations show support for decomplexation of the two HF molecules prior to undergoing C-F bond formation from the $Me_3NH^+ \bullet\bullet F^-$ complex. Consequently, $Me_3NH^+ \bullet\bullet F^-$ was used as the fluoride source for this mechanistic study.

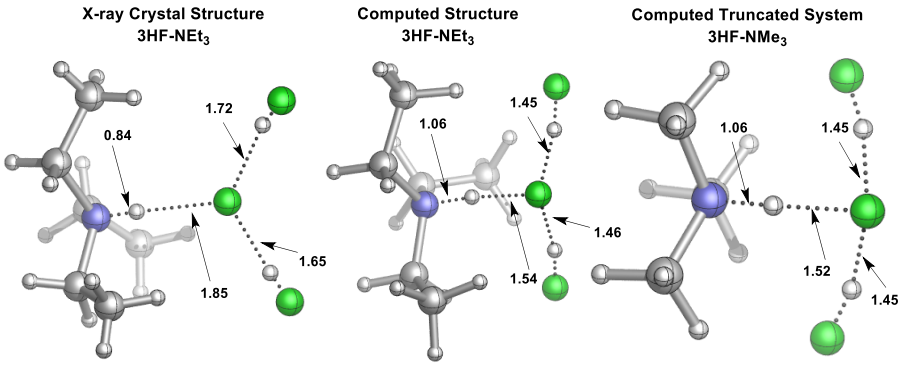


Figure A3.10 Comparison between x-ray crystal structure of 3HF-NEt_3 (left) and the computed structure of 3HF-NEt_3 (middle) optimized with M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether). To reduce the computational cost, the computed truncated system of 3HF-NMe_3 (right) optimized with M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) is used in the calculations. Key bond distances in Å (N-H and F-H) are shown in black.

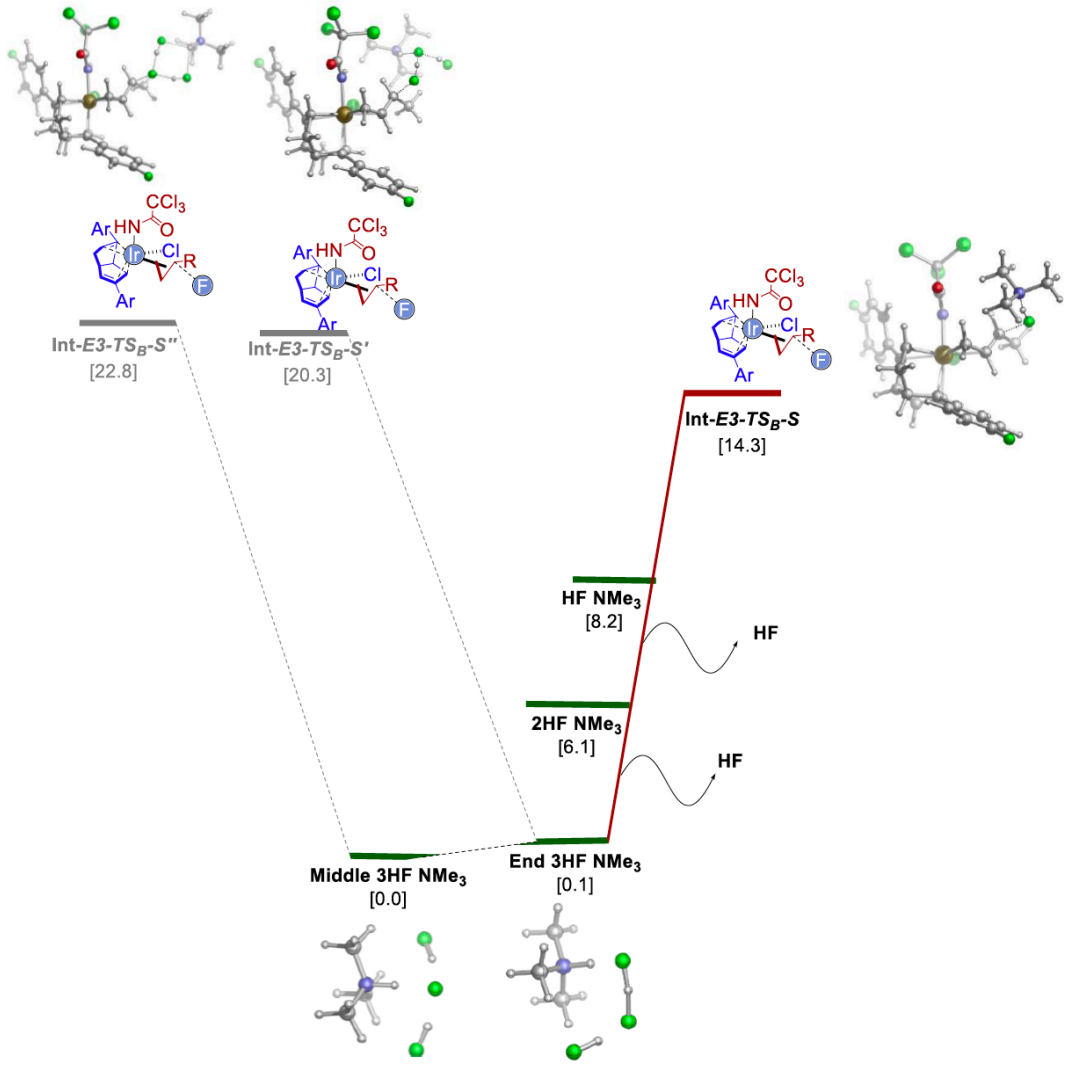


Figure A3.11 Relative energetics for allylic fluorination and the formation of various fluoride sources from 3HF-NMe_3. Free energies (kcal/mol) were computed at the B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) level of theory.

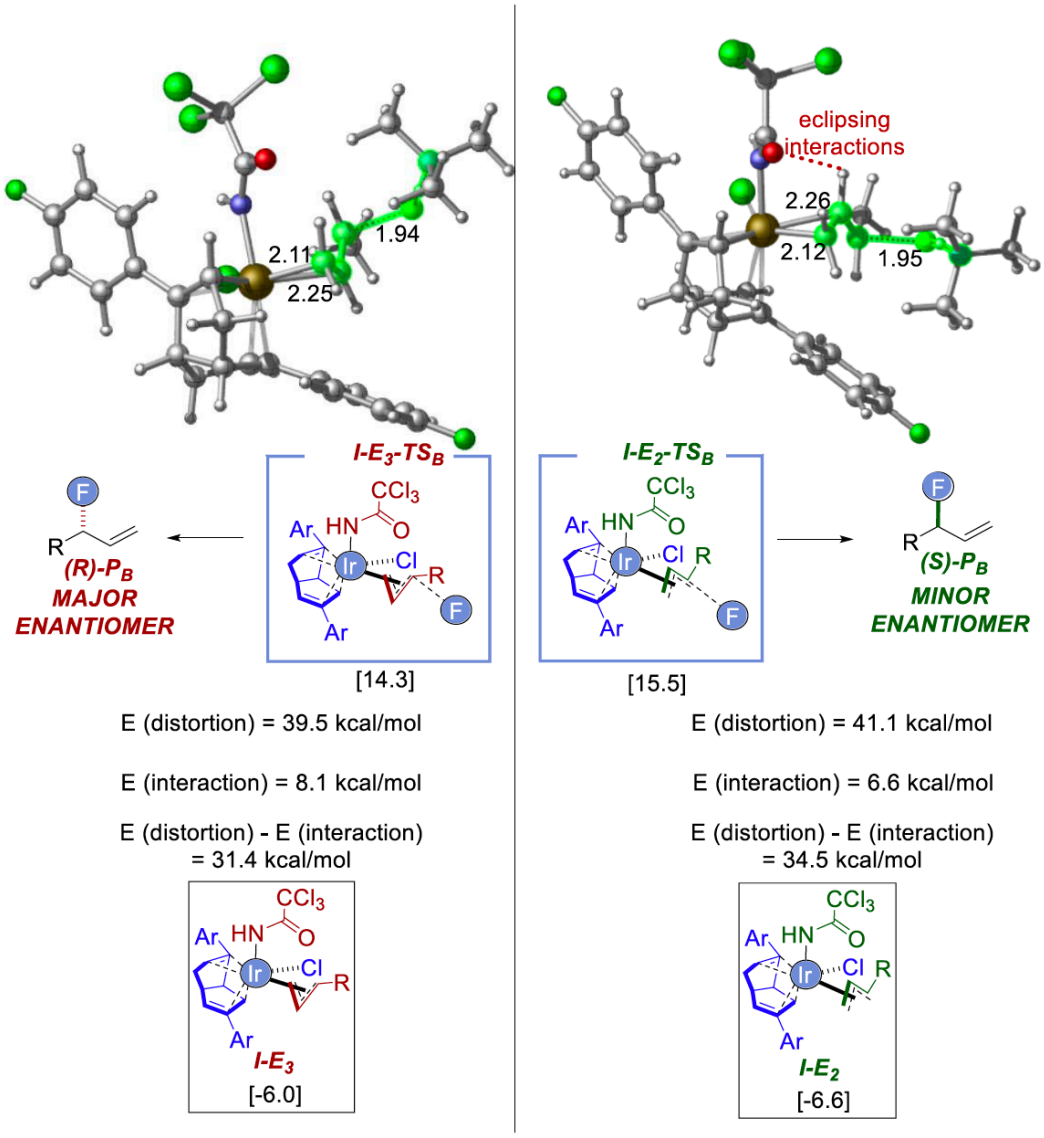


Figure A3.12 Interaction-distortion analysis (calculated using B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethylether)//M06/6-31G(d,p)-LANL2DZ(Ir) CPCM(diethyl ether) level of theory) of lowest energy diastereomeric transition states leading to major and minor branched-selective allylic fluorides with relative energies of fluoride addition. Free energies (kcal/mol) were computed using B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether) levels of theory.

A3.3 Coordinates and Energies

6-Ir-A

M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether)
Zero-point correction= 0.322197 (Hartree/Particle)
Thermal correction to Energy= 0.344469
Thermal correction to Enthalpy= 0.345414
Thermal correction to Gibbs Free Energy= 0.270504
Sum of electronic and zero-point Energies= -2620.065472
Sum of electronic and thermal Energies= -2620.043200
Sum of electronic and thermal Enthalpies= -2620.042256
Sum of electronic and thermal Free Energies= -2620.117166

Ir	0.38641	-0.79192	-0.02806
C	0.81751	-1.68196	-1.95788
H	1.80948	-2.13043	-1.87397
C	0.74888	-0.28679	-2.12527
H	1.70383	0.23948	-2.16939
C	-1.63987	-1.35779	-0.59696
H	-2.13496	-1.8079	0.2671
C	-1.53599	0.06244	-0.57816
H	-1.97852	0.56082	0.28949
C	-0.40827	0.42331	-2.80179
H	-0.01613	1.24712	-3.40911
H	-0.8945	-0.2637	-3.505
C	-1.41039	0.96039	-1.78403
H	-2.39497	1.12745	-2.2493
H	-1.06947	1.94197	-1.42524
C	-1.67889	-2.19619	-1.86511
H	-2.28265	-3.09061	-1.67483
H	-2.21011	-1.64949	-2.65577
C	-0.28624	-2.63598	-2.34281
H	-0.04457	-3.6049	-1.89334
H	-0.27425	-2.78418	-3.4345
Cl	0.80914	-3.19933	0.82467
C	1.56743	0.96817	0.33651
H	1.56125	1.64429	-0.52155
C	2.42093	-0.18124	0.33184
H	3.06728	-0.38608	-0.52247
H	2.8073	-0.55223	1.28254
C	1.3416	1.66932	1.65056
H	1.89027	1.13912	2.44357
C	1.73266	3.12387	1.60521
H	1.59358	3.59844	2.58132
H	2.78464	3.21047	1.31663
H	1.12661	3.65466	0.86205
O	-0.05761	1.68098	2.12867
C	-0.51953	0.52211	2.5362
C	-1.37685	0.6528	3.79294
Cl	-2.02382	-0.91311	4.32486
Cl	-0.35729	1.34771	5.08413
Cl	-2.72975	1.75741	3.4211
N	-0.25732	-0.57966	1.94781
H	-0.58682	-1.43885	2.38733

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0739305

6-Ir-B

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.321480 (Hartree/Particle)
Thermal correction to Energy= 0.344330
Thermal correction to Enthalpy= 0.345274
Thermal correction to Gibbs Free Energy= 0.269007
Sum of electronic and zero-point Energies= -2620.048771
Sum of electronic and thermal Energies= -2620.025920
Sum of electronic and thermal Enthalpies= -2620.024976
Sum of electronic and thermal Free Energies= -2620.10124

Ir	-0.28189	-1.09423	0.36899
C	-0.13006	-2.30755	-1.37307
H	0.74588	-2.95718	-1.29253
C	0.10888	-0.96205	-1.75907
H	1.15206	-0.70097	-1.93749
C	-2.40982	-1.29979	-0.08733
H	-2.90375	-1.5414	0.8547
C	-2.01522	0.04225	-0.26398
H	-2.20587	0.71678	0.57502
C	-0.88791	-0.10701	-2.51923
H	-0.34561	0.5583	-3.20154
H	-1.51449	-0.7443	-3.15624
C	-1.74647	0.73366	-1.57077
H	-2.69511	1.02587	-2.04797
H	-1.2196	1.66938	-1.33758
C	-2.66459	-2.24787	-1.24169
H	-3.47925	-2.92925	-0.97378
H	-3.0201	-1.68366	-2.11263
C	-1.41672	-3.06356	-1.59102
H	-1.38437	-3.95725	-0.95439
H	-1.46207	-3.43115	-2.62872
Cl	-0.94006	-0.78922	2.68154
C	1.75675	-0.36278	1.27013
H	1.52131	-0.42382	2.33107
C	1.90937	-1.54438	0.57535
H	1.86166	-2.48821	1.12233
H	2.39818	-1.58517	-0.39726
C	2.2271	0.99866	0.84391
H	3.13017	1.19787	1.44317
C	2.5122	1.24136	-0.61616
H	2.96387	2.2295	-0.74099
H	3.21176	0.49586	-1.00715
H	1.58767	1.20859	-1.20187
O	1.24677	1.99661	1.21588
C	1.20793	2.39101	2.48643
C	0.16473	3.5185	2.61113
Cl	-0.0376	4.0229	4.30613
Cl	0.74534	4.92001	1.65527
Cl	-1.41128	2.97538	1.97771
N	1.94474	1.92084	3.39535
H	1.77546	2.35742	4.29838

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0549907

6-Ir-C

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.320292 (Hartree/Particle)
Thermal correction to Energy= 0.343886
Thermal correction to Enthalpy= 0.344831
Thermal correction to Gibbs Free Energy= 0.265823
Sum of electronic and zero-point Energies= -2620.048889
Sum of electronic and thermal Energies= -2620.025295
Sum of electronic and thermal Enthalpies= -2620.024351
Sum of electronic and thermal Free Energies= -2620.103358

Ir	-1.50522	0.16639	0.701
C	-1.12458	-0.13336	-1.34964
H	-0.202	-0.71163	-1.47213
C	-0.9625	1.24963	-1.04242
H	0.06987	1.59989	-0.94149
C	-3.52412	0.02533	0.01612
H	-4.04736	-0.65936	0.68702
C	-3.26498	1.32311	0.52116
H	-3.61816	1.53105	1.53472
C	-1.97284	2.31746	-1.42689
H	-1.44716	3.25564	-1.63924
H	-2.46943	2.03609	-2.36503
C	-3.00253	2.55358	-0.31377
H	-3.94463	2.94835	-0.72627
H	-2.62043	3.327	0.36558
C	-3.64542	-0.27704	-1.46669
H	-4.40626	-1.05093	-1.61941
H	-4.01384	0.6119	-1.99465
C	-2.31106	-0.7438	-2.05571
H	-2.23062	-1.83312	-1.94339
H	-2.26572	-0.54343	-3.13813
Cl	-2.10455	-0.48166	2.96656
C	3.09536	-1.5814	-0.46376
H	2.2842	-1.00388	-0.9141
C	4.05055	-2.07895	-1.24208
H	4.03051	-1.92336	-2.31694
H	4.88033	-2.66391	-0.85149
C	3.02128	-1.75083	1.02341
H	2.16788	-2.3881	1.30593
C	4.26289	-2.28189	1.69123
H	4.13076	-2.28637	2.77606
H	4.45329	-3.30849	1.36598
H	5.13004	-1.66305	1.4403
O	2.80152	-0.42986	1.60989
C	1.63112	0.17006	1.51142
C	1.79663	1.65809	1.847
Cl	0.2752	2.50751	2.10771
Cl	2.81122	1.83355	3.30317
Cl	2.65068	2.3709	0.42916
N	0.52526	-0.34646	1.13547
H	0.61474	-1.34468	0.94435

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0596254

6-Ir-TS

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -140.88 cm^{-1}
Zero-point correction= 0.318772 (Hartree/Particle)
Thermal correction to Energy= 0.341502
Thermal correction to Enthalpy= 0.342447
Thermal correction to Gibbs Free Energy= 0.266861
Sum of electronic and zero-point Energies= -2620.043161
Sum of electronic and thermal Energies= -2620.020430
Sum of electronic and thermal Enthalpies= -2620.019486
Sum of electronic and thermal Free Energies= -2620.095071

Ir	0.31663	-0.76807	0.00743
C	0.68121	-1.74354	-1.95039
H	1.58513	-2.34104	-1.81942
C	0.84859	-0.36612	-2.11946
H	1.88243	-0.01771	-2.13203
C	-1.74665	-1.06416	-0.66341
H	-2.3034	-1.45809	0.18896
C	-1.4463	0.32364	-0.62426
H	-1.82587	0.88098	0.23349
C	-0.15706	0.5397	-2.80535
H	0.38561	1.32377	-3.34567
H	-0.69054	-0.03522	-3.57262
C	-1.14139	1.18575	-1.82543
H	-2.07203	1.46806	-2.34276
H	-0.7097	2.12318	-1.44741
C	-1.86114	-1.86042	-1.95005
H	-2.6239	-2.63654	-1.8227
H	-2.23524	-1.20867	-2.75022
C	-0.54122	-2.52437	-2.35758
H	-0.4712	-3.50828	-1.88198
H	-0.50839	-2.69864	-3.44468
Cl	0.49659	-3.16829	0.76512
C	1.90387	0.79873	0.34969
H	2.05544	1.33436	-0.5886
C	2.3676	-0.5658	0.49617
H	3.04861	-0.95135	-0.26426
H	2.57797	-0.92938	1.50392
C	1.66123	1.62693	1.45922
H	1.79229	1.19602	2.45154
C	1.66207	3.09584	1.32908
H	1.18416	3.58667	2.1774
H	2.7099	3.4275	1.28304
H	1.18224	3.40579	0.39442
O	-0.42643	1.66213	2.22819
C	-0.67543	0.49835	2.5999
C	-1.28754	0.37938	4.02623
Cl	0.03053	0.79836	5.17292
Cl	-2.61925	1.551	4.20132
Cl	-1.90703	-1.24769	4.4279
N	-0.3765	-0.59558	1.95095
H	-0.58775	-1.48533	2.3944

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0564027

6-Ir-D

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.320591 (Hartree/Particle)
Thermal correction to Energy= 0.343934
Thermal correction to Enthalpy= 0.344878
Thermal correction to Gibbs Free Energy= 0.267845
Sum of electronic and zero-point Energies= -2620.072738
Sum of electronic and thermal Energies= -2620.049396
Sum of electronic and thermal Enthalpies= -2620.048451

Sum of electronic and thermal Free Energies= -2620.125485

Ir	-0.03558	-0.14778	0.24763
C	-0.40996	1.00589	-1.56037
H	0.19434	1.90765	-1.45942
C	-1.59657	0.93128	-0.78837
H	-1.807	1.79138	-0.15179
C	-0.3355	-1.80217	-1.27014
H	0.48927	-2.50097	-1.13217
C	-1.36894	-1.86214	-0.33878
H	-1.27845	-2.58323	0.47549
C	-2.7979	0.08205	-1.16518
H	-3.7023	0.58341	-0.80516
H	-2.88646	0.05735	-2.25909
C	-2.76009	-1.34067	-0.5882
H	-3.28285	-2.04297	-1.25576
H	-3.29493	-1.35803	0.36542
C	-0.50785	-1.26713	-2.67822
H	0.11206	-1.86182	-3.35795
H	-1.54533	-1.43404	-2.99343
C	-0.13525	0.21095	-2.80726
H	0.9339	0.30406	-3.03409
H	-0.66256	0.67152	-3.65681
Cl	-1.60918	-0.18496	2.21857
C	2.04328	-0.67371	0.96501
H	2.39175	0.07071	1.68245
C	1.34367	-1.76849	1.45069
H	1.15827	-2.61304	0.78583
C	2.01655	-0.33659	-0.43287
O	1.92589	2.74704	-0.2464
C	1.29212	2.62632	0.79902
C	1.55242	3.73134	1.8945
Cl	0.17879	3.99134	3.01895
Cl	2.97206	3.15184	2.83984
Cl	1.9512	5.28147	1.12769
N	0.48508	1.64923	1.17232
H	0.04426	1.73731	2.08262
H	2.12076	-1.13126	-1.16992
H	2.45112	0.62002	-0.7175
C	1.13141	-2.00821	2.9026
H	0.111	-2.35495	3.09841
H	1.82034	-2.78507	3.25844
H	1.29717	-1.09492	3.48344

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0883548

(S)-II

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.445263 (Hartree/Particle)
Thermal correction to Energy= 0.477632
Thermal correction to Enthalpy= 0.478576
Thermal correction to Gibbs Free Energy= 0.381196
Sum of electronic and zero-point Energies= -3278.923573
Sum of electronic and thermal Energies= -3278.891204
Sum of electronic and thermal Enthalpies= -3278.890260
Sum of electronic and thermal Free Energies= -3278.987640

C	0.41003	-1.75148	-1.73319
C	1.37637	-0.63539	-1.45296
C	2.47271	-1.11998	-0.67258
C	2.19714	-2.55728	1.36279
C	1.00188	-1.71568	1.72564
C	0.00716	-1.84376	0.73477
H	-0.61639	-1.40051	-1.89325
H	0.71674	-2.30911	-2.63195
H	1.49437	0.1682	-2.18106
H	2.05202	-3.57755	1.75209
H	3.13235	-2.16339	1.77188
H	0.78338	-1.48745	2.76706
C	0.59442	-2.57902	-0.46652
H	0.20699	-3.60563	-0.52727
C	2.11443	-2.51615	-0.16216
H	2.68563	-3.307	-0.66834
C	3.87469	-0.68748	-0.8382
C	4.92577	-1.41029	-0.25512
C	4.21746	0.44264	-1.60033
C	6.25157	-1.01977	-0.40079
H	4.71099	-2.30363	0.32559
C	5.53586	0.85283	-1.7492
H	3.44238	1.01509	-2.10807
C	6.53778	0.11434	-1.14064
H	7.06173	-1.58314	0.05366
H	5.794	1.72791	-2.33972
C	-1.44564	-1.86668	1.01094
C	-2.35967	-2.28849	0.03421
C	-1.95692	-1.53343	2.27599
C	-3.72467	-2.34498	0.28889
H	-2.00691	-2.59741	-0.94555
C	-3.3165	-1.57603	2.54643
H	-1.28006	-1.24871	3.07769
C	-4.18378	-1.97651	1.54175
H	-4.43033	-2.67627	-0.46742
H	-3.7096	-1.31831	3.52565
F	-5.49551	-2.02359	1.79579
F	7.81336	0.50133	-1.28246
Ir	1.11844	0.13397	0.5601
Cl	2.91144	0.6298	2.35821
C	-0.77972	1.08131	0.27064
H	-1.57159	0.34821	0.10084
C	-0.3593	1.32235	1.61187
H	-0.85151	0.78937	2.42269
H	0.0417	2.29772	1.89202
C	-0.83925	2.13853	-0.79677
O	0.08065	3.25525	-0.5925
C	1.36049	3.05153	-0.42165
C	2.16112	4.3337	-0.67879
Cl	3.86529	4.15303	-0.20699
Cl	2.06447	4.65913	-2.43636
Cl	1.43944	5.67787	0.2335
N	1.9057	1.94095	-0.11846
H	2.91884	1.97222	-0.00148
H	-0.57384	1.70643	-1.774
C	-2.20148	2.79287	-0.85674
H	-2.22677	3.57236	-1.62363
H	-2.96159	2.04293	-1.09405
H	-2.44295	3.23755	0.11508

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6580262
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.663614227847
ΔG_{solv} = -0.014918

(S)-II'

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.446431 (Hartree/Particle)

Thermal correction to Energy= 0.478216
Thermal correction to Enthalpy= 0.479160
Thermal correction to Gibbs Free Energy= 0.384211
Sum of electronic and zero-point Energies= -3278.917119
Sum of electronic and thermal Energies= -3278.885335
Sum of electronic and thermal Enthalpies= -3278.884390
Sum of electronic and thermal Free Energies= -3278.979339

C	-0.27825	-2.23542	-1.81213
C	0.68475	-1.08505	-1.69171
C	1.5572	-1.30755	-0.61094
C	0.86327	-2.08277	1.66244
C	-0.33753	-1.18694	1.53303
C	-1.16667	-1.63114	0.46546
H	-1.22459	-1.9464	-2.27563
H	0.18389	-3.02434	-2.42692
H	0.95203	-0.4938	-2.56533
H	0.62236	-2.94875	2.2986
H	1.73456	-1.58123	2.09886
H	-0.72774	-0.68429	2.4181
C	-0.3912	-2.66475	-0.35036
H	-0.78631	-3.68098	-0.21164
C	1.04705	-2.49041	0.20535
H	1.67912	-3.37613	0.05239
C	2.98958	-0.93992	-0.61207
C	3.86952	-1.46256	0.3467
C	3.53356	-0.11372	-1.6084
C	5.22518	-1.156	0.33631
H	3.50083	-2.13445	1.11676
C	4.88194	0.21128	-1.62966
H	2.89606	0.27484	-2.39888
C	5.70948	-0.31276	-0.64841
H	5.906	-1.56415	1.07767
H	5.3002	0.8513	-2.40111
C	-2.64	-1.58632	0.47955
C	-3.39738	-2.20013	-0.53006
C	-3.34682	-0.95781	1.51872
C	-4.78549	-2.16343	-0.52618
H	-2.8954	-2.72375	-1.33887
C	-4.73569	-0.90128	1.53316
H	-2.8096	-0.53042	2.36436
C	-5.43681	-1.50298	0.50234
H	-5.36647	-2.64049	-1.31054
H	-5.27663	-0.41839	2.34277
F	-6.7761	-1.46145	0.51059
F	7.01081	-0.00602	-0.66387
Ir	-0.04476	0.24664	-0.09639
Cl	-1.74541	0.73173	-1.98333
C	1.24541	1.94553	-0.33194
H	1.96749	1.81616	-1.14143
C	0.68108	3.33455	-0.36282
C	1.5149	1.28125	0.91142
O	-0.3144	3.60974	0.69117
C	-1.29638	2.81867	1.01455
Cl	-3.73089	2.61883	2.3057
N	-1.34831	1.54923	0.87924
H	-2.24457	1.13176	1.13496
H	1.15577	1.73201	1.83903
C	-2.46059	3.64198	1.59497
Cl	-3.14837	4.57019	0.23081
Cl	-1.84697	4.7503	2.84409
H	2.42758	0.70344	1.03672
H	1.46767	4.04338	-0.06742
C	0.08818	3.75754	-1.684
H	-0.24521	4.79936	-1.64417
H	0.85671	3.67132	-2.46036
H	-0.74762	3.105	-1.96127

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6515807
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.657628344849
ΔG_{solv} = -0.0128618

(S)-II-TS'

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -241.49 cm^{-1}
Zero-point correction= 0.442707 (Hartree/Particle)
Thermal correction to Energy= 0.475015
Thermal correction to Enthalpy= 0.475959
Thermal correction to Gibbs Free Energy= 0.380147
Sum of electronic and zero-point Energies= -3278.900871
Sum of electronic and thermal Energies= -3278.868562
Sum of electronic and thermal Enthalpies= -3278.867618
Sum of electronic and thermal Free Energies= -3278.963430

C	-0.44158	-2.40544	-1.56472
C	0.60563	-1.325	-1.64443
C	1.51123	-1.44414	-0.58349
C	0.8853	-1.88722	1.81053
C	-0.24185	-0.91325	1.60981
C	-1.14642	-1.408	0.60561
H	-1.40435	-2.11946	-2.00024
H	-0.07672	-3.29642	-2.09925
H	0.85437	-0.85748	-2.59312
H	0.58751	-2.6524	2.54479
H	1.8118	-1.42748	2.17194
H	-0.59085	-0.31054	2.45065
C	-0.48924	-2.62193	-0.0601
H	-0.95843	-3.56224	0.25886
C	0.98058	-2.47586	0.40807
H	1.55132	-3.41254	0.34163
C	2.94627	-1.10782	-0.67232
C	3.85358	-1.5643	0.29381
C	3.45972	-0.37145	-1.7525
C	5.21174	-1.28	0.20771
H	3.50558	-2.16576	1.12907
C	4.80951	-0.07054	-1.8501
H	2.79386	-0.03262	-2.54347
C	5.66746	-0.52765	-0.86073
H	5.91561	-1.63701	0.95381
H	5.2061	0.49998	-2.68492
C	-2.62517	-1.34113	0.76393
C	-3.49425	-0.99734	-0.27989
C	-3.17887	-1.67558	2.00752
C	-4.87092	-0.98934	-0.09024
H	-3.0796	-0.68281	-1.23649
C	-4.55428	-1.67504	2.21276
H	-2.51717	-1.95272	2.82725
C	-5.37786	-1.33168	1.15368
H	-5.55302	-0.71129	-0.889
H	-4.99069	-1.93618	3.17276
F	-6.7044	-1.32594	1.33868
F	6.97041	-0.24317	-0.9495
Ir	-0.03359	0.2554	-0.16954
Cl	-1.31848	0.82538	-2.32982
C	1.41308	1.96826	-0.49213

H	1.97552	1.65317	-1.372
C	0.89149	3.28603	-0.55581
C	1.57084	1.27834	0.76016
O	-1.09229	3.4654	-0.48449
C	-1.71524	2.72952	0.31026
Cl	-3.88015	2.36464	2.06623
N	-1.36052	1.54797	0.73808
H	-2.01587	1.11846	1.38415
H	1.23088	1.80155	1.65738
C	-3.08012	3.32139	0.77663
Cl	-4.14972	3.35297	-0.6528
Cl	-2.82818	4.98049	1.37901
H	2.44932	0.65528	0.91696
H	0.84332	3.8446	0.37859
C	1.02581	4.0576	-1.81236
H	0.43943	4.97743	-1.79494
H	2.08375	4.31727	-1.94967
H	0.71885	3.43764	-2.66225

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6389865
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.633770453789
ΔG_{solv} = -0.0138696

I-E$_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.444411 (Hartree/Particle)
Thermal correction to Energy= 0.477465
Thermal correction to Enthalpy= 0.478410
Thermal correction to Gibbs Free Energy= 0.380813
Sum of electronic and zero-point Energies= -3278.926085
Sum of electronic and thermal Energies= -3278.893031
Sum of electronic and thermal Enthalpies= -3278.892087
Sum of electronic and thermal Free Energies= -3278.989684

C	0.3255	-1.59445	-1.64809
C	1.24893	-0.45691	-1.32745
C	2.37062	-0.94136	-0.59202
C	2.17253	-2.5223	1.36637
C	0.94106	-1.77133	1.7976
C	-0.05575	-1.90239	0.82468
H	-0.71049	-1.28641	-1.81212
H	0.66988	-2.08082	-2.57368
H	1.28419	0.41773	-1.97351
H	2.06902	-3.575	1.67141
H	3.0907	-2.12626	1.80484
H	0.73798	-1.59113	2.85179
C	0.55406	-2.49437	-0.4404
H	0.2184	-3.53145	-0.57514
C	2.07124	-2.37631	-0.14884
H	2.67581	-3.09745	-0.71444
C	3.75796	-0.47041	-0.79064
C	4.83574	-1.123	-0.17804
C	4.04607	0.59803	-1.65412
C	6.14676	-0.71567	-0.38933
H	4.65745	-1.97018	0.47775
C	5.34837	1.02274	-1.87242
H	3.2408	1.1033	-2.18351
C	6.38159	0.36025	-1.22854
H	6.98262	-1.22007	0.08665
H	5.57131	1.85156	-2.53909
C	-1.5012	-2.01348	1.10838
C	-2.42764	-2.28078	0.09029
C	-1.98444	-1.95514	2.42742
C	-3.78012	-2.44826	0.36238
H	-2.09833	-2.38127	-0.93914
C	-3.33019	-2.1137	2.71735
H	-1.29368	-1.78934	3.25102
C	-4.21228	-2.35294	1.67323
H	-4.49621	-2.65599	-0.42701
H	-3.70216	-2.06908	3.73656
F	-5.50894	-2.51101	1.94497
F	7.64105	0.76138	-1.43682
Ir	1.03252	0.22246	0.73403
Cl	2.87739	0.46704	2.44884
C	-0.94812	1.08059	1.5129
H	-1.56597	0.34323	2.02439
C	-0.11381	1.85988	2.28974
H	0.40406	2.70101	1.82827
C	-0.84962	1.01665	0.07925
O	1.0379	2.59705	-1.93712
C	1.76263	2.76531	-0.95794
C	2.64005	4.0767	-0.96104
Cl	4.1211	3.97418	0.04681
Cl	3.12654	4.47722	-2.62337
Cl	1.58421	5.37967	-0.31301
N	1.86219	2.03417	0.13522
H	2.56831	2.32735	0.80424
H	-0.62117	1.91116	-0.4991
C	-0.04241	1.7376	3.76607
H	-0.62469	0.88455	4.13244
H	1.00123	1.61551	4.08197
H	-0.42105	2.65168	4.24009
H	-1.53751	0.33228	-0.41645

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6672426
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.660683349553
ΔG_{solv} = -0.0143758

TS-E$_2$-E$_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -91.65 cm^{-1}
Zero-point correction= 0.442525 (Hartree/Particle)
Thermal correction to Energy= 0.475536
Thermal correction to Enthalpy= 0.476480
Thermal correction to Gibbs Free Energy= 0.378281
Sum of electronic and zero-point Energies= -3278.901358
Sum of electronic and thermal Energies= -3278.868348
Sum of electronic and thermal Enthalpies= -3278.867403
Sum of electronic and thermal Free Energies= -3278.965603

C	0.12028	-3.80027	-1.05566
C	0.99416	-2.74984	-1.67773
C	2.01941	-2.37856	-0.80349
C	1.74435	-1.98578	1.67692
C	0.45824	-1.26661	1.3621
C	-0.44474	-2.19177	0.78906
H	-0.91515	-3.76048	-1.40804
H	0.51521	-4.79754	-1.29999

H	1.0717	-2.65011	-2.75675
H	1.64863	-2.47165	2.65925
H	2.62688	-1.34186	1.72768
H	0.13643	-0.39685	1.93104
C	0.29977	-3.47168	0.42553
H	0.03346	-4.28583	1.11219
C	1.77401	-3.02073	0.55815
H	2.46525	-3.85698	0.7277
C	3.33411	-1.87097	-1.23146
C	4.43392	-1.90117	-0.36464
C	3.52007	-1.34741	-2.52073
C	5.67495	-1.41256	-0.75737
H	4.33464	-2.32021	0.63389
C	4.75072	-0.86053	-2.92894
H	2.67776	-1.29019	-3.20748
C	5.81067	-0.89424	-2.03375
H	6.53178	-1.43227	-0.0904
H	4.89833	-0.44502	-3.9216
C	-1.91205	-2.15809	0.89536
C	-2.68721	-3.26549	0.51131
C	-2.57556	-1.05543	1.4657
C	-4.06762	-3.26747	0.65165
H	-2.2159	-4.15994	0.11607
C	-3.95202	-1.04094	1.60492
H	-2.00685	-0.1951	1.81199
C	-4.68032	-2.14683	1.187
H	-4.66862	-4.12339	0.35972
H	-4.46846	-0.19168	2.04281
F	-6.00636	-2.13536	1.32209
F	6.99748	-0.41625	-2.4182
Ir	0.29975	-0.80475	-0.80915
Cl	0.00356	-0.21323	-3.16597
C	2.36096	1.37617	-1.29004
H	2.04855	1.17213	-2.31285
C	3.26851	2.33006	-1.06913
C	1.81618	0.54271	-0.17149
O	-0.72693	1.59879	1.59363
C	-1.12711	1.6787	0.43162
Cl	-3.5144	2.73286	1.14255
N	-0.92014	0.83977	-0.56717
H	-1.28497	1.14217	-1.46562
H	1.33055	1.14233	0.6061
C	-2.04299	2.92236	0.13574
Cl	-2.55296	3.11324	-1.57341
Cl	-1.16853	4.3962	0.62882
H	2.61627	-0.04235	0.28387
H	3.58992	2.53193	-0.04292
C	3.91938	3.1275	-2.14919
H	3.53331	2.84315	-3.13486
H	3.75918	4.20499	-2.01637
H	5.00662	2.97174	-2.15495

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6468396
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.631590895520
ΔG_{solv} = -0.0159637

I-E$_2$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.443248 (Hartree/Particle)
Thermal correction to Energy= 0.476676
Thermal correction to Enthalpy= 0.477620
Thermal correction to Gibbs Free Energy= 0.378583
Sum of electronic and zero-point Energies= -3278.924810
Sum of electronic and thermal Energies= -3278.891383
Sum of electronic and thermal Enthalpies= -3278.890439
Sum of electronic and thermal Free Energies= -3278.989476

C	0.27397	-1.57129	-1.60705
C	1.2147	-0.44107	-1.31382
C	2.35057	-0.92336	-0.60295
C	2.20136	-2.50901	1.3541
C	0.96868	-1.78319	1.81735
C	-0.04915	-1.92313	0.87317
H	-0.76504	-1.25054	-1.72606
H	0.57739	-2.05407	-2.54861
H	1.2345	0.4318	-1.96351
H	2.12302	-3.56374	1.66013
H	3.12074	-2.0969	1.77472
H	0.79244	-1.6081	2.87721
C	0.5389	-2.48465	-0.41527
H	0.20921	-3.52224	-0.56085
C	2.06274	-2.35931	-0.15686
H	2.65816	-3.07643	-0.73725
C	3.73314	-0.44965	-0.82772
C	4.82536	-1.08021	-0.21788
C	4.00144	0.60784	-1.71015
C	6.12904	-0.65928	-0.44908
H	4.6654	-1.91946	0.4525
C	5.29502	1.04816	-1.94781
H	3.18566	1.09218	-2.24181
C	6.34279	0.40827	-1.30477
H	6.97578	-1.14634	0.02586
H	5.49344	1.87532	-2.62495
C	-1.485	-2.05057	1.18827
C	-2.42899	-2.31388	0.18356
C	-1.94589	-2.00981	2.51547
C	-3.77576	-2.48414	0.47605
H	-2.11688	-2.40362	-0.8522
C	-3.28776	-2.16892	2.82579
H	-1.24027	-1.87947	3.33244
C	-4.18714	-2.39613	1.79498
H	-4.50437	-2.6873	-0.30298
H	-3.64149	-2.13928	3.85199
F	-5.47935	-2.55447	2.08541
F	7.59524	0.82279	-1.52911
Ir	1.02436	0.24391	0.75213
Cl	2.8688	0.48248	2.45848
C	-0.61503	1.73534	1.25548
H	-0.25032	2.7569	1.14132
C	-0.478	1.12123	2.49023
H	-1.01274	0.18757	2.65822
C	-0.9066	0.95848	0.0831
O	0.90628	2.65244	-1.84057
C	1.72566	2.77406	-0.93123
C	2.6603	4.03981	-1.02144
Cl	4.12707	3.97375	0.00859
Cl	3.18151	4.26435	-2.71093
Cl	1.659	5.43881	-0.50959
N	1.9003	2.01776	0.13325
H	2.65478	2.27274	0.76323
H	-1.65039	0.16596	0.15685
C	0.05838	1.81967	3.68736
H	0.63373	2.70824	3.40623
H	-0.76776	2.12548	4.34259
H	0.71357	1.15964	4.26556
H	-0.86249	1.47666	-0.87265

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6658612
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.659844664588
ΔG_{solv} = -0.0143604

TS-E_1-E_2

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -45.09 cm^{-1}
Zero-point correction= 0.442999 (Hartree/Particle)
Thermal correction to Energy= 0.475911
Thermal correction to Enthalpy= 0.476855
Thermal correction to Gibbs Free Energy= 0.379475
Sum of electronic and zero-point Energies= -3278.910575
Sum of electronic and thermal Energies= -3278.877663
Sum of electronic and thermal Enthalpies= -3278.876719
Sum of electronic and thermal Free Energies= -3278.974099

C	0.04554	-3.93214	-1.14984
C	0.95675	-3.00936	-1.90869
C	2.12489	-2.77468	-1.17466
C	2.19685	-2.22287	1.26812
C	0.95153	-1.39002	1.09323
C	-0.10896	-2.23197	0.68355
H	-1.01348	-3.77791	-1.3778
H	0.29066	-4.9741	-1.40544
H	0.92297	-2.95197	-2.99381
H	2.22543	-2.63002	2.28977
H	3.13347	-1.67649	1.10913
H	0.78755	-0.47646	1.66066
C	0.43946	-3.59544	0.28944
H	0.163	-4.35788	1.02928
C	1.95794	-3.32128	0.2343
H	2.56147	-4.22546	0.38639
C	3.45688	-2.56089	-1.76927
C	4.61373	-2.86276	-1.03952
C	3.60556	-2.0855	-3.08245
C	5.87926	-2.71335	-1.59618
H	4.53567	-3.23408	-0.02055
C	4.85945	-1.92372	-3.64764
H	2.72465	-1.80263	-3.65583
C	5.98056	-2.24568	-2.89421
H	6.7788	-2.95506	-1.03774
H	4.98297	-1.54956	-4.65979
C	-1.54602	-2.05933	0.96462
C	-2.45514	-3.10569	0.73159
C	-2.03965	-0.88539	1.55892
C	-3.80377	-2.97611	1.03361
H	-2.1159	-4.055	0.32944
C	-3.38361	-0.73689	1.85677
H	-1.35932	-0.07249	1.79422
C	-4.25027	-1.78423	1.57969
H	-4.50688	-3.78444	0.85683
H	-3.76665	0.17469	2.30711
F	-5.54651	-1.64656	1.86511
F	7.19118	-2.09433	-3.4393
Ir	0.62284	-0.98177	-1.05268
Cl	0.47512	-0.28357	-3.3906
C	2.56467	1.08857	0.31535
H	2.86551	0.61442	1.25203
C	2.42004	2.42377	0.2994
C	2.42297	0.25554	-0.86676
O	-0.22937	1.59085	1.36327
C	-0.57671	1.65927	0.18908
Cl	-1.17279	4.2441	0.97039
N	-0.46	0.75204	-0.77173
H	-0.77024	1.08001	-1.68342
H	3.2211	-0.47799	-0.96507
C	-1.30623	2.98345	-0.26911
Cl	-3.04056	2.59967	-0.53428
Cl	-0.59802	3.6115	-1.7998
H	2.31165	0.84246	-1.78448
H	2.10987	2.90099	-0.63584
C	2.6349	3.30935	1.47008
H	2.93586	2.73793	2.3546
H	3.3982	4.07119	1.2682
H	1.70664	3.84592	1.70804

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6559825
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.637567228433
ΔG_{solv} = -0.0136845

I-E_1

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.443958 (Hartree/Particle)
Thermal correction to Energy= 0.477025
Thermal correction to Enthalpy= 0.477969
Thermal correction to Gibbs Free Energy= 0.380816
Sum of electronic and zero-point Energies= -3278.918940
Sum of electronic and thermal Energies= -3278.885873
Sum of electronic and thermal Enthalpies= -3278.884928
Sum of electronic and thermal Free Energies= -3278.982082

C	0.20384	-1.5294	-1.58952
C	1.15244	-0.39453	-1.31838
C	2.27973	-0.87178	-0.60364
C	2.11269	-2.43125	1.38818
C	0.88611	-1.68135	1.83831
C	-0.12378	-1.8304	0.88527
H	-0.83998	-1.22503	-1.70165
H	0.50259	-2.02442	-2.52646
H	1.18093	0.47702	-1.97025
H	2.00652	-3.48285	1.69711
H	3.03983	-2.04202	1.81127
H	0.69693	-1.50761	2.89595
C	0.47026	-2.42117	-0.38591
H	0.14333	-3.46265	-0.50873
C	1.98823	-2.29607	-0.12557
H	2.58182	-3.02703	-0.69053
C	3.66782	-0.4088	-0.81776
C	4.74644	-1.06423	-0.21027
C	3.95702	0.6504	-1.69174
C	6.05902	-0.66726	-0.43518
H	4.57	-1.90704	0.4513
C	5.26014	1.06686	-1.92139
H	3.15144	1.1556	-2.21992
C	6.29472	0.40211	-1.28159
H	6.89485	-1.17471	0.0377
H	5.48005	1.89305	-2.59257

C	-1.55945	-1.97374	1.19397
C	-2.46025	-2.43213	0.22251
C	-2.0508	-1.76316	2.4937
C	-3.80141	-2.64309	0.51909
H	-2.11752	-2.64182	-0.78708
C	-3.38664	-1.95916	2.80551
H	-1.37689	-1.43484	3.28271
C	-4.24546	-2.39589	1.80669
H	-4.49966	-3.00165	-0.23125
H	-3.76839	-1.79277	3.80846
F	-5.53155	-2.59499	2.10036
F	7.55535	0.79451	-1.50167
Ir	0.96854	0.33815	0.77749
Cl	2.881	0.49025	2.41688
C	-1.01193	1.18011	1.46413
H	-1.72894	0.42988	1.79203
C	-0.01619	1.62183	2.34653
H	-0.00058	1.23257	3.3624
H	0.48194	2.5772	2.19137
C	-0.92534	1.46665	0.08109
O	1.12585	2.6476	-1.91295
C	1.80845	2.83638	-0.90693
C	2.6682	4.15657	-0.9098
Cl	3.98825	4.20585	0.3052
Cl	3.38509	4.39119	-2.52241
Cl	1.51656	5.4915	-0.56526
N	1.8557	2.12779	0.2045
H	2.53794	2.42109	0.89689
C	-1.94491	0.98789	-0.89522
H	-1.51295	0.86608	-1.89398
H	-2.42745	0.05451	-0.58608
H	-2.72796	1.75254	-0.98677
H	-0.438	2.39488	-0.20822

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6597755
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.653833911274
ΔG_{solv} = -0.014478

(R)-II-TS

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -147.94 cm^{-1}
Zero-point correction= 0.441824 (Hartree/Particle)
Thermal correction to Energy= 0.474453
Thermal correction to Enthalpy= 0.475398
Thermal correction to Gibbs Free Energy= 0.378218
Sum of electronic and zero-point Energies= -3278.898989
Sum of electronic and thermal Energies= -3278.866359
Sum of electronic and thermal Enthalpies= -3278.865415
Sum of electronic and thermal Free Energies= -3278.962595

C	-0.39815	-1.54248	-1.67087
C	0.52009	-0.39218	-1.36136
C	1.6159	-0.84245	-0.57271
C	1.36674	-2.33884	1.43517
C	0.11168	-1.59287	1.79579
C	-0.84915	-1.76122	0.78965
H	-1.43551	-1.22891	-1.83501
H	-0.06051	-2.06266	-2.58074
H	0.59048	0.43782	-2.0615
H	1.27763	-3.37787	1.78903
H	2.26429	-1.90183	1.88001
H	-0.13372	-1.39434	2.83705
C	-0.19358	-2.40193	-0.42768
H	-0.51564	-3.44678	-0.53711
C	1.3132	-2.26051	-0.08904
H	1.94025	-3.00471	-0.59911
C	3.0016	-0.34339	-0.6788
C	4.05684	-0.98313	-0.01315
C	3.32319	0.76252	-1.48085
C	5.3662	-0.52771	-0.11468
H	3.86532	-1.86256	0.5951
C	4.62144	1.23832	-1.58787
H	2.54549	1.26166	-2.05322
C	5.62831	0.58536	-0.89429
H	6.18148	-1.02603	0.40212
H	4.85726	2.10079	-2.20651
C	-2.3039	-1.87147	1.02821
C	-3.1808	-2.25205	0.00097
C	-2.85424	-1.64163	2.29934
C	-4.54998	-2.35553	0.21489
H	-2.79663	-2.48294	-0.98826
C	-4.21907	-1.73129	2.52925
H	-2.2055	-1.39982	3.13695
C	-5.0503	-2.07915	1.4758
H	-5.22815	-2.64999	-0.58064
H	-4.64347	-1.55086	3.51258
F	-6.36633	-2.16821	1.68849
F	6.88682	1.03355	-0.99242
Ir	0.15382	0.33952	0.67472
Cl	1.81829	0.80248	2.49915
C	-1.92004	1.16619	0.56978
H	-2.58198	0.32396	0.36684
C	-1.30572	1.3018	1.87232
H	-1.69975	0.69039	2.68404
H	-0.97351	2.29429	2.18379
C	-2.10206	2.25907	-0.30509
O	-0.46728	2.66905	-1.6947
C	0.54698	2.86209	-0.9915
C	1.3972	4.09737	-1.40316
Cl	2.8653	4.34899	-0.41821
Cl	1.88987	3.87949	-3.1113
Cl	0.34814	5.53851	-1.2603
N	0.90997	2.15315	0.04198
H	1.74141	2.4449	0.54993
C	-3.08874	2.17955	-1.39856
H	-2.92815	2.94346	-2.16013
H	-3.08463	1.18255	-1.85369
H	-4.08638	2.33332	-0.96128
H	-1.7823	3.24523	0.03072

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6372486
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.625739708569
ΔG_{solv} = -0.0133637

(R)-II

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.445778 (Hartree/Particle)
Thermal correction to Energy= 0.477857
Thermal correction to Enthalpy= 0.478802
Thermal correction to Gibbs Free Energy= 0.382362

Sum of electronic and zero-point Energies= -3278.922949
Sum of electronic and thermal Energies= -3278.890870
Sum of electronic and thermal Enthalpies= -3278.889925
Sum of electronic and thermal Free Energies= -3278.986365

C	-0.33039	-1.69799	-1.73607
C	0.63875	-0.59025	-1.43679
C	1.69847	-1.07568	-0.61547
C	1.35182	-2.50541	1.41778
C	0.16095	-1.64301	1.74447
C	-0.80917	-1.76078	0.72507
H	-1.34616	-1.3396	-1.93766
H	0.00314	-2.27131	-2.61547
H	0.80278	0.19778	-2.17152
H	1.17928	-3.52325	1.8019
H	2.28138	-2.12648	1.85181
H	-0.08113	-1.41113	2.77998
C	-0.19781	-2.51254	-0.45502
H	-0.59794	-3.53424	-0.51753
C	1.31298	-2.46553	-0.10785
H	1.89096	-3.2619	-0.59742
C	3.10766	-0.64997	-0.73395
C	4.13199	-1.36668	-0.09913
C	3.48332	0.46833	-1.49765
C	5.46324	-0.98017	-0.19496
H	3.89197	-2.25149	0.48456
C	4.80781	0.8748	-1.5974
H	2.73114	1.03525	-2.04511
C	5.7819	0.14376	-0.93718
H	6.25311	-1.53818	0.30008
H	5.09213	1.74034	-2.18998
C	-2.27025	-1.76721	0.95932
C	-3.16877	-2.10941	-0.06266
C	-2.80865	-1.48659	2.22554
C	-4.54171	-2.13262	0.15064
H	-2.79874	-2.37953	-1.04714
C	-4.1766	-1.49839	2.45602
H	-2.14824	-1.2699	3.06101
C	-5.02626	-1.81379	1.40761
H	-5.23477	-2.39967	-0.64183
H	-4.58949	-1.28233	3.43712
F	-6.34593	-1.82891	1.6213
F	7.06264	0.52783	-1.02988
Ir	0.32726	0.19978	0.5832
Cl	2.15607	0.66283	2.35097
C	-1.57275	1.20238	0.40951
H	-2.38763	0.49345	0.24905
C	-1.07069	1.35912	1.7346
H	-1.52735	0.7956	2.54601
H	-0.63435	2.31059	2.0416
C	-1.70508	2.33784	-0.56503
O	-0.70509	3.39626	-0.41861
C	0.57363	3.13828	-0.34989
C	1.3982	4.38856	-0.68412
Cl	3.11108	4.18567	-0.25623
Cl	1.24883	4.61904	-2.45574
Cl	0.74484	5.79927	0.17364
N	1.10879	2.01027	-0.09462
H	2.128	2.01896	-0.04473
C	-1.76516	1.93766	-2.02026
H	-1.99571	2.80246	-2.64955
H	-2.55206	1.18789	-2.1589
H	-0.81864	1.49882	-2.35162
H	-2.62098	2.88533	-0.30293

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6568098
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.662579791963
ΔG_{solv} = -0.0146715

I-E$_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.444411 (Hartree/Particle)
Thermal correction to Energy= 0.477465
Thermal correction to Enthalpy= 0.478410
Thermal correction to Gibbs Free Energy= 0.380813
Sum of electronic and zero-point Energies= -3278.926085
Sum of electronic and thermal Energies= -3278.893031
Sum of electronic and thermal Enthalpies= -3278.892087
Sum of electronic and thermal Free Energies= -3278.989684

C	0.3255	-1.59445	-1.64809
C	1.24893	-0.45691	-1.32745
C	2.37062	-0.94136	-0.59202
C	2.17253	-2.5223	1.36637
C	0.94106	-1.77133	1.7976
C	-0.05575	-1.90239	0.82468
H	-0.71049	-1.28641	-1.81212
H	0.66988	-2.08082	-2.57368
H	1.28419	0.41773	-1.97351
H	2.06902	-3.575	1.67141
H	3.0907	-2.12626	1.80484
H	0.73798	-1.59113	2.85179
C	0.55406	-2.49437	-0.4404
H	0.2184	-3.53145	-0.57514
C	2.07124	-2.37631	-0.14884
H	2.67581	-3.09745	-0.71444
C	3.75796	-0.47041	-0.79064
C	4.83574	-1.123	-0.17804
C	4.04607	0.59803	-1.65412
C	6.14676	-0.71567	-0.38933
H	4.65745	-1.97018	0.47775
C	5.34837	1.02274	-1.87242
H	3.2408	1.1033	-2.18351
C	6.38159	0.36025	-1.22854
H	6.98262	-1.22007	0.08665
H	5.57131	1.85156	-2.53909
C	-1.5012	-2.01348	1.10838
C	-2.42764	-2.28078	0.09029
C	-1.98444	-1.95514	2.42742
C	-3.78012	-2.44826	0.36238
H	-2.09833	-2.38127	-0.93914
C	-3.33019	-2.1137	2.71735
H	-1.29368	-1.78934	3.25102
C	-4.21228	-2.35294	1.67323
H	-4.49621	-2.65599	-0.42701
H	-3.70216	-2.06908	3.73656
F	-5.50894	-2.51101	1.94497
F	7.64105	0.76138	-1.43682
Ir	1.03252	0.22246	0.73403
Cl	2.87739	0.46704	2.44884
C	-0.94812	1.08059	1.5129
H	-1.56597	0.34323	2.02439
C	-0.11381	1.85988	2.28974

H	0.40406	2.70101	1.82827
C	-0.84962	1.01665	0.07925
O	1.0379	2.59705	-1.93712
C	1.76263	2.76531	-0.95794
C	2.64005	4.0767	-0.96104
Cl	4.1211	3.97418	0.04681
Cl	3.12654	4.47722	-2.62337
Cl	1.58421	5.37967	-0.31301
N	1.86219	2.03417	0.13522
H	2.56831	2.32735	0.80424
H	-0.62117	1.91116	-0.4991
C	-0.04241	1.7376	3.76607
H	-0.62469	0.88455	4.13244
H	1.00123	1.61551	4.08197
H	-0.42105	2.65168	4.24009
H	-1.53751	0.33228	-0.41645

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6672426
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.660683349553
ΔG_{solv} = -0.0143758

I-E$_3$-TS$_L$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -374.86 cm^{-1}
Zero-point correction= 0.578165 (Hartree/Particle)
Thermal correction to Energy= 0.619739
Thermal correction to Enthalpy= 0.620684
Thermal correction to Gibbs Free Energy= 0.504003
Sum of electronic and zero-point Energies= -3553.541927
Sum of electronic and thermal Energies= -3553.500353
Sum of electronic and thermal Enthalpies= -3553.499409
Sum of electronic and thermal Free Energies= -3553.616089

C	-0.28993	-1.44755	-2.1869
C	0.62559	-0.42548	-1.57633
C	1.90608	-1.01659	-1.33934
C	2.22846	-3.26347	-0.25351
C	1.11101	-2.90324	0.68816
C	-0.08266	-2.73909	-0.03331
H	-1.35155	-1.24184	-2.01713
H	-0.13526	-1.47812	-3.27715
H	0.49381	0.63022	-1.80666
H	2.23181	-4.35479	-0.40264
H	3.20987	-2.96408	0.1218
H	1.15029	-3.20731	1.73199
C	0.23608	-2.71495	-1.52602
H	-0.08891	-3.64926	-2.00465
C	1.77531	-2.53205	-1.51361
H	2.25731	-2.87871	-2.43809
C	3.19741	-0.32872	-1.57311
C	4.41136	-1.02611	-1.50599
C	3.25218	1.03033	-1.921
C	5.62922	-0.39674	-1.73615
H	4.41696	-2.0868	-1.27241
C	4.45881	1.67821	-2.14661
H	2.33173	1.59821	-2.03588
C	5.63458	0.95288	-2.04207
H	6.56833	-0.94002	-1.68059
H	4.49656	2.73262	-2.40861
C	-1.41297	-3.156	0.46515
C	-2.57652	-2.99889	-0.30047
C	-1.54366	-3.77859	1.71823
C	-3.82131	-3.39685	0.17364
H	-2.52407	-2.56765	-1.29491
C	-2.77716	-4.17679	2.21091
H	-0.66217	-3.96224	2.32725
C	-3.90468	-3.96988	1.43041
H	-4.72132	-3.27107	-0.42111
H	-2.87478	-4.6545	3.18138
F	-5.09736	-4.35005	1.89779
F	6.80477	1.56984	-2.25912
Ir	0.86415	-0.69591	0.57852
Cl	3.03356	-0.90537	1.9547
O	0.35924	2.64664	-0.78457
C	1.22935	2.42154	0.06805
C	2.04717	3.67401	0.55674
Cl	3.7051	3.28807	1.10534
Cl	2.15218	4.89159	-0.7354
Cl	1.11229	4.35554	1.94151
N	1.50173	1.29867	0.68806
H	2.28983	1.32981	1.32983
H	-2.29172	5.02774	0.96247
H	-1.11349	4.28483	-0.16732
C	-2.14755	4.61972	-0.04071
H	-2.38611	5.38574	-0.78671
F	-3.00449	1.4697	1.20902
C	-0.03447	-0.15092	2.6293
H	0.37855	0.85462	2.73085
H	-2.88877	2.6645	0.52365
N	-3.04773	3.4626	-0.22628
H	-4.59568	4.31066	0.91855
C	-4.46758	3.83058	-0.05428
C	-1.0756	-0.35838	1.71252
H	-1.76565	2.52361	-1.60082
C	-2.82257	2.79738	-1.52864
H	-1.67085	-1.26242	1.82199
H	-4.77566	4.5157	-0.85045
H	-3.09282	3.47764	-2.3428
H	-5.06552	2.91669	-0.08694
C	-1.40181	0.49691	0.63636
H	-3.44771	1.90105	-1.56492
H	-0.90165	1.44231	0.48098
H	-1.98144	0.0986	-0.18937
C	0.15123	-1.05958	3.80005
H	1.21496	-1.25022	3.98065
H	-0.26409	-0.6002	4.70675
H	-0.35957	-2.01837	3.64999

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3555.702673
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3550.165976616739
ΔG_{solv} = -0.0207448

I-E$_3$-TS$_B$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -877.03 cm^{-1}
Zero-point correction= 0.576008 (Hartree/Particle)
Thermal correction to Energy= 0.617235
Thermal correction to Enthalpy= 0.618179
Thermal correction to Gibbs Free Energy= 0.502580
Sum of electronic and zero-point Energies= -3553.560080

Sum of electronic and thermal Energies= -3553.518853
Sum of electronic and thermal Enthalpies= -3553.517909
Sum of electronic and thermal Free Energies= -3553.633508

C	1.16844	-0.85494	-2.80479
C	1.51884	0.18586	-1.77986
C	2.70772	-0.20812	-1.08272
C	3.07017	-2.517	-0.15712
C	1.61969	-2.52722	0.2435
C	0.81134	-2.44869	-0.90031
H	0.10286	-0.87632	-3.05598
H	1.72337	-0.66061	-3.7359
H	1.25186	1.22663	-1.95753
H	3.38731	-3.54853	-0.37804
H	3.72392	-2.11566	0.6209
H	1.30129	-2.99237	1.17435
C	1.68006	-2.10905	-2.10575
H	1.79738	-2.9834	-2.76062
C	3.00186	-1.6705	-1.42589
H	3.87767	-1.76662	-2.08199
C	3.79328	0.71275	-0.68407
C	5.01489	0.22499	-0.19781
C	3.66333	2.10315	-0.82449
C	6.05112	1.07852	0.16058
H	5.17354	-0.84529	-0.09897
C	4.68384	2.97198	-0.46584
H	2.75115	2.52258	-1.24204
C	5.86527	2.44395	0.02922
H	6.99639	0.69774	0.53719
H	4.57928	4.04807	-0.57888
C	-0.48093	-3.14949	-1.0616
C	-1.11123	-3.23286	-2.31228
C	-1.07596	-3.83608	0.00949
C	-2.29748	-3.93592	-2.48567
H	-0.66807	-2.75536	-3.18145
C	-2.26346	-4.53585	-0.14198
H	-0.5945	-3.84187	0.98456
C	-2.86177	-4.56957	-1.3924
H	-2.78124	-4.00236	-3.45586
H	-2.7211	-5.0667	0.68768
F	-4.004	-5.24618	-1.54793
F	6.85795	3.27547	0.37379
Ir	0.93792	-0.40407	0.2066
Cl	2.32513	-0.45835	2.36947
O	-0.35476	2.80873	-0.77633
C	0.45089	2.71246	0.15464
C	0.8906	4.0919	0.78329
Cl	2.10922	3.99838	2.09484
Cl	1.55714	5.10994	-0.53301
Cl	-0.57757	4.88168	1.44245
N	0.97583	1.63136	0.68782
H	1.6428	1.7785	1.43937
H	-3.18216	3.15565	1.83855
H	-2.49475	2.75009	0.23907
C	-3.42325	2.91646	0.79815
H	-3.96891	3.7531	0.34414
F	-3.1089	0.39941	2.44375
C	-1.20084	0.14096	2.20567
H	-1.04862	1.2084	2.04222
H	-3.64205	0.92903	1.5113
N	-4.24536	1.69331	0.78335
H	-5.29324	2.18761	2.53102
C	-5.51556	1.90812	1.49755
C	-1.11221	-0.70019	1.07551
H	-3.51087	1.03187	-1.07267
C	-4.47335	1.20695	-0.58444
H	-1.31164	-1.75724	1.25041
H	-6.09744	2.7029	1.01529
H	-5.03954	1.95103	-1.15902
H	-6.09267	0.97983	1.49653
C	-1.11082	-0.20055	-0.27617
H	-5.0357	0.27037	-0.55007
H	-1.30338	0.85805	-0.45689
H	-1.47879	-0.86224	-1.05957
C	-0.96105	-0.37031	3.56881
H	-1.42162	0.27272	4.32071
H	-1.32789	-1.39571	3.67909
H	0.12929	-0.37533	3.7251

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3555.714091
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3550.180473817605
ΔG_{solv} = -0.0191866

I-E$_2$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.443248 (Hartree/Particle)
Thermal correction to Energy= 0.476676
Thermal correction to Enthalpy= 0.477620
Thermal correction to Gibbs Free Energy= 0.378583
Sum of electronic and zero-point Energies= -3278.924810
Sum of electronic and thermal Energies= -3278.891383
Sum of electronic and thermal Enthalpies= -3278.890439
Sum of electronic and thermal Free Energies= -3278.989476

C	0.27397	-1.57129	-1.60705
C	1.2147	-0.44107	-1.31382
C	2.35057	-0.92336	-0.60295
C	2.20136	-2.50901	1.3541
C	0.96868	-1.78319	1.81735
C	-0.04915	-1.92313	0.87317
H	-0.76504	-1.25054	-1.72606
H	0.57739	-2.05407	-2.54861
H	1.2345	0.4318	-1.96351
H	2.12302	-3.56374	1.66013
H	3.12074	-2.0969	1.77472
H	0.79244	-1.6081	2.87721
C	0.5389	-2.48465	-0.41527
H	0.20921	-3.52224	-0.56085
C	2.06274	-2.35931	-0.15686
H	2.65816	-3.07643	-0.73725
C	3.73314	-0.44965	-0.82772
C	4.82536	-1.08021	-0.21788
C	4.00144	0.60784	-1.71015
C	6.12904	-0.65928	-0.44908
H	4.6654	-1.91946	0.4525
C	5.29502	1.04816	-1.94781
H	3.18566	1.09218	-2.24181
C	6.34279	0.40827	-1.30477
H	6.97578	-1.14634	0.02586
H	5.49344	1.87532	-2.62495
C	-1.485	-2.05057	1.18827
C	-2.42899	-2.31388	0.18356
C	-1.94589	-2.00981	2.51547
C	-3.77576	-2.48414	0.47605
H	-2.11688	-2.40362	-0.8522
C	-3.28776	-2.16892	2.82579

H	-1.24027	-1.87947	3.33244
C	-4.18714	-2.39613	1.79498
H	-4.50437	-2.6873	-0.30298
H	-3.64149	-2.13928	3.85199
F	-5.47935	-2.55447	2.08541
F	7.59524	0.82279	-1.52911
Ir	1.02436	0.24391	0.75213
Cl	2.8688	0.48248	2.45848
C	-0.61503	1.73534	1.25548
H	-0.25032	2.7569	1.14132
C	-0.478	1.12123	2.49023
H	-1.01274	0.18757	2.65822
C	-0.9066	0.95848	0.0831
O	0.90628	2.65244	-1.84057
C	1.72566	2.77406	-0.93123
C	2.6603	4.03981	-1.02144
Cl	4.12707	3.97375	0.00859
Cl	3.18151	4.26435	-2.71093
Cl	1.659	5.43881	-0.50959
N	1.9003	2.01776	0.13325
H	2.65478	2.27274	0.76323
H	-1.65039	0.16596	0.15685
C	0.05838	1.81967	3.68736
H	0.63373	2.70824	3.40623
H	-0.76776	2.12548	4.34259
H	0.71357	1.15964	4.26556
H	-0.86249	1.47666	-0.87265

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6658612
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.659844664588
ΔG_{solv} = -0.0143604

I-E$_2$-TS$_L$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -294.60 cm^{-1}
Zero-point correction= 0.575485 (Hartree/Particle)
Thermal correction to Energy= 0.617398
Thermal correction to Enthalpy= 0.618342
Thermal correction to Gibbs Free Energy= 0.500644
Sum of electronic and zero-point Energies= -3553.541293
Sum of electronic and thermal Energies= -3553.499380
Sum of electronic and thermal Enthalpies= -3553.498435
Sum of electronic and thermal Free Energies= -3553.616133

C	-1.9082	-1.28321	-0.99624
C	-0.81632	-0.25598	-1.13958
C	0.19297	-0.7651	-2.0094
C	1.16045	-3.06027	-1.91239
C	1.18015	-2.86076	-0.42191
C	-0.14277	-2.69799	0.06346
H	-2.46781	-1.20723	-0.05658
H	-2.63516	-1.18221	-1.81772
H	-1.0374	0.80634	-1.08174
H	1.03079	-4.12681	-2.15359
H	2.07525	-2.71365	-2.40496
H	1.97806	-3.28647	0.1825
C	-1.08549	-2.55927	-1.12977
H	-1.66799	-3.47468	-1.30386
C	-0.07927	-2.24573	-2.26368
H	-0.48701	-2.42091	-3.26891
C	0.98059	0.04473	-2.96541
C	1.68533	-0.55783	-4.01731
C	1.00147	1.44774	-2.88634
C	2.40944	0.19529	-4.93538
H	1.66279	-1.63673	-4.14374
C	1.72209	2.21272	-3.78993
H	0.43522	1.95593	-2.10947
C	2.42465	1.57162	-4.80017
H	2.95314	-0.27259	-5.75116
H	1.73977	3.2974	-3.72779
C	-0.62496	-3.18747	1.37424
C	-1.9941	-3.36137	1.62229
C	0.27235	-3.55637	2.39147
C	-2.45884	-3.86802	2.83351
H	-2.72359	-3.11868	0.85362
C	-0.17288	-4.07057	3.60027
H	1.34089	-3.41908	2.24103
C	-1.53825	-4.21755	3.80517
H	-3.51959	-4.00812	3.02129
H	0.52172	-4.36404	4.38321
F	-1.97222	-4.71982	4.96772
F	3.12199	2.30662	-5.67552
Ir	0.91134	-0.76876	0.03376
Cl	2.67375	-1.08245	1.72598
O	-0.35798	2.62021	-0.05064
C	0.79139	2.38332	0.35387
C	1.50516	3.62507	0.99371
Cl	3.20493	3.36403	1.49028
Cl	1.45178	4.97185	-0.1775
Cl	0.55701	4.0622	2.45813
N	1.43271	1.23839	0.35429
H	2.34259	1.27369	0.80544
H	-5.22141	2.17863	2.23901
H	-4.70876	3.72087	2.96265
C	-4.8181	3.1727	2.02247
H	-5.51392	3.7141	1.36664
F	-2.55535	1.41368	2.88565
C	-1.02993	0.32351	2.08498
H	-1.70826	-0.51898	1.9723
H	-2.87215	2.22958	2.21312
N	-3.50306	3.02823	1.38627
H	-3.97771	1.25127	0.37543
C	-3.61007	2.25668	0.14064
C	-0.11008	0.32043	3.15576
H	-2.75548	4.85919	2.09881
C	-2.87863	4.33604	1.14571
H	0.64278	1.10673	3.21532
H	-4.30342	2.74067	-0.56143
H	-3.5123	4.94326	0.48293
H	-2.61697	2.18773	-0.31329
C	-0.15733	-0.65982	4.08794
H	-1.89738	4.18281	0.68569
H	-0.92862	-1.42815	3.98534
C	0.78482	-0.79761	5.21323
H	0.25168	-0.83007	6.17177
H	1.3136	-1.75743	5.12668
H	1.52321	0.00892	5.23357
H	-0.99854	1.06634	1.29422

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3555.6952996
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3550.147507210888
ΔG_{solv} = -0.0158056

I-E_2-TS_B

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -1092.01 cm^{-1}
Zero-point correction= 0.575108 (Hartree/Particle)
Thermal correction to Energy= 0.616991
Thermal correction to Enthalpy= 0.617935
Thermal correction to Gibbs Free Energy= 0.499641
Sum of electronic and zero-point Energies= -3553.554224
Sum of electronic and thermal Energies= -3553.512341
Sum of electronic and thermal Enthalpies= -3553.511397
Sum of electronic and thermal Free Energies= -3553.629691

C	-0.10891	-2.09807	-2.1629
C	1.04283	-1.15525	-1.97317
C	2.0884	-1.8128	-1.24867
C	1.7074	-3.17942	0.82159
C	0.70024	-2.14655	1.24974
C	-0.36956	-2.11788	0.343
H	-1.06604	-1.58374	-2.29589
H	0.0601	-2.71455	-3.05974
H	1.22079	-0.369	-2.70327
H	1.40606	-4.15795	1.22818
H	2.72116	-2.9641	1.16793
H	0.61313	-1.86369	2.29693
C	0.00553	-2.93242	-0.89336
H	-0.55387	-3.87794	-0.91519
C	1.53106	-3.12415	-0.6922
H	1.93081	-3.99661	-1.22712
C	3.53167	-1.64528	-1.52425
C	4.48681	-2.46534	-0.90784
C	3.99632	-0.69248	-2.44562
C	5.84561	-2.32511	-1.16453
H	4.17275	-3.23916	-0.21323
C	5.34898	-0.53401	-2.71095
H	3.28783	-0.0709	-2.98757
C	6.25754	-1.3506	-2.05669
H	6.58325	-2.96105	-0.68334
H	5.70369	0.20767	-3.42177
C	-1.78942	-1.95685	0.73577
C	-2.82694	-1.98621	-0.20906
C	-2.15744	-1.89342	2.09037
C	-4.16345	-1.9194	0.16859
H	-2.60017	-2.07775	-1.26638
C	-3.48449	-1.81273	2.48802
H	-1.39277	-1.93268	2.86246
C	-4.47159	-1.82231	1.5149
H	-4.96245	-1.94594	-0.56679
H	-3.76152	-1.76586	3.53713
F	-5.75291	-1.74226	1.88635
F	7.5656	-1.20505	-2.30834
Ir	1.08647	-0.3151	0.01282
Cl	2.97778	-0.1856	1.73706
O	1.2553	1.89325	-2.78187
C	2.08795	1.9716	-1.87735
C	3.11818	3.15706	-2.01984
Cl	4.57376	3.04174	-0.97514
Cl	3.66269	3.26945	-3.71321
Cl	2.22051	4.65088	-1.57675
N	2.20823	1.2393	-0.79103
H	2.9873	1.45663	-0.17813
H	-4.56772	3.48553	2.58075
H	-3.84027	4.80574	1.63185
C	-4.39288	3.8652	1.57067
H	-5.34964	4.03238	1.06291
F	-1.99019	2.27478	2.52079
H	-2.68553	2.64181	1.54922
N	-3.58475	2.87774	0.83241
H	-4.47966	1.22228	1.75671
C	-4.28217	1.58305	0.74317
H	-2.60937	4.30166	-0.36899
C	-3.18416	3.38054	-0.49129
H	-5.22427	1.68663	0.1923
H	-4.07386	3.58164	-1.09992
H	-3.63711	0.86153	0.23079
H	-2.56299	2.63247	-0.99062
C	-0.6196	0.8646	-0.41289
H	-1.55063	0.29784	-0.35089
C	-0.08633	1.44721	0.79515
H	0.57056	2.31518	0.71545
C	-0.50197	1.0887	2.0901
H	-1.17026	0.23536	2.17811
C	0.28126	1.4728	3.28449
H	-0.32653	1.42326	4.18943
H	1.13294	0.78281	3.37737
H	0.69013	2.48189	3.17067
H	-0.47922	1.40896	-1.34744

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3555.709258
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3550.171106818992
ΔG_{solv} = -0.0238011

I-E_2-TS_B

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -1092.01 cm^{-1}
Zero-point correction= 0.575108 (Hartree/Particle)
Thermal correction to Energy= 0.616991
Thermal correction to Enthalpy= 0.617935
Thermal correction to Gibbs Free Energy= 0.499641
Sum of electronic and zero-point Energies= -3553.554224
Sum of electronic and thermal Energies= -3553.512341
Sum of electronic and thermal Enthalpies= -3553.511397
Sum of electronic and thermal Free Energies= -3553.629691

C	-0.10891	-2.09807	-2.1629
C	1.04283	-1.15525	-1.97317
C	2.0884	-1.8128	-1.24867
C	1.7074	-3.17942	0.82159
C	0.70024	-2.14655	1.24974
C	-0.36956	-2.11788	0.343
H	-1.06604	-1.58374	-2.29589
H	0.0601	-2.71455	-3.05974
H	1.22079	-0.369	-2.70327
H	1.40606	-4.15795	1.22818
H	2.72116	-2.9641	1.16793
H	0.61313	-1.86369	2.29693
C	0.00553	-2.93242	-0.89336
H	-0.55387	-3.87794	-0.91519
C	1.53106	-3.12415	-0.6922
H	1.93081	-3.99661	-1.22712
C	3.53167	-1.64528	-1.52425
C	4.48681	-2.46534	-0.90784
C	3.99632	-0.69248	-2.44562
C	5.84561	-2.32511	-1.16453

H	4.17275	-3.23916	-0.21323
C	5.34898	-0.53401	-2.71095
H	3.28783	-0.0709	-2.98757
C	6.25754	-1.3506	-2.05669
H	6.58325	-2.96105	-0.68334
H	5.70369	0.20767	-3.42177
C	-1.78942	-1.95685	0.73577
C	-2.82694	-1.98621	-0.20906
C	-2.15744	-1.89342	2.09037
C	-4.16345	-1.9194	0.16859
H	-2.60017	-2.07775	-1.26638
C	-3.48449	-1.81273	2.48802
H	-1.39277	-1.93268	2.86246
C	-4.47159	-1.82231	1.5149
H	-4.96245	-1.94594	-0.56679
H	-3.76152	-1.76586	3.53713
F	-5.75291	-1.74226	1.88635
F	7.5656	-1.20505	-2.30834
Ir	1.08647	-0.3151	0.01282
Cl	2.97778	-0.1856	1.73706
O	1.2553	1.89325	-2.78187
C	2.08795	1.9716	-1.87735
C	3.11818	3.15706	-2.01984
Cl	4.57376	3.04174	-0.97514
Cl	3.66269	3.26945	-3.71321
Cl	2.22051	4.65088	-1.57675
N	2.20823	1.2393	-0.79103
H	2.9873	1.45663	-0.17813
H	-4.56772	3.48553	2.58075
H	-3.84027	4.80574	1.63185
C	-4.39288	3.8652	1.57067
H	-5.34964	4.03238	1.06291
F	-1.99019	2.27478	2.52079
H	-2.68553	2.64181	1.54922
N	-3.58475	2.87774	0.83241
H	-4.47966	1.22228	1.75671
C	-4.28217	1.58305	0.74317
H	-2.60937	4.30166	-0.36899
C	-3.18416	3.38054	-0.49129
H	-5.22427	1.68663	0.1923
H	-4.07386	3.58164	-1.09992
H	-3.63711	0.86153	0.23079
H	-2.56299	2.63247	-0.99062
C	-0.6196	0.8646	-0.41289
H	-1.55063	0.29784	-0.35089
C	-0.08633	1.44721	0.79515
H	0.57056	2.31518	0.71545
C	-0.50197	1.0887	2.0901
H	-1.17026	0.23536	2.17811
C	0.28126	1.4728	3.28449
H	-0.32653	1.42326	4.18943
H	1.13294	0.78281	3.37737
H	0.69013	2.48189	3.17067
H	-0.47922	1.40896	-1.34744

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3555.709258
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3550.171106818992
ΔG_{solv} = -0.0238011

I-E$_3$-TS$_B$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -877.03 cm^{-1}

Zero-point correction= 0.576008 (Hartree/Particle)
Thermal correction to Energy= 0.617235
Thermal correction to Enthalpy= 0.618179
Thermal correction to Gibbs Free Energy= 0.502580
Sum of electronic and zero-point Energies= -3553.560080
Sum of electronic and thermal Energies= -3553.518853
Sum of electronic and thermal Enthalpies= -3553.517909
Sum of electronic and thermal Free Energies= -3553.633508

C	1.16844	-0.85494	-2.80479
C	1.51884	0.18586	-1.77986
C	2.70772	-0.20812	-1.08272
C	3.07017	-2.517	-0.15712
C	1.61969	-2.52722	0.2435
C	0.81134	-2.44869	-0.90031
H	0.10286	-0.87632	-3.05598
H	1.72337	-0.66061	-3.7359
H	1.25186	1.22663	-1.95753
H	3.38731	-3.54853	-0.37804
H	3.72392	-2.11566	0.6209
H	1.30129	-2.99237	1.17435
C	1.68006	-2.10905	-2.10575
H	1.79738	-2.9834	-2.76062
C	3.00186	-1.6705	-1.42589
H	3.87767	-1.76662	-2.08199
C	3.79328	0.71275	-0.68407
C	5.01489	0.22499	-0.19781
C	3.66333	2.10315	-0.82449
C	6.05112	1.07852	0.16058
H	5.17354	-0.84529	-0.09897
C	4.68384	2.97198	-0.46584
H	2.75115	2.52258	-1.24204
C	5.86527	2.44395	0.02922
H	6.99639	0.69774	0.53719
H	4.57928	4.04807	-0.57888
C	-0.48093	-3.14949	-1.0616
C	-1.11123	-3.23286	-2.31228
C	-1.07596	-3.83608	0.00949
C	-2.29748	-3.93592	-2.48567
H	-0.66807	-2.75536	-3.18145
C	-2.26346	-4.53585	-0.14198
H	-0.5945	-3.84187	0.98456
C	-2.86177	-4.56957	-1.3924
H	-2.78124	-4.00236	-3.45586
H	-2.7211	-5.0667	0.68768
F	-4.004	-5.24618	-1.54793
F	6.85795	3.27547	0.37379
Ir	0.93792	-0.40407	0.2066
Cl	2.32513	-0.45835	2.36947
O	-0.35476	2.80873	-0.77633
C	0.45089	2.71246	0.15464
C	0.8906	4.0919	0.78329
Cl	2.10922	3.99838	2.09484
Cl	1.55714	5.10994	-0.53301
Cl	-0.57757	4.88168	1.44245
N	0.97583	1.63136	0.68782
H	1.6428	1.7785	1.43937
H	-3.18216	3.15565	1.83855
H	-2.49475	2.75009	0.23907
C	-3.42325	2.91646	0.79815
H	-3.96891	3.7531	0.34414
F	-3.1089	0.39941	2.44375
C	-1.20084	0.14096	2.20567
H	-1.04862	1.2084	2.04222
H	-3.64205	0.92903	1.5113

N	-4.24536	1.69331	0.78335
H	-5.29324	2.18761	2.53102
C	-5.51556	1.90812	1.49755
C	-1.11221	-0.70019	1.07551
H	-3.51087	1.03187	-1.07267
C	-4.47335	1.20695	-0.58444
H	-1.31164	-1.75724	1.25041
H	-6.09744	2.7029	1.01529
H	-5.03954	1.95103	-1.15902
H	-6.09267	0.97983	1.49653
C	-1.11082	-0.20055	-0.27617
H	-5.0357	0.27037	-0.55007
H	-1.30338	0.85805	-0.45689
H	-1.47879	-0.86224	-1.05957
C	-0.96105	-0.37031	3.56881
H	-1.42162	0.27272	4.32071
H	-1.32789	-1.39571	3.67909
H	0.12929	-0.37533	3.7251

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3555.714091
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3550.180473817605
ΔG_{solv} = -0.0191866

X-ray-1

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.410787 (Hartree/Particle)
Thermal correction to Energy= 0.441457
Thermal correction to Enthalpy= 0.442401
Thermal correction to Gibbs Free Energy= 0.349352
Sum of electronic and zero-point Energies= -3138.549671
Sum of electronic and thermal Energies= -3138.519001
Sum of electronic and thermal Enthalpies= -3138.518057
Sum of electronic and thermal Free Energies= -3138.611106

C	-4.40582	9.28864	-13.87630
C	-4.59765	8.78516	-12.59327
C	-5.49718	7.62441	-12.26149
C	-5.30659	6.40599	-13.17400
C	-3.90338	6.27590	-13.73916
C	-3.50633	6.83592	-14.97725
C	-4.37444	7.69085	-15.85998
C	-5.13881	8.77895	-15.10178
C	-1.71452	9.20831	-14.91602
C	-0.96293	9.46602	-13.72242
C	-1.58975	10.00943	-12.60663
C	-0.95958	10.07123	-11.25987
C	0.65564	8.92371	-10.01009
C	1.72464	7.90508	-10.06218
C	2.43442	7.64676	-8.88566
C	3.44717	6.70143	-8.86797
C	3.73068	6.01867	-10.04277
C	3.03964	6.24623	-11.22363
C	2.03003	7.19814	-11.22946
C	-0.35669	6.17230	-14.46731
C	0.42647	4.82557	-14.23934
Cl	-2.56762	7.18520	-10.95724
Cl	0.43490	4.20571	-12.55646
Cl	2.11545	5.04968	-14.77230
Cl	-0.37751	3.60347	-15.27665
F	4.70288	5.10460	-10.03431
H	-0.94390	6.14039	-12.55646
H	-4.33905	9.42871	-11.75038
H	-3.33083	5.40945	-13.40209
H	-2.67406	6.35802	-15.49556
H	0.00397	8.98343	-13.59149
H	-2.43059	10.69133	-12.73171
H	2.17540	8.20226	-7.98837
H	4.01588	6.48178	-7.96948
H	3.29004	5.67214	-12.11193
H	1.46325	7.38448	-12.14041
H	-4.03193	10.30945	-13.94756
H	-6.54102	7.97281	-12.29328
H	-5.29299	7.33577	-11.22690
H	-5.53650	5.50016	-12.60357
H	-6.02300	6.42407	-14.00538
H	-5.32471	9.62413	-15.77337
H	-6.12857	8.41972	-14.79499
H	-1.22289	8.60787	-15.67868
H	-2.41467	9.95642	-15.28190
H	-0.63610	11.09918	-11.03903
H	-1.68106	9.78148	-10.48458
Ir	-2.62248	7.98654	-13.34602
N	-1.02902	6.64502	-13.43336
O	-0.28880	6.61804	-15.61033
O	0.15612	9.19560	-11.22878
O	0.26595	9.46960	-9.00008
H	-3.72682	8.15559	-16.61322
H	-5.07027	7.04675	-16.41879

X-ray-2

M06/6-31G(d,p)-LANL2DZ (Ir)-SMD (diethyl ether)
Zero-point correction= 0.410316 (Hartree/Particle)
Thermal correction to Energy= 0.441119
Thermal correction to Enthalpy= 0.442063
Thermal correction to Gibbs Free Energy= 0.348431
Sum of electronic and zero-point Energies= -3138.568144
Sum of electronic and thermal Energies= -3138.537341
Sum of electronic and thermal Enthalpies= -3138.536396
Sum of electronic and thermal Free Energies= -3138.630029

C	-4.39136	9.30160	-13.87390
C	-4.54012	8.81606	-12.57616
C	-5.46941	7.69572	-12.19100
C	-5.37415	6.46918	-13.10646
C	-4.00880	6.28336	-13.74361
C	-3.65149	6.81986	-15.00291
C	-4.51932	7.71000	-15.84807
C	-5.20754	8.82048	-15.05620
C	-1.70956	9.13679	-14.97471
C	-0.93696	9.37209	-13.78515
C	-1.54190	9.94474	-12.67487
C	-0.92799	10.00680	-11.32321
C	0.57460	8.80245	-10.00058
C	1.66515	7.80470	-9.98950
C	2.16875	7.41095	-8.74575
C	3.20283	6.49262	-8.66238
C	3.72385	5.98116	-9.84202
C	3.24511	6.34720	-11.09077
C	2.20418	7.26194	-11.15915
C	-0.46688	6.09437	-14.68087
C	0.69887	5.06536	-14.41863
Cl	-2.49744	7.09471	-11.04522
Cl	0.69267	4.30301	-12.79602

Cl	2.23186	5.99376	-14.62225
Cl	0.63803	3.77118	-15.63937
F	4.72620	5.10052	-9.77254
H	-0.76792	6.22841	-12.70241
H	-4.22079	9.46046	-11.75453
H	-3.45272	5.40120	-13.42403
H	-2.85733	6.31555	-15.55296
H	0.01992	8.86812	-13.65464
H	-2.36843	10.64314	-12.80674
H	1.73419	7.83829	-7.84593
H	3.60963	6.16739	-7.70908
H	3.68453	5.91176	-11.98452
H	1.80824	7.55408	-12.12951
H	-3.98174	10.30589	-13.97434
H	-6.49915	8.08560	-12.17049
H	-5.22375	7.40296	-11.16597
H	-5.60630	5.57361	-12.52025
H	-6.13261	6.51373	-13.89896
H	-5.40001	9.67313	-15.71709
H	-6.19096	8.49307	-14.69783
H	-1.24673	8.53186	-15.75220
H	-2.37753	9.91858	-15.33309
H	-0.59937	11.03608	-11.11186
H	-1.66600	9.74206	-10.55519
Ir	-2.64008	7.93982	-13.41451
N	-1.06689	6.57873	-13.60763
O	-0.65079	6.37380	-15.86269
O	0.18016	9.12256	-11.24903
O	0.09088	9.30101	-9.00814
H	-3.88293	8.15159	-16.62507
H	-5.26023	7.09448	-16.38127

6-Ir-A (TCA)

M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether)
Zero-point correction= 0.322197 (Hartree/Particle)
Thermal correction to Energy= 0.344469
Thermal correction to Enthalpy= 0.345414
Thermal correction to Gibbs Free Energy= 0.270504
Sum of electronic and zero-point Energies= -2620.065472
Sum of electronic and thermal Energies= -2620.043200
Sum of electronic and thermal Enthalpies= -2620.042256
Sum of electronic and thermal Free Energies= -2620.117166

Ir	0.38641	-0.79192	-0.02806
C	0.81751	-1.68196	-1.95788
H	1.80948	-2.13043	-1.87397
C	0.74888	-0.28679	-2.12527
H	1.70383	0.23948	-2.16939
C	-1.63987	-1.35779	-0.59696
H	-2.13496	-1.8079	0.2671
C	-1.53599	0.06244	-0.57816
H	-1.97852	0.56082	0.28949
C	-0.40827	0.42331	-2.80179
H	-0.01613	1.24712	-3.40911
H	-0.8945	-0.2637	-3.505
C	-1.41039	0.96039	-1.78403
H	-2.39497	1.12745	-2.2493
H	-1.06947	1.94197	-1.42524
C	-1.67889	-2.19619	-1.86511
H	-2.28265	-3.09061	-1.67483
H	-2.21011	-1.64949	-2.65577
C	-0.28624	-2.63598	-2.34281
H	-0.04457	-3.6049	-1.89334
H	-0.27425	-2.78418	-3.4345
Cl	0.80914	-3.19933	0.82467
C	1.56743	0.96817	0.33651
H	1.56125	1.64429	-0.52155
C	2.42093	-0.18124	0.33184
H	3.06728	-0.38608	-0.52247
H	2.8073	-0.55223	1.28254
C	1.3416	1.66932	1.65056
H	1.89027	1.13912	2.44357
C	1.73266	3.12387	1.60521
H	1.59358	3.59844	2.58132
H	2.78464	3.21047	1.31663
H	1.12661	3.65466	0.86205
O	-0.05761	1.68098	2.12867
C	-0.51953	0.52211	2.5362
C	-1.37685	0.6528	3.79294
Cl	-2.02382	-0.91311	4.32486
Cl	-0.35729	1.34771	5.08413
Cl	-2.72975	1.75741	3.4211
N	-0.25732	-0.57966	1.94781
H	-0.58682	-1.43885	2.38733

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0739305

6-Ir-B (TCA)

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.321480 (Hartree/Particle)
Thermal correction to Energy= 0.344330
Thermal correction to Enthalpy= 0.345274
Thermal correction to Gibbs Free Energy= 0.269007
Sum of electronic and zero-point Energies= -2620.048771
Sum of electronic and thermal Energies= -2620.025920
Sum of electronic and thermal Enthalpies= -2620.024976
Sum of electronic and thermal Free Energies= -2620.10124

Ir	-0.28189	-1.09423	0.36899
C	-0.13006	-2.30755	-1.37307
H	0.74588	-2.95718	-1.29253
C	0.10888	-0.96205	-1.75907
H	1.15206	-0.70097	-1.93749
C	-2.40982	-1.29979	-0.08733
H	-2.90375	-1.5414	0.8547
C	-2.01522	0.04225	-0.26398
H	-2.20587	0.71678	0.57502
C	-0.88791	-0.10701	-2.51923
H	-0.34561	0.5583	-3.20154
H	-1.51449	-0.7443	-3.15624
C	-1.74647	0.73366	-1.57077
H	-2.69511	1.02587	-2.04797
H	-1.2196	1.66938	-1.33758
C	-2.66459	-2.24787	-1.24169
H	-3.47925	-2.92925	-0.97378
H	-3.0201	-1.68366	-2.11263
C	-1.41672	-3.06356	-1.59102
H	-1.38437	-3.95725	-0.95439
H	-1.46207	-3.43115	-2.62872
Cl	-0.94006	-0.78922	2.68154
C	1.75675	-0.36278	1.27013
H	1.52131	-0.42382	2.33107

C	1.90937	-1.54438	0.57535
H	1.86166	-2.48821	1.12233
H	2.39818	-1.58517	-0.39726
C	2.2271	0.99866	0.84391
H	3.13017	1.19787	1.44317
C	2.5122	1.24136	-0.61616
H	2.96387	2.2295	-0.74099
H	3.21176	0.49586	-1.00715
H	1.58767	1.20859	-1.20187
O	1.24677	1.99661	1.21588
C	1.20793	2.39101	2.48643
C	0.16473	3.5185	2.61113
Cl	-0.0376	4.0229	4.30613
Cl	0.74534	4.92001	1.65527
Cl	-1.41128	2.97538	1.97771
N	1.94474	1.92084	3.39535
H	1.77546	2.35742	4.29838

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0549907

6-Ir-C (TCA)

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.320292 (Hartree/Particle)
Thermal correction to Energy= 0.343886
Thermal correction to Enthalpy= 0.344831
Thermal correction to Gibbs Free Energy= 0.265823
Sum of electronic and zero-point Energies= -2620.048889
Sum of electronic and thermal Energies= -2620.025295
Sum of electronic and thermal Enthalpies= -2620.024351
Sum of electronic and thermal Free Energies= -2620.103358

Ir	-1.50522	0.16639	0.701
C	-1.12458	-0.13336	-1.34964
H	-0.202	-0.71163	-1.47213
C	-0.9625	1.24963	-1.04242
H	0.06987	1.59989	-0.94149
C	-3.52412	0.02533	0.01612
H	-4.04736	-0.65936	0.68702
C	-3.26498	1.32311	0.52116
H	-3.61816	1.53105	1.53472
C	-1.97284	2.31746	-1.42689
H	-1.44716	3.25564	-1.63924
H	-2.46943	2.03609	-2.36503
C	-3.00253	2.55358	-0.31377
H	-3.94463	2.94835	-0.72627
H	-2.62043	3.327	0.36558
C	-3.64542	-0.27704	-1.46669
H	-4.40626	-1.05093	-1.61941
H	-4.01384	0.6119	-1.99465
C	-2.31106	-0.7438	-2.05571
H	-2.23062	-1.83312	-1.94339
H	-2.26572	-0.54343	-3.13813
Cl	-2.10455	-0.48166	2.96656
C	3.09536	-1.5814	-0.46376
H	2.2842	-1.00388	-0.9141
C	4.05055	-2.07895	-1.24208
H	4.03051	-1.92336	-2.31694
H	4.88033	-2.66391	-0.85149
C	3.02128	-1.75083	1.02341
H	2.16788	-2.3881	1.30593
C	4.26289	-2.28189	1.69123
H	4.13076	-2.28637	2.77606
H	4.45329	-3.30849	1.36598
H	5.13004	-1.66305	1.4403
O	2.80152	-0.42986	1.60989
C	1.63112	0.17006	1.51142
C	1.79663	1.65809	1.847
Cl	0.2752	2.50751	2.10771
Cl	2.81122	1.83355	3.30317
Cl	2.65068	2.3709	0.42916
N	0.52526	-0.34646	1.13547
H	0.61474	-1.34468	0.94435

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0596254

6-Ir-A' (TCA)

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.322081 (Hartree/Particle)
Thermal correction to Energy= 0.344336
Thermal correction to Enthalpy= 0.345280
Thermal correction to Gibbs Free Energy= 0.270934
Sum of electronic and zero-point Energies= -2620.063056
Sum of electronic and thermal Energies= -2620.040801
Sum of electronic and thermal Enthalpies= -2620.039857
Sum of electronic and thermal Free Energies= -2620.114203

Ir	0.54274	-0.56747	-0.12926
C	-0.12598	0.38361	-1.93894
H	0.22445	1.41843	-1.96531
C	-1.23885	0.14215	-1.09343
H	-1.60625	1.00923	-0.53483
C	0.59487	-2.24187	-1.504
H	1.54315	-2.76449	-1.37077
C	-0.39236	-2.44954	-0.49056
H	-0.12485	-3.14172	0.31086
C	-2.26661	-0.95052	-1.34542
H	-3.23412	-0.62325	-0.94712
H	-2.41208	-1.05469	-2.42959
C	-1.88133	-2.29821	-0.71848
H	-2.27196	-3.13078	-1.32475
H	-2.37643	-2.39441	0.25792
C	0.21282	-1.90751	-2.93476
H	0.90026	-2.40569	-3.62777
H	-0.78204	-2.31765	-3.15502
C	0.24462	-0.40161	-3.17209
H	1.26499	-0.10466	-3.44984
H	-0.39928	-0.10585	-4.01607
Cl	2.13937	-1.80909	1.30363
C	1.31872	1.40164	0.39293
H	0.68929	2.19747	-0.02449
C	2.26997	0.78196	-0.44634
H	2.38355	1.10928	-1.4775
H	3.14465	0.30224	-0.01049
C	1.52507	1.55548	1.87054
H	1.95383	0.6407	2.3015
C	2.34316	2.77388	2.22755
H	2.4223	2.8931	3.31242
H	3.34927	2.66261	1.81127
H	1.89022	3.67747	1.80352
O	0.23093	1.78652	2.52148
C	-0.71322	0.87974	2.45188
C	-1.94472	1.35866	3.24267
Cl	-3.24926	0.1435	3.22493
Cl	-1.4888	1.70602	4.92648

Cl	-2.53886	2.84674	2.44395
N	-0.6561	-0.21135	1.79954
H	-1.48511	-0.79005	1.90379

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0700636

6-Ir-B' (TCA)

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.320904 (Hartree/Particle)
Thermal correction to Energy= 0.344074
Thermal correction to Enthalpy= 0.345018
Thermal correction to Gibbs Free Energy= 0.267648
Sum of electronic and zero-point Energies= -2620.048032
Sum of electronic and thermal Energies= -2620.024861
Sum of electronic and thermal Enthalpies= -2620.023917
Sum of electronic and thermal Free Energies= -2620.101288

Ir	-0.05069	-1.12881	0.36926
C	0.22028	-0.61099	-1.68428
H	1.24518	-0.28355	-1.86312
C	-0.64294	0.33606	-1.07698
H	-0.19511	1.28942	-0.78884
C	-1.45245	-2.57602	-0.60351
H	-1.1776	-3.52699	-0.14444
C	-2.16276	-1.66352	0.18829
H	-2.44376	-1.99625	1.18962
C	-2.14166	0.38686	-1.32242
H	-2.48019	1.42562	-1.23125
H	-2.34585	0.09709	-2.36199
C	-2.94283	-0.48863	-0.34902
H	-3.87378	-0.83852	-0.82163
H	-3.25333	0.11926	0.50964
C	-1.40995	-2.50593	-2.11038
H	-1.40119	-3.52173	-2.52062
H	-2.32939	-2.03253	-2.47735
C	-0.17725	-1.74328	-2.59719
H	0.67633	-2.43439	-2.63605
H	-0.32415	-1.3777	-3.62568
Cl	-0.03213	-2.39336	2.44337
C	1.88986	-0.20994	1.10986
H	1.72576	-0.3543	2.18109
C	2.204	-1.34342	0.37224
H	2.312	-2.30278	0.87337
H	2.64442	-1.27762	-0.6213
C	2.2675	1.21122	0.78447
H	3.05982	1.48313	1.49721
C	2.71889	1.55963	-0.61232
H	3.08885	2.58888	-0.62882
H	3.5358	0.90264	-0.92677
H	1.90559	1.48641	-1.34024
O	1.13579	2.07474	1.07192
C	0.90207	2.3903	2.34183
C	-0.50587	3.0085	2.44702
Cl	-0.7024	3.88923	3.98283
Cl	-0.84375	4.12307	1.09774
Cl	-1.66377	1.63782	2.39861
N	1.68901	2.13816	3.29498
H	1.33163	2.46216	4.1909

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0564996

6-Ir-C' (TCA)

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.320245 (Hartree/Particle)
Thermal correction to Energy= 0.343799
Thermal correction to Enthalpy= 0.344743
Thermal correction to Gibbs Free Energy= 0.266018
Sum of electronic and zero-point Energies= -2620.049064
Sum of electronic and thermal Energies= -2620.025510
Sum of electronic and thermal Enthalpies= -2620.024566
Sum of electronic and thermal Free Energies= -2620.103291

Ir	-1.55711	-0.50407	0.39887
C	-0.90051	0.1751	-1.48332
H	0.15167	-0.09496	-1.62613
C	-1.15561	1.30183	-0.64726
H	-0.27546	1.7887	-0.21502
C	-3.38319	-0.74367	-0.68422
H	-3.77162	-1.73725	-0.45016
C	-3.5347	0.241	0.3236
H	-4.03285	-0.07772	1.24323
C	-2.37511	2.19478	-0.80132
H	-2.10597	3.2272	-0.55003
H	-2.68857	2.21628	-1.85316
C	-3.52475	1.7345	0.10232
H	-4.49632	2.07441	-0.29014
H	-3.41124	2.2051	1.08835
C	-3.26416	-0.41159	-2.16081
H	-3.76785	-1.18696	-2.74909
H	-3.80163	0.52165	-2.37318
C	-1.79903	-0.30602	-2.5967
H	-1.44125	-1.29917	-2.89873
H	-1.69735	0.33861	-3.48439
Cl	-2.19427	-2.18612	2.03594
C	3.42882	-0.42224	-0.38878
H	2.5255	0.11379	-0.69044
C	4.54406	-0.27022	-1.09498
H	4.5657	0.37195	-1.97081
H	5.47166	-0.77902	-0.84237
C	3.2892	-1.29261	0.82311
H	2.65083	-2.16504	0.6105
C	4.57552	-1.77463	1.44182
H	4.36391	-2.33379	2.35676
H	5.09841	-2.4386	0.74792
H	5.22659	-0.92851	1.68291
O	2.63309	-0.49993	1.86137
C	1.35065	-0.20257	1.78053
C	1.04031	0.973	2.71776
Cl	1.69438	2.42934	1.87959
Cl	-0.67779	1.1961	3.0412
Cl	1.8923	0.75808	4.2689
N	0.48115	-0.72529	1.00407
H	0.87258	-1.48145	0.44232

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0595359

(R)-6-Ir*-A

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.445778 (Hartree/Particle)
Thermal correction to Energy= 0.477857

Thermal correction to Enthalpy= 0.478802
Thermal correction to Gibbs Free Energy= 0.382362
Sum of electronic and zero-point Energies= -3278.922949
Sum of electronic and thermal Energies= -3278.890870
Sum of electronic and thermal Enthalpies= -3278.889925
Sum of electronic and thermal Free Energies= -3278.986365

C	-0.33039	-1.69799	-1.73607
C	0.63875	-0.59025	-1.43679
C	1.69847	-1.07568	-0.61547
C	1.35182	-2.50541	1.41778
C	0.16095	-1.64301	1.74447
C	-0.80917	-1.76078	0.72507
H	-1.34616	-1.3396	-1.93766
H	0.00314	-2.27131	-2.61547
H	0.80278	0.19778	-2.17152
H	1.17928	-3.52325	1.8019
H	2.28138	-2.12648	1.85181
H	-0.08113	-1.41113	2.77998
C	-0.19781	-2.51254	-0.45502
H	-0.59794	-3.53424	-0.51753
C	1.31298	-2.46553	-0.10785
H	1.89096	-3.2619	-0.59742
C	3.10766	-0.64997	-0.73395
C	4.13199	-1.36668	-0.09913
C	3.48332	0.46833	-1.49765
C	5.46324	-0.98017	-0.19496
H	3.89197	-2.25149	0.48456
C	4.80781	0.8748	-1.5974
H	2.73114	1.03525	-2.04511
C	5.7819	0.14376	-0.93718
H	6.25311	-1.53818	0.30008
H	5.09213	1.74034	-2.18998
C	-2.27025	-1.76721	0.95932
C	-3.16877	-2.10941	-0.06266
C	-2.80865	-1.48659	2.22554
C	-4.54171	-2.13262	0.15064
H	-2.79874	-2.37953	-1.04714
C	-4.1766	-1.49839	2.45602
H	-2.14824	-1.2699	3.06101
C	-5.02626	-1.81379	1.40761
H	-5.23477	-2.39967	-0.64183
H	-4.58949	-1.28233	3.43712
F	-6.34593	-1.82891	1.6213
F	7.06264	0.52783	-1.02988
Ir	0.32726	0.19978	0.5832
Cl	2.15607	0.66283	2.35097
C	-1.57275	1.20238	0.40951
H	-2.38763	0.49345	0.24905
C	-1.07069	1.35912	1.7346
H	-1.52735	0.7956	2.54601
H	-0.63435	2.31059	2.0416
C	-1.70508	2.33784	-0.56503
O	-0.70509	3.39626	-0.41861
C	0.57363	3.13828	-0.34989
C	1.3982	4.38856	-0.68412
Cl	3.11108	4.18567	-0.25623
Cl	1.24883	4.61904	-2.45574
Cl	0.74484	5.79927	0.17364
N	1.10879	2.01027	-0.09462
H	2.128	2.01896	-0.04473
C	-1.76516	1.93766	-2.02026
H	-1.99571	2.80246	-2.64955
H	-2.55206	1.18789	-2.1589
H	-0.81864	1.49882	-2.35162
H	-2.62098	2.88533	-0.30293

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6568098
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.662579791963
ΔG_{solv} = -0.0146715

(S)-6-Ir*-A

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.445263 (Hartree/Particle)
Thermal correction to Energy= 0.477632
Thermal correction to Enthalpy= 0.478576
Thermal correction to Gibbs Free Energy= 0.381196
Sum of electronic and zero-point Energies= -3278.923573
Sum of electronic and thermal Energies= -3278.891204
Sum of electronic and thermal Enthalpies= -3278.890260
Sum of electronic and thermal Free Energies= -3278.987640

C	0.41003	-1.75148	-1.73319
C	1.37637	-0.63539	-1.45296
C	2.47271	-1.11998	-0.67258
C	2.19714	-2.55728	1.36279
C	1.00188	-1.71568	1.72564
C	0.00716	-1.84376	0.73477
H	-0.61639	-1.40051	-1.89325
H	0.71674	-2.30911	-2.63195
H	1.49437	0.1682	-2.18106
H	2.05202	-3.57755	1.75209
H	3.13235	-2.16339	1.77188
H	0.78338	-1.48745	2.76706
C	0.59442	-2.57902	-0.46652
H	0.20699	-3.60563	-0.52727
C	2.11443	-2.51615	-0.16216
H	2.68563	-3.307	-0.66834
C	3.87469	-0.68748	-0.8382
C	4.92577	-1.41029	-0.25512
C	4.21746	0.44264	-1.60033
C	6.25157	-1.01977	-0.40079
H	4.71099	-2.30363	0.32559
C	5.53586	0.85283	-1.7492
H	3.44238	1.01509	-2.10807
C	6.53778	0.11434	-1.14064
H	7.06173	-1.58314	0.05366
H	5.794	1.72791	-2.33972
C	-1.44564	-1.86668	1.01094
C	-2.35967	-2.28849	0.03421
C	-1.95692	-1.53343	2.27599
C	-3.72467	-2.34498	0.28889
H	-2.00691	-2.59741	-0.94555
C	-3.3165	-1.57603	2.54643
H	-1.28006	-1.24871	3.07769
C	-4.18378	-1.97651	1.54175
H	-4.43033	-2.67627	-0.46742
H	-3.7096	-1.31831	3.52565
F	-5.49551	-2.02359	1.79579
F	7.81336	0.50133	-1.28246
Ir	1.11844	0.13397	0.5601
Cl	2.91144	0.6298	2.35821
C	-0.77972	1.08131	0.27064
H	-1.57159	0.34821	0.10084
C	-0.3593	1.32235	1.61187

H	-0.85151	0.78937	2.42269
H	0.0417	2.29772	1.89202
C	-0.83925	2.13853	-0.79677
O	0.08065	3.25525	-0.5925
C	1.36049	3.05153	-0.42165
C	2.16112	4.3337	-0.67879
Cl	3.86529	4.15303	-0.20699
Cl	2.06447	4.65913	-2.43636
Cl	1.43944	5.67787	0.2335
N	1.9057	1.94095	-0.11846
H	2.91884	1.97222	-0.00148
H	-0.57384	1.70643	-1.774
C	-2.20148	2.79287	-0.85674
H	-2.22677	3.57236	-1.62363
H	-2.96159	2.04293	-1.09405
H	-2.44295	3.23755	0.11508

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6580262
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.663614227847
ΔG_{solv} = -0.014918

(R)-6-Ir*-B

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.444002 (Hartree/Particle)
Thermal correction to Energy= 0.476745
Thermal correction to Enthalpy= 0.477690
Thermal correction to Gibbs Free Energy= 0.379560
Sum of electronic and zero-point Energies= -3278.909078
Sum of electronic and thermal Energies= -3278.876335
Sum of electronic and thermal Enthalpies= -3278.875391
Sum of electronic and thermal Free Energies= -3278.973520

C	-0.5162	-2.86565	0.60991
C	0.73386	-2.24724	1.18393
C	0.41762	-1.52105	2.34427
C	-1.57954	-0.08564	2.75655
C	-1.27929	0.49377	1.39828
C	-1.39274	-0.52111	0.39966
H	-0.50625	-2.98068	-0.47861
H	-0.66777	-3.86522	1.04605
H	1.73121	-2.63349	0.985
H	-2.66411	-0.05798	2.94304
H	-1.08959	0.42177	3.5937
H	-1.52137	1.53702	1.18952
C	-1.55672	-1.87304	1.11157
H	-2.59602	-2.22364	1.05669
C	-1.09364	-1.5078	2.53709
H	-1.39713	-2.23119	3.30579
C	1.37416	-1.26715	3.44767
C	1.5201	-0.01338	4.05661
C	2.15767	-2.33	3.91347
C	2.41087	0.17372	5.10486
H	0.96199	0.83936	3.67615
C	3.05031	-2.16093	4.96462
H	2.05573	-3.30886	3.44929
C	3.15909	-0.90768	5.54435
H	2.54106	1.14352	5.57637
H	3.65925	-2.98055	5.33495
C	-2.00036	-0.32864	-0.94139
C	-1.48554	-0.93197	-2.09507
C	-3.16407	0.44317	-1.05907
C	-2.10863	-0.77688	-3.32837
H	-0.56512	-1.51048	-2.0378
C	-3.80428	0.60333	-2.28135
H	-3.57972	0.91433	-0.16986
C	-3.26427	-0.01556	-3.39738
H	-1.70641	-1.22845	-4.23152
H	-4.70692	1.19956	-2.38186
F	-3.87448	0.13451	-4.57919
F	4.01611	-0.73281	6.55623
Ir	0.67555	-0.07188	0.67856
Cl	3.06827	-0.32977	0.36896
C	0.41945	1.69545	-0.70844
H	-0.65275	1.88088	-0.7811
C	1.1112	2.11674	0.41643
H	0.58223	2.6078	1.2313
H	2.19131	2.23705	0.40598
C	1.04814	1.39869	-2.0499
O	0.12354	1.97709	-3.00739
C	0.11722	1.46385	-4.23294
C	-0.65824	2.41817	-5.16363
Cl	-1.11182	1.59683	-6.6782
Cl	-2.13045	3.05679	-4.39337
Cl	0.45805	3.77528	-5.53042
N	0.73447	0.41715	-4.57326
H	0.601	0.19239	-5.55666
C	2.41399	2.0045	-2.27869
H	2.74117	1.80471	-3.30377
H	2.38231	3.08785	-2.11692
H	3.14203	1.5582	-1.59473
H	1.07449	0.31525	-2.236

DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.639643228945
ΔG_{solv} = -0.0132165

(S)-6-Ir*-B

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.443519 (Hartree/Particle)
Thermal correction to Energy= 0.476762
Thermal correction to Enthalpy= 0.477706
Thermal correction to Gibbs Free Energy= 0.375870
Sum of electronic and zero-point Energies= -3278.906517
Sum of electronic and thermal Energies= -3278.873274
Sum of electronic and thermal Enthalpies= -3278.872330
Sum of electronic and thermal Free Energies= -3278.974166

C	-0.49569	-3.1204	1.14985
C	0.76046	-2.30718	1.34504
C	0.55811	-1.36525	2.37144
C	-1.48419	0.01674	2.77137
C	-1.45146	0.28247	1.28995
C	-1.61535	-0.92967	0.56366
H	-0.6305	-3.52131	0.14163
H	-0.49106	-3.97923	1.83906
H	1.74877	-2.67944	1.08274
H	-2.52417	0.02918	3.13136
H	-0.91935	0.73251	3.37801
H	-1.80487	1.23839	0.90322
C	-1.54237	-2.0948	1.56319
H	-2.54037	-2.50877	1.7593
C	-0.90955	-1.38765	2.78614
H	-1.0371	-1.93685	3.72897

C	1.64211	-0.86118	3.24572
C	1.77355	0.48575	3.60898
C	2.57198	-1.7791	3.75048
C	2.79319	0.90518	4.45218
H	1.09466	1.22605	3.19411
C	3.59459	-1.3776	4.60067
H	2.48361	-2.82927	3.48051
C	3.68611	-0.03754	4.93835
H	2.91075	1.94883	4.72906
H	4.3164	-2.08412	4.99995
C	-2.35601	-1.03727	-0.7151
C	-2.0278	-1.99392	-1.68633
C	-3.43036	-0.17603	-0.97671
C	-2.73842	-2.09046	-2.87505
H	-1.17736	-2.65349	-1.53267
C	-4.14989	-0.25373	-2.16298
H	-3.71842	0.56045	-0.22956
C	-3.78977	-1.21432	-3.09438
H	-2.48281	-2.82368	-3.63454
H	-4.98508	0.40915	-2.36949
F	-4.47926	-1.30075	-4.23698
F	4.66856	0.36088	5.75334
Ir	0.4366	-0.31971	0.39836
Cl	2.75238	-0.52285	-0.27334
C	0.03605	1.38627	-0.98685
H	-1.04515	1.52508	-1.06998
C	0.71047	1.87053	0.13659
H	0.18275	2.37548	0.94352
H	1.78449	2.04619	0.0882
C	0.72766	1.25796	-2.31572
H	1.80267	1.09594	-2.1785
C	0.12986	0.21377	-3.22622
H	0.62586	0.22235	-4.20101
H	0.25128	-0.78093	-2.7826
H	-0.94317	0.39598	-3.36713
O	0.54711	2.57164	-2.92924
C	1.40609	2.93242	-3.87535
C	0.99351	4.32705	-4.39312
Cl	2.06366	4.87041	-5.70967
Cl	-0.68334	4.25312	-5.01008
Cl	1.08785	5.5039	-3.04898
N	2.38328	2.23189	-4.2588
H	2.92842	2.69097	-4.98459

DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.634536131226
ΔG_{solv} = -0.0147892

(R)-6-Ir*-C

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.443817 (Hartree/Particle)
Thermal correction to Energy= 0.477000
Thermal correction to Enthalpy= 0.477944
Thermal correction to Gibbs Free Energy= 0.378342
Sum of electronic and zero-point Energies= -3278.909186
Sum of electronic and thermal Energies= -3278.876003
Sum of electronic and thermal Enthalpies= -3278.875059
Sum of electronic and thermal Free Energies= -3278.974661

C	-0.62923	-1.26191	-2.01108
C	0.29558	-0.22723	-1.42792
C	1.49651	-0.85463	-0.96468
C	1.59344	-2.9969	0.33314
C	0.47316	-2.38857	1.14299
C	-0.64968	-2.16872	0.29818
H	-1.6912	-1.00018	-1.94231
H	-0.39406	-1.43426	-3.07271
H	0.29106	0.79181	-1.81785
H	1.48774	-4.09246	0.30117
H	2.59604	-2.77585	0.71328
H	0.37668	-2.582	2.20986
C	-0.23951	-2.45116	-1.14574
H	-0.59707	-3.42945	-1.49578
C	1.29952	-2.37433	-1.02515
H	1.83609	-2.82366	-1.87144
C	2.84057	-0.22936	-1.06367
C	3.80877	-0.37882	-0.06002
C	3.16989	0.53656	-2.18849
C	5.06603	0.19937	-0.17984
H	3.56561	-0.93217	0.84486
C	4.42427	1.12123	-2.32651
H	2.43286	0.663	-2.9794
C	5.35575	0.93556	-1.31854
H	5.82022	0.08921	0.59423
H	4.6862	1.71311	-3.19923
C	-2.07368	-2.1847	0.70005
C	-3.06374	-2.5795	-0.21029
C	-2.48211	-1.8044	1.98862
C	-4.41087	-2.58337	0.1363
H	-2.78835	-2.90211	-1.21125
C	-3.82227	-1.79746	2.34799
H	-1.73694	-1.47604	2.71099
C	-4.76977	-2.18491	1.41143
H	-5.17836	-2.89139	-0.56802
H	-4.14136	-1.49595	3.34203
F	-6.06464	-2.17529	1.75279
F	6.56785	1.4901	-1.44188
Ir	0.3684	-0.28329	0.71902
Cl	0.27154	0.04687	3.1446
C	-1.77633	3.04175	1.5612
H	-1.2843	3.98084	1.8233
C	-2.24841	2.24914	2.51754
H	-2.74946	1.3058	2.3061
H	-2.14631	2.5164	3.56553
C	-1.91725	2.7974	0.09654
O	-0.61822	3.00454	-0.59304
C	0.55679	2.79528	-0.04533
C	1.5007	3.97119	-0.3643
Cl	3.1058	3.78555	0.37821
Cl	1.68787	4.02163	-2.1439
Cl	0.76094	5.48979	0.20913
N	0.94811	1.75146	0.57755
H	1.89494	1.84781	0.9475
H	-2.49094	3.62781	-0.33807
C	-2.53223	1.49103	-0.33215
H	-3.56076	1.42863	0.04062
H	-2.55951	1.43437	-1.42497
H	-1.96238	0.63283	0.04881

DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.643341643491
ΔG_{solv} = -0.0117191

(S)-6-Ir*-C

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.444357 (Hartree/Particle)
Thermal correction to Energy= 0.477580
Thermal correction to Enthalpy= 0.478524
Thermal correction to Gibbs Free Energy= 0.378519

Sum of electronic and zero-point Energies= -3278.917601
Sum of electronic and thermal Energies= -3278.884379
Sum of electronic and thermal Enthalpies= -3278.883435
Sum of electronic and thermal Free Energies= -3278.983440

C	-0.66245	-1.16548	-1.91919
C	0.33066	-0.20211	-1.32896
C	1.50528	-0.899	-0.90593
C	1.52912	-3.08972	0.30858
C	0.45172	-2.46371	1.16165
C	-0.67768	-2.16979	0.34868
H	-1.70552	-0.85059	-1.79117
H	-0.48003	-1.30457	-2.99573
H	0.37514	0.82951	-1.68357
H	1.37072	-4.17717	0.23922
H	2.54843	-2.93171	0.6764
H	0.36584	-2.69493	2.22203
C	-0.30618	-2.40746	-1.11281
H	-0.71482	-3.35277	-1.49592
C	1.2388	-2.40423	-1.01978
H	1.73982	-2.84427	-1.89219
C	2.86959	-0.31567	-0.98368
C	3.83337	-0.53975	0.00984
C	3.21765	0.50205	-2.06557
C	5.10361	0.01507	-0.07904
H	3.57583	-1.12917	0.88711
C	4.48603	1.06234	-2.1744
H	2.48297	0.69535	-2.84549
C	5.41183	0.80281	-1.17761
H	5.85293	-0.14989	0.69005
H	4.76165	1.69329	-3.01476
C	-2.0911	-2.16991	0.78514
C	-3.11898	-2.46158	-0.1222
C	-2.44731	-1.91512	2.11935
C	-4.45216	-2.48964	0.27409
H	-2.88403	-2.69245	-1.1583
C	-3.77184	-1.93644	2.52975
H	-1.6722	-1.67075	2.84275
C	-4.75776	-2.2217	1.59652
H	-5.24912	-2.71967	-0.42732
H	-4.04998	-1.73506	3.56057
F	-6.03858	-2.23941	1.98687
F	6.63608	1.33573	-1.27178
Ir	0.41763	-0.3429	0.81447
Cl	0.28008	-0.05384	3.23379
C	-2.1613	2.95297	1.16373
H	-2.33388	4.02774	1.06983
C	-2.4176	2.302	2.29451
H	-2.23088	1.23161	2.38518
H	-2.81662	2.81101	3.16793
C	-1.67355	2.27083	-0.06877
O	-0.42771	2.93146	-0.49648
C	0.71479	2.72319	0.11401
C	1.64023	3.93249	-0.09203
Cl	3.25844	3.66305	0.59577
Cl	1.80222	4.2104	-1.85104
Cl	0.88967	5.3497	0.68658
N	1.06505	1.67476	0.75276
H	1.9886	1.75438	1.17769
H	-1.45256	1.21069	0.13419
C	-2.60669	2.41417	-1.24503
H	-3.54833	1.90385	-1.0198
H	-2.82118	3.47056	-1.44302
H	-2.17377	1.96945	-2.14742

DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.654015420317
ΔG_{solv} = -0.0119175

6-Ir-TS-[3,3]

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -427.75 cm^{-1}
Zero-point correction= 0.319741 (Hartree/Particle)
Thermal correction to Energy= 0.342242
Thermal correction to Enthalpy= 0.343186
Thermal correction to Gibbs Free Energy= 0.266446
Sum of electronic and zero-point Energies= -2620.029901
Sum of electronic and thermal Energies= -2620.007401
Sum of electronic and thermal Enthalpies= -2620.006456
Sum of electronic and thermal Free Energies= -2620.083197

Ir	-1.00279	-0.43826	-0.28101
C	0.58812	-1.26944	-1.3833
H	1.51269	-1.25944	-0.79608
C	0.20464	-0.03059	-1.97498
H	0.85175	0.82688	-1.76412
C	-2.12802	-1.9092	-1.44655
H	-2.7597	-2.43708	-0.72889
C	-2.5286	-0.60438	-1.79731
H	-3.45848	-0.24217	-1.35201
C	-0.5752	0.06507	-3.27633
H	-0.25317	0.95584	-3.82839
H	-0.3234	-0.78744	-3.92054
C	-2.08804	0.13912	-3.03539
H	-2.64089	-0.21399	-3.92057
H	-2.37431	1.19055	-2.89988
C	-1.23189	-2.77333	-2.30947
H	-1.54192	-3.82094	-2.22041
H	-1.37255	-2.50715	-3.36474
C	0.24215	-2.64131	-1.91043
H	0.45771	-3.35785	-1.10556
H	0.90037	-2.918	-2.74991
Cl	-2.74104	-0.25353	1.41441
C	0.49731	0.41635	1.04976
H	1.42952	0.59723	0.49372
C	0.52664	-0.72002	1.89423
H	1.16338	-1.57137	1.66034
H	-0.33198	-0.93019	2.52605
C	0.05602	1.65532	1.77118
H	-0.79605	1.43557	2.42772
C	-0.20203	2.8492	0.89461
H	-1.09801	2.6579	0.29404
H	-0.36116	3.75379	1.48885
H	0.64189	3.01427	0.2139
O	1.16412	2.08931	2.67018
C	1.85831	1.22089	3.35409
C	3.10019	1.90464	3.9647
Cl	3.94034	0.82581	5.10414
Cl	4.19437	2.29453	2.60309
Cl	2.62401	3.39231	4.81191
N	1.59385	-0.02365	3.44835
H	2.26189	-0.5753	3.98059

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0330304

6-Int-[3,3]

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.321876 (Hartree/Particle)
Thermal correction to Energy= 0.345184
Thermal correction to Enthalpy= 0.346129
Thermal correction to Gibbs Free Energy= 0.267714
Sum of electronic and zero-point Energies= -2620.079223
Sum of electronic and thermal Energies= -2620.055915
Sum of electronic and thermal Enthalpies= -2620.054971
Sum of electronic and thermal Free Energies= -2620.133386

Ir	-0.93434	-0.60405	-0.17726
C	0.60574	-1.31767	-1.43845
H	1.531	-1.40835	-0.86006
C	0.25157	-0.01288	-1.8721
H	0.94214	0.78051	-1.58521
C	-2.1627	-1.83493	-1.51928
H	-2.81888	-2.41837	-0.87066
C	-2.5078	-0.48341	-1.70122
H	-3.3857	-0.12683	-1.1578
C	-0.55396	0.27731	-3.12522
H	-0.19839	1.21214	-3.57333
H	-0.36798	-0.50384	-3.87318
C	-2.05244	0.40213	-2.82811
H	-2.64877	0.19395	-3.73073
H	-2.28	1.43719	-2.54373
C	-1.30745	-2.61781	-2.49551
H	-1.66121	-3.65418	-2.52902
H	-1.44211	-2.2235	-3.51024
C	0.17345	-2.60552	-2.09655
H	0.35599	-3.41728	-1.37987
H	0.81584	-2.81944	-2.96571
Cl	-2.59567	-0.88333	1.55014
C	0.61847	0.25944	1.14916
H	1.56651	0.34339	0.60437
C	0.71708	-0.54327	2.42418
H	0.95551	-1.594	2.22939
H	-0.22605	-0.50887	2.97855
C	-0.30406	1.29195	0.99241
H	-1.11288	1.34778	1.72212
C	-0.08268	2.5329	0.19667
H	-0.96545	2.81063	-0.39007
H	0.10662	3.35337	0.90396
H	0.78215	2.4668	-0.46983
O	0.60928	1.81704	3.94081
C	1.64793	1.19542	3.84539
C	2.97483	1.85941	4.32757
Cl	4.2138	0.67431	4.84541
Cl	3.58069	2.76106	2.89275
Cl	2.65508	2.98213	5.65252
N	1.79186	-0.00594	3.25992
H	2.71295	-0.41541	3.17783

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0888963

6-Ir-TS-O

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -261.64 cm^{-1}
Zero-point correction= 0.318541 (Hartree/Particle)
Thermal correction to Energy= 0.341096
Thermal correction to Enthalpy= 0.342041
Thermal correction to Gibbs Free Energy= 0.267315
Sum of electronic and zero-point Energies= -2620.013169
Sum of electronic and thermal Energies= -2619.990613
Sum of electronic and thermal Enthalpies= -2619.989669
Sum of electronic and thermal Free Energies= -2620.064395

Ir	0.31121	-0.57141	0.17375
C	0.7728	-2.28349	-1.01548
H	1.47233	-2.90435	-0.45163
C	1.30157	-1.13084	-1.64933
H	2.37289	-0.96768	-1.5151
C	-1.60327	-0.79491	-0.86413
H	-2.3735	-0.70527	-0.0983
C	-0.98577	0.41189	-1.27373
H	-1.35296	1.32429	-0.7954
C	0.70569	-0.51694	-2.90539
H	1.51712	-0.14391	-3.54026
H	0.20938	-1.30467	-3.48541
C	-0.26409	0.62012	-2.58406
H	-0.98532	0.76633	-3.40324
H	0.30155	1.5595	-2.50926
C	-1.66101	-2.04734	-1.72018
H	-2.59292	-2.58102	-1.50383
H	-1.72053	-1.76771	-2.77992
C	-0.47808	-2.99423	-1.46947
H	-0.74757	-3.70768	-0.68411
H	-0.24852	-3.58785	-2.36855
Cl	-0.47105	-2.31789	1.79772
C	1.97107	0.79563	0.44187
H	2.40366	1.0472	-0.52844
C	2.23811	-0.42882	1.13896
H	2.98148	-1.11599	0.73462
H	2.12034	-0.44215	2.22211
C	1.30259	1.86457	1.12251
O	-0.5242	0.97497	1.53734
C	-0.66594	0.87163	2.83726
C	-2.11978	1.24205	3.23868
Cl	-2.43758	0.95502	4.97154
Cl	-2.32224	2.99965	2.89817
Cl	-3.30532	0.31954	2.28496
N	0.27414	0.63799	3.65706
H	-0.04372	0.64539	4.62367
H	1.39998	1.9017	2.20994
C	0.87923	3.09241	0.43232
H	-0.03112	3.49657	0.88745
H	1.66761	3.8453	0.57699
H	0.73175	2.94242	-0.64166

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0234331

6-Int-O

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.320595 (Hartree/Particle)
Thermal correction to Energy= 0.343650
Thermal correction to Enthalpy= 0.344594
Thermal correction to Gibbs Free Energy= 0.268695
Sum of electronic and zero-point Energies= -2620.040962
Sum of electronic and thermal Energies= -2620.017907

Sum of electronic and thermal Enthalpies= -2620.016963
Sum of electronic and thermal Free Energies= -2620.092862

Ir	0.29425	-0.42364	0.3062
C	0.99171	-1.88616	-1.15434
H	1.82065	-2.43091	-0.69734
C	1.25711	-0.61268	-1.68995
H	2.28265	-0.25915	-1.6123
C	-1.58856	-0.8149	-0.6966
H	-2.28636	-0.92078	0.13376
C	-1.21158	0.50579	-1.02119
H	-1.65585	1.30042	-0.41858
C	0.46328	-0.00848	-2.83515
H	1.1518	0.55141	-3.47823
H	0.0683	-0.82072	-3.45729
C	-0.65819	0.91252	-2.36044
H	-1.47693	0.94338	-3.09542
H	-0.2843	1.93867	-2.28849
C	-1.51049	-1.98551	-1.65951
H	-2.30986	-2.68952	-1.40695
H	-1.7334	-1.63193	-2.67465
C	-0.1657	-2.73407	-1.62286
H	-0.24789	-3.58608	-0.944
H	0.07828	-3.14012	-2.61671
Cl	-0.28619	-2.53578	1.54955
C	2.33035	0.4707	0.81107
H	3.12228	0.28952	0.08331
C	2.0671	-0.49351	1.77905
H	2.65617	-1.40813	1.77433
H	1.49679	-0.26183	2.68155
C	1.39079	1.51325	0.54351
O	-0.98999	0.46415	1.73696
C	-0.9849	0.64003	3.00849
C	-2.41524	1.11931	3.43171
Cl	-2.5396	1.49836	5.17545
Cl	-2.83657	2.59884	2.50615
Cl	-3.59553	-0.17201	3.04823
N	-0.02003	0.48845	3.83033
H	-0.29379	0.70312	4.78527
H	0.81749	1.8771	1.39836
C	1.64504	2.53569	-0.51542
H	0.72415	3.05922	-0.7894
H	2.33821	3.29452	-0.12859
H	2.09452	2.11148	-1.41992

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0566934

6-Ir-TS

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -140.88 cm^{-1}
Zero-point correction= 0.318772 (Hartree/Particle)
Thermal correction to Energy= 0.341502
Thermal correction to Enthalpy= 0.342447
Thermal correction to Gibbs Free Energy= 0.266861
Sum of electronic and zero-point Energies= -2620.043161
Sum of electronic and thermal Energies= -2620.020430
Sum of electronic and thermal Enthalpies= -2620.019486
Sum of electronic and thermal Free Energies= -2620.095071

Ir	0.31663	-0.76807	0.00743
C	0.68121	-1.74354	-1.95039
H	1.58513	-2.34104	-1.81942
C	0.84859	-0.36612	-2.11946
H	1.88243	-0.01771	-2.13203
C	-1.74665	-1.06416	-0.66341
H	-2.3034	-1.45809	0.18896
C	-1.4463	0.32364	-0.62426
H	-1.82587	0.88098	0.23349
C	-0.15706	0.5397	-2.80535
H	0.38561	1.32377	-3.34567
H	-0.69054	-0.03522	-3.57262
C	-1.14139	1.18575	-1.82543
H	-2.07203	1.46806	-2.34276
H	-0.7097	2.12318	-1.44741
C	-1.86114	-1.86042	-1.95005
H	-2.6239	-2.63654	-1.8227
H	-2.23524	-1.20867	-2.75022
C	-0.54122	-2.52437	-2.35758
H	-0.4712	-3.50828	-1.88198
H	-0.50839	-2.69864	-3.44468
Cl	0.49659	-3.16829	0.76512
C	1.90387	0.79873	0.34969
H	2.05544	1.33436	-0.5886
C	2.3676	-0.5658	0.49617
H	3.04861	-0.95135	-0.26426
H	2.57797	-0.92938	1.50392
C	1.66123	1.62693	1.45922
H	1.79229	1.19602	2.45154
C	1.66207	3.09584	1.32908
H	1.18416	3.58667	2.1774
H	2.7099	3.4275	1.28304
H	1.18224	3.40579	0.39442
O	-0.42643	1.66213	2.22819
C	-0.67543	0.49835	2.5999
C	-1.28754	0.37938	4.02623
Cl	0.03053	0.79836	5.17292
Cl	-2.61925	1.551	4.20132
Cl	-1.90703	-1.24769	4.4279
N	-0.3765	-0.59558	1.95095
H	-0.58775	-1.48533	2.3944

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0564027

6-Ir-D

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.320591 (Hartree/Particle)
Thermal correction to Energy= 0.343934
Thermal correction to Enthalpy= 0.344878
Thermal correction to Gibbs Free Energy= 0.267845
Sum of electronic and zero-point Energies= -2620.072738
Sum of electronic and thermal Energies= -2620.049396
Sum of electronic and thermal Enthalpies= -2620.048451
Sum of electronic and thermal Free Energies= -2620.125485

Ir	-0.03558	-0.14778	0.24763
C	-0.40996	1.00589	-1.56037
H	0.19434	1.90765	-1.45942
C	-1.59657	0.93128	-0.78837
H	-1.807	1.79138	-0.15179
C	-0.3355	-1.80217	-1.27014
H	0.48927	-2.50097	-1.13217

C	-1.36894	-1.86214	-0.33878
H	-1.27845	-2.58323	0.47549
C	-2.7979	0.08205	-1.16518
H	-3.7023	0.58341	-0.80516
H	-2.88646	0.05735	-2.25909
C	-2.76009	-1.34067	-0.5882
H	-3.28285	-2.04297	-1.25576
H	-3.29493	-1.35803	0.36542
C	-0.50785	-1.26713	-2.67822
H	0.11206	-1.86182	-3.35795
H	-1.54533	-1.43404	-2.99343
C	-0.13525	0.21095	-2.80726
H	0.9339	0.30406	-3.03409
H	-0.66256	0.67152	-3.65681
Cl	-1.60918	-0.18496	2.21857
C	2.04328	-0.67371	0.96501
H	2.39175	0.07071	1.68245
C	1.34367	-1.76849	1.45069
H	1.15827	-2.61304	0.78583
C	2.01655	-0.33659	-0.43287
O	1.92589	2.74704	-0.2464
C	1.29212	2.62632	0.79902
C	1.55242	3.73134	1.8945
Cl	0.17879	3.99134	3.01895
Cl	2.97206	3.15184	2.83984
Cl	1.9512	5.28147	1.12769
N	0.48508	1.64923	1.17232
H	0.04426	1.73731	2.08262
H	2.12076	-1.13126	-1.16992
H	2.45112	0.62002	-0.7175
C	1.13141	-2.00821	2.9026
H	0.111	-2.35495	3.09841
H	1.82034	-2.78507	3.25844
H	1.29717	-1.09492	3.48344

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0883548

6-Ir-TS-N

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -140.88 cm^{-1}
Zero-point correction= 0.318772 (Hartree/Particle)
Thermal correction to Energy= 0.341502
Thermal correction to Enthalpy= 0.342447
Thermal correction to Gibbs Free Energy= 0.266861
Sum of electronic and zero-point Energies= -2620.043161
Sum of electronic and thermal Energies= -2620.020430
Sum of electronic and thermal Enthalpies= -2620.019486
Sum of electronic and thermal Free Energies= -2620.095071

Ir	0.31663	-0.76807	0.00743
C	0.68121	-1.74354	-1.95039
H	1.58513	-2.34104	-1.81942
C	0.84859	-0.36612	-2.11946
H	1.88243	-0.01771	-2.13203
C	-1.74665	-1.06416	-0.66341
H	-2.3034	-1.45809	0.18896
C	-1.4463	0.32364	-0.62426
H	-1.82587	0.88098	0.23349
C	-0.15706	0.5397	-2.80535
H	0.38561	1.32377	-3.34567
H	-0.69054	-0.03522	-3.57262
C	-1.14139	1.18575	-1.82543
H	-2.07203	1.46806	-2.34276
H	-0.7097	2.12318	-1.44741
C	-1.86114	-1.86042	-1.95005
H	-2.6239	-2.63654	-1.8227
H	-2.23524	-1.20867	-2.75022
C	-0.54122	-2.52437	-2.35758
H	-0.4712	-3.50828	-1.88198
H	-0.50839	-2.69864	-3.44468
Cl	0.49659	-3.16829	0.76512
C	1.90387	0.79873	0.34969
H	2.05544	1.33436	-0.5886
C	2.3676	-0.5658	0.49617
H	3.04861	-0.95135	-0.26426
H	2.57797	-0.92938	1.50392
C	1.66123	1.62693	1.45922
H	1.79229	1.19602	2.45154
C	1.66207	3.09584	1.32908
H	1.18416	3.58667	2.1774
H	2.7099	3.4275	1.28304
H	1.18224	3.40579	0.39442
O	-0.42643	1.66213	2.22819
C	-0.67543	0.49835	2.5999
C	-1.28754	0.37938	4.02623
Cl	0.03053	0.79836	5.17292
Cl	-2.61925	1.551	4.20132
Cl	-1.90703	-1.24769	4.4279
N	-0.3765	-0.59558	1.95095
H	-0.58775	-1.48533	2.3944

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0564027

6-Ir-A, $NHCCl_3$

M06/6-31G(d,p)-LANL2DZ(Ir)-CPCM(diethyl ether)
Zero-point correction= 0.322197 (Hartree/Particle)
Thermal correction to Energy= 0.344469
Thermal correction to Enthalpy= 0.345414
Thermal correction to Gibbs Free Energy= 0.270504
Sum of electronic and zero-point Energies= -2620.065472
Sum of electronic and thermal Energies= -2620.043200
Sum of electronic and thermal Enthalpies= -2620.042256
Sum of electronic and thermal Free Energies= -2620.117166

Ir	0.38641	-0.79192	-0.02806
C	0.81751	-1.68196	-1.95788
H	1.80948	-2.13043	-1.87397
C	0.74888	-0.28679	-2.12527
H	1.70383	0.23948	-2.16939
C	-1.63987	-1.35779	-0.59696
H	-2.13496	-1.8079	0.2671
C	-1.53599	0.06244	-0.57816
H	-1.97852	0.56082	0.28949
C	-0.40827	0.42331	-2.80179
H	-0.01613	1.24712	-3.40911
H	-0.8945	-0.2637	-3.505
C	-1.41039	0.96039	-1.78403
H	-2.39497	1.12745	-2.2493
H	-1.06947	1.94197	-1.42524
C	-1.67889	-2.19619	-1.86511
H	-2.28265	-3.09061	-1.67483
H	-2.21011	-1.64949	-2.65577
C	-0.28624	-2.63598	-2.34281
H	-0.04457	-3.6049	-1.89334

H	-0.27425	-2.78418	-3.4345
Cl	0.80914	-3.19933	0.82467
C	1.56743	0.96817	0.33651
H	1.56125	1.64429	-0.52155
C	2.42093	-0.18124	0.33184
H	3.06728	-0.38608	-0.52247
H	2.8073	-0.55223	1.28254
C	1.3416	1.66932	1.65056
H	1.89027	1.13912	2.44357
C	1.73266	3.12387	1.60521
H	1.59358	3.59844	2.58132
H	2.78464	3.21047	1.31663
H	1.12661	3.65466	0.86205
O	-0.05761	1.68098	2.12867
C	-0.51953	0.52211	2.5362
C	-1.37685	0.6528	3.79294
Cl	-2.02382	-0.91311	4.32486
Cl	-0.35729	1.34771	5.08413
Cl	-2.72975	1.75741	3.4211
N	-0.25732	-0.57966	1.94781
H	-0.58682	-1.43885	2.38733

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0739305
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2617.33746919552
ΔG_{solv} = -0.0121938

6-Ir-B, $NHCCl_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.321480 (Hartree/Particle)
Thermal correction to Energy= 0.344330
Thermal correction to Enthalpy= 0.345274
Thermal correction to Gibbs Free Energy= 0.269007
Sum of electronic and zero-point Energies= -2620.048771
Sum of electronic and thermal Energies= -2620.025920
Sum of electronic and thermal Enthalpies= -2620.024976
Sum of electronic and thermal Free Energies= -2620.10124

Ir	-0.28189	-1.09423	0.36899
C	-0.13006	-2.30755	-1.37307
H	0.74588	-2.95718	-1.29253
C	0.10888	-0.96205	-1.75907
H	1.15206	-0.70097	-1.93749
C	-2.40982	-1.29979	-0.08733
H	-2.90375	-1.5414	0.8547
C	-2.01522	0.04225	-0.26398
H	-2.20587	0.71678	0.57502
C	-0.88791	-0.10701	-2.51923
H	-0.34561	0.5583	-3.20154
H	-1.51449	-0.7443	-3.15624
C	-1.74647	0.73366	-1.57077
H	-2.69511	1.02587	-2.04797
H	-1.2196	1.66938	-1.33758
C	-2.66459	-2.24787	-1.24169
H	-3.47925	-2.92925	-0.97378
H	-3.0201	-1.68366	-2.11263
C	-1.41672	-3.06356	-1.59102
H	-1.38437	-3.95725	-0.95439
H	-1.46207	-3.43115	-2.62872
Cl	-0.94006	-0.78922	2.68154
C	1.75675	-0.36278	1.27013
H	1.52131	-0.42382	2.33107
C	1.90937	-1.54438	0.57535
H	1.86166	-2.48821	1.12233
H	2.39818	-1.58517	-0.39726
C	2.2271	0.99866	0.84391
H	3.13017	1.19787	1.44317
C	2.5122	1.24136	-0.61616
H	2.96387	2.2295	-0.74099
H	3.21176	0.49586	-1.00715
H	1.58767	1.20859	-1.20187
O	1.24677	1.99661	1.21588
C	1.20793	2.39101	2.48643
C	0.16473	3.5185	2.61113
Cl	-0.0376	4.0229	4.30613
Cl	0.74534	4.92001	1.65527
Cl	-1.41128	2.97538	1.97771
N	1.94474	1.92084	3.39535
H	1.77546	2.35742	4.29838

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0549907
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2617.30956607119
ΔG_{solv} = -0.0111192

6-Ir-C, $NHCCl_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.320292 (Hartree/Particle)
Thermal correction to Energy= 0.343886
Thermal correction to Enthalpy= 0.344831
Thermal correction to Gibbs Free Energy= 0.265823
Sum of electronic and zero-point Energies= -2620.048889
Sum of electronic and thermal Energies= -2620.025295
Sum of electronic and thermal Enthalpies= -2620.024351
Sum of electronic and thermal Free Energies= -2620.103358

Ir	-1.50522	0.16639	0.701
C	-1.12458	-0.13336	-1.34964
H	-0.202	-0.71163	-1.47213
C	-0.9625	1.24963	-1.04242
H	0.06987	1.59989	-0.94149
C	-3.52412	0.02533	0.01612
H	-4.04736	-0.65936	0.68702
C	-3.26498	1.32311	0.52116
H	-3.61816	1.53105	1.53472
C	-1.97284	2.31746	-1.42689
H	-1.44716	3.25564	-1.63924
H	-2.46943	2.03609	-2.36503
C	-3.00253	2.55358	-0.31377
H	-3.94463	2.94835	-0.72627
H	-2.62043	3.327	0.36558
C	-3.64542	-0.27704	-1.46669
H	-4.40626	-1.05093	-1.61941
H	-4.01384	0.6119	-1.99465
C	-2.31106	-0.7438	-2.05571
H	-2.23062	-1.83312	-1.94339
H	-2.26572	-0.54343	-3.13813
Cl	-2.10455	-0.48166	2.96656
C	3.09536	-1.5814	-0.46376
H	2.2842	-1.00388	-0.9141

C	4.05055	-2.07895	-1.24208
H	4.03051	-1.92336	-2.31694
H	4.88033	-2.66391	-0.85149
C	3.02128	-1.75083	1.02341
H	2.16788	-2.3881	1.30593
C	4.26289	-2.28189	1.69123
H	4.13076	-2.28637	2.77606
H	4.45329	-3.30849	1.36598
H	5.13004	-1.66305	1.4403
O	2.80152	-0.42986	1.60989
C	1.63112	0.17006	1.51142
C	1.79663	1.65809	1.847
Cl	0.2752	2.50751	2.10771
Cl	2.81122	1.83355	3.30317
Cl	2.65068	2.3709	0.42916
N	0.52526	-0.34646	1.13547
H	0.61474	-1.34468	0.94435

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2621.0596254
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -2617.31015404877
ΔG_{solv} = -0.0152828

6-Ir-A, $COOCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.343848 (Hartree/Particle)
Thermal correction to Energy= 0.363719
Thermal correction to Enthalpy= 0.364663
Thermal correction to Gibbs Free Energy= 0.296763
Sum of electronic and zero-point Energies= -1336.444580
Sum of electronic and thermal Energies= -1336.424709
Sum of electronic and thermal Enthalpies= -1336.423765
Sum of electronic and thermal Free Energies= -1336.491665

Ir	0.55143	-0.68935	-0.07915
C	0.87281	-1.46371	-2.02148
H	1.9063	-1.81213	-2.08228
C	0.65517	-0.06136	-2.12253
H	1.55255	0.5464	-2.25537
C	-1.44628	-1.43714	-0.45023
H	-1.78508	-1.96313	0.44499
C	-1.48344	-0.01383	-0.39424
H	-1.88307	0.41964	0.52758
C	-0.61597	0.54978	-2.68591
H	-0.35769	1.43959	-3.27112
H	-1.0703	-0.15388	-3.39475
C	-1.59055	0.92063	-1.5734
H	-2.62622	0.96523	-1.94574
H	-1.35044	1.92896	-1.20892
C	-1.53961	-2.22764	-1.74528
H	-2.03848	-3.18196	-1.54363
H	-2.18988	-1.70027	-2.45622
C	-0.16262	-2.50746	-2.3647
H	0.21155	-3.46494	-1.98666
H	-0.23096	-2.60728	-3.45983
Cl	1.31153	-3.00296	0.69584
C	1.67787	1.12478	0.26756
H	1.54938	1.8546	-0.53594
C	2.58298	0.03538	0.1151
H	3.14005	-0.09666	-0.8129
H	3.07595	-0.37467	0.99724
C	1.53943	1.71101	1.65009
H	2.06144	1.06503	2.36846
C	2.06645	3.12347	1.71432
H	1.99666	3.5254	2.72917
H	3.11519	3.13422	1.40219
H	1.49848	3.77133	1.03733
O	0.1576	1.80121	2.13514
C	-0.39645	0.65784	2.44792
O	-1.4428	0.83865	3.21921
O	-0.00555	-0.4562	2.08341
C	-2.18434	-0.34086	3.56952
H	-3.03237	0.01219	4.15388
H	-1.5624	-1.01425	4.16313
H	-2.52827	-0.85572	2.66819

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.3495129
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1239.98297586214
ΔG_{solv} = -0.0144487

6-Ir-B, $COOCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.341920 (Hartree/Particle)
Thermal correction to Energy= 0.362849
Thermal correction to Enthalpy= 0.363793
Thermal correction to Gibbs Free Energy= 0.292278
Sum of electronic and zero-point Energies= -1336.448522
Sum of electronic and thermal Energies= -1336.427593
Sum of electronic and thermal Enthalpies= -1336.426649
Sum of electronic and thermal Free Energies= -1336.498164

Ir	-0.10889	-1.36892	0.48981
C	-0.14567	-1.7923	-1.58186
H	0.76238	-2.3317	-1.86753
C	-0.02693	-0.38689	-1.41422
H	0.96624	0.03191	-1.57096
C	-2.26703	-1.58786	0.25036
H	-2.58251	-2.22994	1.07499
C	-1.9936	-0.24393	0.56086
H	-2.08006	0.04878	1.61034
C	-1.15412	0.59528	-1.67939
H	-0.72493	1.53584	-2.04406
H	-1.78452	0.21529	-2.49435
C	-1.99625	0.88563	-0.43076
H	-3.03536	1.12309	-0.70984
H	-1.60376	1.77695	0.06993
C	-2.63651	-2.04058	-1.14842
H	-3.36975	-2.85173	-1.08093
H	-3.14183	-1.22333	-1.67883
C	-1.41543	-2.52621	-1.93781
H	-1.24944	-3.58987	-1.72164
H	-1.6002	-2.46165	-3.02196
Cl	-0.33592	-1.93753	2.83196
C	2.01494	-0.61972	1.14426
H	1.80242	-0.61281	2.21149
C	2.07821	-1.83492	0.49217
H	2.01843	-2.76219	1.06539
H	2.50664	-1.91784	-0.50596
C	2.60872	0.67388	0.6318

H	3.2253	1.05202	1.46124
C	3.46625	0.58041	-0.60704
H	3.87114	1.56783	-0.84625
H	4.303	-0.10156	-0.42777
H	2.91381	0.21925	-1.48051
O	1.60767	1.67898	0.36517
C	0.98946	2.17671	1.43558
O	0.14184	3.11576	1.01785
O	1.17179	1.84957	2.58456
C	-0.64635	3.708	2.05214
H	-1.23911	4.48364	1.56762
H	-0.00693	4.14295	2.82456
H	-1.30315	2.95968	2.50797

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.3556051
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1334.959475456219
ΔG_{solv} = -0.0127336

6-Ir-C, $COOCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.342209 (Hartree/Particle)
Thermal correction to Energy= 0.363237
Thermal correction to Enthalpy= 0.364181
Thermal correction to Gibbs Free Energy= 0.291315
Sum of electronic and zero-point Energies= -1336.441399
Sum of electronic and thermal Energies= -1336.420371
Sum of electronic and thermal Enthalpies= -1336.419427
Sum of electronic and thermal Free Energies= -1336.492292

Ir	-1.00466	0.48199	0.1966
C	-1.40687	0.12311	-1.83057
H	-0.48156	-0.22441	-2.30116
C	-1.5031	1.52213	-1.57936
H	-0.64054	2.12776	-1.87092
C	-2.98231	-0.19099	0.41535
H	-3.01921	-0.91227	1.236
C	-2.87702	1.18334	0.78987
H	-2.84818	1.38955	1.86381
C	-2.82803	2.26084	-1.49969
H	-2.71041	3.26984	-1.91127
H	-3.56836	1.76387	-2.13957
C	-3.32918	2.35167	-0.0533
H	-4.42554	2.45385	-0.01852
H	-2.9242	3.26092	0.41
C	-3.62387	-0.64683	-0.88566
H	-4.1415	-1.59914	-0.72371
H	-4.40095	0.06992	-1.18059
C	-2.58253	-0.81151	-1.99889
H	-2.18845	-1.83577	-1.97162
H	-3.04428	-0.68786	-2.99141
Cl	-0.3582	-0.04189	2.48574
C	3.3191	-1.79277	-0.73787
H	3.03443	-1.0735	-1.50683
C	4.23229	-2.72149	-1.0031
H	4.70491	-2.77683	-1.98005
H	4.54159	-3.46685	-0.27363
C	2.58563	-1.64382	0.5568
H	1.50473	-1.74446	0.38503
C	3.02496	-2.52986	1.69134
H	2.45278	-2.28808	2.59172
H	2.84056	-3.57853	1.4401
H	4.09157	-2.40006	1.90312
O	2.79336	-0.26646	1.03502
C	1.98091	0.65711	0.59357
O	2.13031	1.83653	1.14253
O	1.1504	0.48466	-0.30726
C	2.97724	1.96433	2.29589
H	2.8987	3.00741	2.59856
H	4.01091	1.7175	2.0432
H	2.61458	1.30702	3.09072

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.349625
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1334.958375760837
ΔG_{solv} = -0.0110629

6-Ir-A, $COCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.337742 (Hartree/Particle)
Thermal correction to Energy= 0.356871
Thermal correction to Enthalpy= 0.357815
Thermal correction to Gibbs Free Energy= 0.291365
Sum of electronic and zero-point Energies= -1261.257023
Sum of electronic and thermal Energies= -1261.237895
Sum of electronic and thermal Enthalpies= -1261.236950
Sum of electronic and thermal Free Energies= -1261.303400

Ir	0.43634	-0.80527	0.03086
C	0.79166	-1.64589	-1.88346
H	1.81355	-2.03136	-1.89763
C	0.62716	-0.24214	-2.03115
H	1.54776	0.33286	-2.14877
C	-1.57162	-1.49635	-0.38184
H	-1.96175	-1.9758	0.51836
C	-1.55846	-0.07086	-0.37248
H	-1.97192	0.40106	0.5234
C	-0.6055	0.39206	-2.65162
H	-0.30092	1.25469	-3.25512
H	-1.06186	-0.31817	-3.35271
C	-1.60226	0.82707	-1.58263
H	-2.62428	0.88651	-1.98942
H	-1.34704	1.84074	-1.24469
C	-1.65261	-2.32352	-1.65486
H	-2.18385	-3.25684	-1.43793
H	-2.26959	-1.80109	-2.39865
C	-0.26969	-2.66212	-2.2313
H	0.06253	-3.62343	-1.82521
H	-0.31348	-2.78239	-3.3257
Cl	1.12086	-3.12612	0.8656
C	1.58986	0.98535	0.37574
H	1.4973	1.70695	-0.44
C	2.47764	-0.12437	0.26318
H	3.05787	-0.28219	-0.6464
H	2.93866	-0.52855	1.16504
C	1.43397	1.58644	1.74927
H	1.9416	0.9387	2.47682
C	1.97616	2.99413	1.80852
H	1.89843	3.40564	2.81904
H	3.02854	2.9926	1.50856

H	1.42289	3.64264	1.11993
O	0.05469	1.69619	2.2404
C	-0.55212	0.5745	2.55215
C	-1.71004	0.75309	3.46917
O	-0.19797	-0.5367	2.14358
H	-2.34148	-0.13605	3.45326
H	-2.28105	1.64035	3.18178
H	-1.33998	0.91762	4.48688

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1048137
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1259.830870530434
ΔG_{solv} = -0.016478

6-Ir-B, $COCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.337810 (Hartree/Particle)
Thermal correction to Energy= 0.357280
Thermal correction to Enthalpy= 0.358224
Thermal correction to Gibbs Free Energy= 0.290673
Sum of electronic and zero-point Energies= -1261.260829
Sum of electronic and thermal Energies= -1261.241359
Sum of electronic and thermal Enthalpies= -1261.240415
Sum of electronic and thermal Free Energies= -1261.307966

Ir	-0.19766	-0.92866	0.47575
C	-0.12888	-2.24528	-1.19541
H	0.72072	-2.92581	-1.09314
C	0.1581	-0.93449	-1.66119
H	1.20726	-0.72789	-1.87278
C	-2.34047	-1.06736	0.06489
H	-2.82767	-1.2332	1.02638
C	-1.88813	0.24356	-0.19386
H	-2.03293	0.97327	0.60745
C	-0.81304	-0.08135	-2.45518
H	-0.25296	0.52058	-3.18055
H	-1.47621	-0.72344	-3.04778
C	-1.61746	0.84775	-1.54321
H	-2.56287	1.15189	-2.01917
H	-1.0479	1.77165	-1.37452
C	-2.65552	-2.06806	-1.02888
H	-3.49321	-2.69719	-0.70863
H	-3.00385	-1.54225	-1.92642
C	-1.44983	-2.95651	-1.34753
H	-1.4429	-3.80979	-0.65706
H	-1.53058	-3.38457	-2.35955
Cl	-0.84248	-0.42884	2.76443
C	1.87593	-0.26241	1.33601
H	1.69243	-0.32028	2.40707
C	1.99277	-1.44233	0.63369
H	1.95575	-2.38722	1.17881
H	2.4445	-1.48405	-0.35626
C	2.29854	1.11062	0.8895
H	3.1969	1.34953	1.48046
C	2.57372	1.33001	-0.57671
H	2.98128	2.33397	-0.7263
H	3.30656	0.60728	-0.95022
H	1.65349	1.24133	-1.16443
O	1.2782	2.06352	1.25566
C	1.19925	2.40984	2.55469
C	0.00151	3.2694	2.79906
O	1.98913	2.04129	3.39425
H	-0.11588	4.01874	2.01207
H	0.0774	3.74586	3.77734
H	-0.88305	2.62092	2.78127

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1101721
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1259.832225914851
ΔG_{solv} = -0.0113795

6-Ir-C, $COCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.335490 (Hartree/Particle)
Thermal correction to Energy= 0.356057
Thermal correction to Enthalpy= 0.357002
Thermal correction to Gibbs Free Energy= 0.285418
Sum of electronic and zero-point Energies= -1261.257915
Sum of electronic and thermal Energies= -1261.237348
Sum of electronic and thermal Enthalpies= -1261.236403
Sum of electronic and thermal Free Energies= -1261.307987

Ir	-0.72166	0.79771	0.61707
C	-0.68719	0.27369	-1.42156
H	0.35633	0.22276	-1.75006
C	-1.24222	1.57761	-1.28776
H	-0.57175	2.41229	-1.51051
C	-2.4155	-0.44799	0.60954
H	-2.346	-1.12108	1.46777
C	-2.79064	0.89809	0.89986
H	-2.98849	1.12787	1.95069
C	-2.72537	1.87168	-1.43571
H	-2.85804	2.85375	-1.90387
H	-3.17749	1.14913	-2.12691
C	-3.437	1.85005	-0.07769
H	-4.50757	1.61849	-0.19497
H	-3.38926	2.85233	0.36788
C	-2.67833	-1.11936	-0.72884
H	-2.91119	-2.17778	-0.56616
H	-3.57347	-0.68226	-1.1902
C	-1.46931	-0.99536	-1.6623
H	-0.78254	-1.83359	-1.47643
H	-1.77436	-1.07693	-2.71745
Cl	-0.31561	0.54615	2.99179
C	2.58142	-1.3046	-0.84172
H	2.59862	-0.36773	-1.40277
C	2.9374	-2.43777	-1.43978
H	3.24292	-2.44963	-2.48227
H	2.93482	-3.39464	-0.92191
C	2.10333	-1.18876	0.57029
H	1.02843	-0.93241	0.57342
C	2.34069	-2.38192	1.45795
H	1.99946	-2.16099	2.47347
H	1.77411	-3.24188	1.08824
H	3.40322	-2.64632	1.48626
O	2.8192	-0.07598	1.19489
C	2.37893	1.15668	1.09522
C	3.23601	2.14449	1.80503
O	1.35822	1.5001	0.49208
H	3.23723	3.09126	1.26174

H	4.25084	1.77124	1.9481
H	2.7818	2.32161	2.78757

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1086777
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1259.831250951304
ΔG_{solv} = -0.0110629

6-Ir-A, $NHCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.350845 (Hartree/Particle)
Thermal correction to Energy= 0.369809
Thermal correction to Enthalpy= 0.370753
Thermal correction to Gibbs Free Energy= 0.304832
Sum of electronic and zero-point Energies= -1241.376821
Sum of electronic and thermal Energies= -1241.357856
Sum of electronic and thermal Enthalpies= -1241.356912
Sum of electronic and thermal Free Energies= -1241.422834

Ir	0.39883	-0.78322	-0.0312
C	0.81983	-1.67533	-1.96042
H	1.81559	-2.11773	-1.88853
C	0.73991	-0.28093	-2.1313
H	1.69035	0.25276	-2.18648
C	-1.62337	-1.36343	-0.57271
H	-2.10977	-1.81103	0.29764
C	-1.52656	0.05867	-0.56379
H	-1.96077	0.56007	0.30533
C	-0.42811	0.41664	-2.80231
H	-0.04846	1.24165	-3.41632
H	-0.91492	-0.27623	-3.49961
C	-1.42603	0.94887	-1.77784
H	-2.41748	1.10154	-2.23417
H	-1.09218	1.93717	-1.43081
C	-1.67264	-2.20792	-1.83702
H	-2.26526	-3.10752	-1.63478
H	-2.22019	-1.67084	-2.62345
C	-0.28247	-2.6372	-2.33279
H	-0.02829	-3.60396	-1.88525
H	-0.28466	-2.78717	-3.42454
Cl	0.85492	-3.19213	0.82379
C	1.56474	0.98058	0.33624
H	1.5377	1.66631	-0.5145
C	2.43173	-0.15768	0.30461
H	3.06675	-0.34772	-0.56186
H	2.83773	-0.53261	1.2456
C	1.36016	1.66332	1.66637
H	1.93485	1.11771	2.4293
C	1.77781	3.11322	1.61943
H	1.67186	3.58726	2.59968
H	2.82292	3.18634	1.30295
H	1.1612	3.65947	0.89599
O	-0.00843	1.68935	2.18817
C	-0.52029	0.52929	2.56854
C	-1.43274	0.63194	3.73846
N	-0.23283	-0.56193	1.95359
H	-0.62111	-1.40962	2.36039
H	-1.91602	-0.32115	3.96071
H	-2.1999	1.38434	3.52739
H	-0.87486	0.97683	4.61489

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1242.2365253
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1239.982975862143
ΔG_{solv} = -0.0144487

6-Ir-B, $NHCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.349993 (Hartree/Particle)
Thermal correction to Energy= 0.369548
Thermal correction to Enthalpy= 0.370492
Thermal correction to Gibbs Free Energy= 0.302732
Sum of electronic and zero-point Energies= -1241.354389
Sum of electronic and thermal Energies= -1241.334833
Sum of electronic and thermal Enthalpies= -1241.333889
Sum of electronic and thermal Free Energies= -1241.401649

Ir	-0.26953	-1.03533	0.38558
C	-0.17408	-2.30928	-1.31261
H	0.67588	-2.98989	-1.20987
C	0.11779	-0.98771	-1.74333
H	1.16983	-0.77685	-1.9341
C	-2.40068	-1.16815	-0.05142
H	-2.90334	-1.35762	0.89791
C	-1.9472	0.151	-0.27211
H	-2.10779	0.86165	0.54326
C	-0.84656	-0.11932	-2.52936
H	-0.28062	0.50083	-3.23475
H	-1.50109	-0.75083	-3.14303
C	-1.66551	0.78621	-1.60565
H	-2.60756	1.09525	-2.08543
H	-1.10309	1.70961	-1.41183
C	-2.70238	-2.13966	-1.17527
H	-3.54373	-2.77749	-0.88297
H	-3.03925	-1.58994	-2.06279
C	-1.49153	-3.01854	-1.5016
H	-1.49285	-3.8899	-0.83392
H	-1.55769	-3.41984	-2.52566
Cl	-0.91629	-0.64611	2.69236
C	1.8072	-0.32012	1.25353
H	1.58271	-0.34804	2.31832
C	1.92609	-1.51933	0.58654
H	1.87161	-2.44897	1.15686
H	2.39403	-1.59076	-0.39447
C	2.2471	1.04054	0.79118
H	3.15013	1.26797	1.38027
C	2.52649	1.24399	-0.67719
H	2.96773	2.23311	-0.83111
H	3.23271	0.49541	-1.05152
H	1.60209	1.18673	-1.2622
O	1.24181	2.00341	1.14912
C	1.18877	2.42173	2.43284
C	-0.03256	3.25854	2.63923
N	2.07318	2.0783	3.27871
H	1.86307	2.49676	4.18229
H	-0.11754	4.01677	1.85478
H	-0.02136	3.74418	3.61751
H	-0.91603	2.6117	2.57188

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1242.2129591
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1239.952987183781
ΔG_{solv} = -0.0110405

6-Ir-C, $NHCH_3$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.348711 (Hartree/Particle)
Thermal correction to Energy= 0.369159
Thermal correction to Enthalpy= 0.370103
Thermal correction to Gibbs Free Energy= 0.298659
Sum of electronic and zero-point Energies= -1241.367110
Sum of electronic and thermal Energies= -1241.346662
Sum of electronic and thermal Enthalpies= -1241.345718
Sum of electronic and thermal Free Energies= -1241.417162

Ir	-1.45996	0.11178	0.63056
C	-1.27137	-0.24006	-1.43281
H	-0.42321	-0.90896	-1.61844
C	-0.95052	1.12279	-1.16123
H	0.11573	1.3716	-1.14205
C	-3.53914	0.19149	0.11038
H	-4.07554	-0.42862	0.83236
C	-3.10229	1.45464	0.57251
H	-3.35287	1.7072	1.60608
C	-1.88095	2.27814	-1.49187
H	-1.28903	3.15311	-1.78523
H	-2.48891	2.02407	-2.36991
C	-2.77154	2.64297	-0.29831
H	-3.69181	3.14758	-0.63347
H	-2.24022	3.36765	0.33356
C	-3.80078	-0.12171	-1.35195
H	-4.64138	-0.82094	-1.42855
H	-4.12347	0.78955	-1.87182
C	-2.56822	-0.72856	-2.03365
H	-2.59222	-1.81932	-1.90852
H	-2.59101	-0.54539	-3.12003
Cl	-1.88484	-0.36324	2.97533
C	3.2829	-1.60116	-0.50166
H	2.45174	-1.12447	-1.02657
C	4.31418	-2.05959	-1.2035
H	4.33584	-1.97086	-2.2861
H	5.17029	-2.54481	-0.74
C	3.14378	-1.68078	0.9904
H	2.33504	-2.37791	1.26502
C	4.39241	-2.07035	1.74191
H	4.20524	-2.03155	2.81819
H	4.69051	-3.09026	1.48295
H	5.21517	-1.38908	1.50152
O	2.78321	-0.36488	1.48876
C	1.53981	0.09253	1.38268
C	1.39999	1.46547	1.93914
N	0.5417	-0.54786	0.88377
H	0.73794	-1.49393	0.56829
H	0.54771	1.97499	1.48069
H	2.32086	2.0325	1.7845
H	1.21522	1.39625	3.01705

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1242.2288786
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1239.965845925151
ΔG_{solv} = -0.014484

6-Ir-A, Ester

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.343848 (Hartree/Particle)
Thermal correction to Energy= 0.363719
Thermal correction to Enthalpy= 0.364663
Thermal correction to Gibbs Free Energy= 0.296763
Sum of electronic and zero-point Energies= -1336.444580
Sum of electronic and thermal Energies= -1336.424709
Sum of electronic and thermal Enthalpies= -1336.423765
Sum of electronic and thermal Free Energies= -1336.491665

Ir	0.55143	-0.68935	-0.07915
C	0.87281	-1.46371	-2.02148
H	1.9063	-1.81213	-2.08228
C	0.65517	-0.06136	-2.12253
H	1.55255	0.5464	-2.25537
C	-1.44628	-1.43714	-0.45023
H	-1.78508	-1.96313	0.44499
C	-1.48344	-0.01383	-0.39424
H	-1.88307	0.41964	0.52758
C	-0.61597	0.54978	-2.68591
H	-0.35769	1.43959	-3.27112
H	-1.0703	-0.15388	-3.39475
C	-1.59055	0.92063	-1.5734
H	-2.62622	0.96523	-1.94574
H	-1.35044	1.92896	-1.20892
C	-1.53961	-2.22764	-1.74528
H	-2.03848	-3.18196	-1.54363
H	-2.18988	-1.70027	-2.45622
C	-0.16262	-2.50746	-2.3647
H	0.21155	-3.46494	-1.98666
H	-0.23096	-2.60728	-3.45983
Cl	1.31153	-3.00296	0.69584
C	1.67787	1.12478	0.26756
H	1.54938	1.8546	-0.53594
C	2.58298	0.03538	0.1151
H	3.14005	-0.09666	-0.8129
H	3.07595	-0.37467	0.99724
C	1.53943	1.71101	1.65009
H	2.06144	1.06503	2.36846
C	2.06645	3.12347	1.71432
H	1.99666	3.5254	2.72917
H	3.11519	3.13422	1.40219
H	1.49848	3.77133	1.03733
O	0.1576	1.80121	2.13514
C	-0.39645	0.65784	2.44792
O	-1.4428	0.83865	3.21921
O	-0.00555	-0.4562	2.08341
C	-2.18434	-0.34086	3.56952
H	-3.03237	0.01219	4.15388
H	-1.5624	-1.01425	4.16313
H	-2.52827	-0.85572	2.66819

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.3495129
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1239.98297586214
ΔG_{solv} = -0.0144487

6-Ir-B, Ester

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.341920 (Hartree/Particle)
Thermal correction to Energy= 0.362849
Thermal correction to Enthalpy= 0.363793
Thermal correction to Gibbs Free Energy= 0.292278
Sum of electronic and zero-point Energies= -1336.448522
Sum of electronic and thermal Energies= -1336.427593
Sum of electronic and thermal Enthalpies= -1336.426649
Sum of electronic and thermal Free Energies= -1336.498164

Ir	-0.10889	-1.36892	0.48981
C	-0.14567	-1.7923	-1.58186
H	0.76238	-2.3317	-1.86753
C	-0.02693	-0.38689	-1.41422
H	0.96624	0.03191	-1.57096
C	-2.26703	-1.58786	0.25036
H	-2.58251	-2.22994	1.07499
C	-1.9936	-0.24393	0.56086
H	-2.08006	0.04878	1.61034
C	-1.15412	0.59528	-1.67939
H	-0.72493	1.53584	-2.04406
H	-1.78452	0.21529	-2.49435
C	-1.99625	0.88563	-0.43076
H	-3.03536	1.12309	-0.70984
H	-1.60376	1.77695	0.06993
C	-2.63651	-2.04058	-1.14842
H	-3.36975	-2.85173	-1.08093
H	-3.14183	-1.22333	-1.67883
C	-1.41543	-2.52621	-1.93781
H	-1.24944	-3.58987	-1.72164
H	-1.6002	-2.46165	-3.02196
Cl	-0.33592	-1.93753	2.83196
C	2.01494	-0.61972	1.14426
H	1.80242	-0.61281	2.21149
C	2.07821	-1.83492	0.49217
H	2.01843	-2.76219	1.06539
H	2.50664	-1.91784	-0.50596
C	2.60872	0.67388	0.6318
H	3.2253	1.05202	1.46124
C	3.46625	0.58041	-0.60704
H	3.87114	1.56783	-0.84625
H	4.303	-0.10156	-0.42777
H	2.91381	0.21925	-1.48051
O	1.60767	1.67898	0.36517
C	0.98946	2.17671	1.43558
O	0.14184	3.11576	1.01785
O	1.17179	1.84957	2.58456
C	-0.64635	3.708	2.05214
H	-1.23911	4.48364	1.56762
H	-0.00693	4.14295	2.82456
H	-1.30315	2.95968	2.50797

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.3556051
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1334.959475456219
ΔG_{solv} = -0.0127336

6-Ir-C, Ester

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.342209 (Hartree/Particle)
Thermal correction to Energy= 0.363237
Thermal correction to Enthalpy= 0.364181
Thermal correction to Gibbs Free Energy= 0.291315
Sum of electronic and zero-point Energies= -1336.441399
Sum of electronic and thermal Energies= -1336.420371
Sum of electronic and thermal Enthalpies= -1336.419427
Sum of electronic and thermal Free Energies= -1336.492292

Ir	-1.00466	0.48199	0.1966
C	-1.40687	0.12311	-1.83057
H	-0.48156	-0.22441	-2.30116
C	-1.5031	1.52213	-1.57936
H	-0.64054	2.12776	-1.87092
C	-2.98231	-0.19099	0.41535
H	-3.01921	-0.91227	1.236
C	-2.87702	1.18334	0.78987
H	-2.84818	1.38955	1.86381
C	-2.82803	2.26084	-1.49969
H	-2.71041	3.26984	-1.91127
H	-3.56836	1.76387	-2.13957
C	-3.32918	2.35167	-0.0533
H	-4.42554	2.45385	-0.01852
H	-2.9242	3.26092	0.41
C	-3.62387	-0.64683	-0.88566
H	-4.1415	-1.59914	-0.72371
H	-4.40095	0.06992	-1.18059
C	-2.58253	-0.81151	-1.99889
H	-2.18845	-1.83577	-1.97162
H	-3.04428	-0.68786	-2.99141
Cl	-0.3582	-0.04189	2.48574
C	3.3191	-1.79277	-0.73787
H	3.03443	-1.0735	-1.50683
C	4.23229	-2.72149	-1.0031
H	4.70491	-2.77683	-1.98005
H	4.54159	-3.46685	-0.27363
C	2.58563	-1.64382	0.5568
H	1.50473	-1.74446	0.38503
C	3.02496	-2.52986	1.69134
H	2.45278	-2.28808	2.59172
H	2.84056	-3.57853	1.4401
H	4.09157	-2.40006	1.90312
O	2.79336	-0.26646	1.03502
C	1.98091	0.65711	0.59357
O	2.13031	1.83653	1.14253
O	1.1504	0.48466	-0.30726
C	2.97724	1.96433	2.29589
H	2.8987	3.00741	2.59856
H	4.01091	1.7175	2.0432
H	2.61458	1.30702	3.09072

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.349625
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1334.958375760837
ΔG_{solv} = -0.0110629

6-Ir-A', Ester

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.343390 (Hartree/Particle)
Thermal correction to Energy= 0.363421
Thermal correction to Enthalpy= 0.364365
Thermal correction to Gibbs Free Energy= 0.296102
Sum of electronic and zero-point Energies= -1336.454067
Sum of electronic and thermal Energies= -1336.434036
Sum of electronic and thermal Enthalpies= -1336.433092
Sum of electronic and thermal Free Energies= -1336.501355

Ir	0.75619	-0.4735	-0.13686
C	-0.03435	0.43383	-1.903
H	0.34349	1.45501	-2.00153
C	-1.07651	0.24966	-0.95721
H	-1.38212	1.14184	-0.40032
C	0.62711	-2.23144	-1.45527
H	1.59312	-2.7336	-1.38384
C	-0.24092	-2.36795	-0.34611
H	0.10658	-3.00686	0.46831
C	-2.13615	-0.83297	-1.08119
H	-3.07653	-0.46424	-0.65448
H	-2.34515	-1.01306	-2.14416
C	-1.73448	-2.13491	-0.37584
H	-2.25668	-2.99454	-0.82454
H	-2.06635	-2.08529	0.66922
C	0.14264	-1.90375	-2.85157
H	0.74945	-2.44665	-3.58486
H	-0.88384	-2.2705	-2.97699
C	0.2215	-0.40416	-3.13019
H	1.23339	-0.1587	-3.48114
H	-0.46278	-0.11193	-3.9425
Cl	2.39867	-1.66256	1.24444
C	1.45304	1.54664	0.35664
H	0.79405	2.30053	-0.08987
C	2.43545	0.95254	-0.44932
H	2.53025	1.22734	-1.49809
H	3.31929	0.50525	0.00208
C	1.61789	1.73591	1.841
H	2.01939	0.82734	2.30884
C	2.47	2.94091	2.17161
H	2.52407	3.095	3.25371
H	3.48257	2.78692	1.78606
H	2.05463	3.84266	1.70715
O	0.31912	2.02852	2.42807
C	-0.57171	1.05471	2.48031
O	-1.68717	1.5271	3.02093
O	-0.42628	-0.09501	2.1016
C	-2.7695	0.5956	3.08208
H	-3.04112	0.26271	2.0751
H	-3.59919	1.13382	3.53935
H	-2.49945	-0.27278	3.68883

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.3582076

6-Ir-B', Ester

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.343611 (Hartree/Particle)
Thermal correction to Energy= 0.364076
Thermal correction to Enthalpy= 0.365020
Thermal correction to Gibbs Free Energy= 0.295227
Sum of electronic and zero-point Energies= -1336.443724
Sum of electronic and thermal Energies= -1336.423258
Sum of electronic and thermal Enthalpies= -1336.422314
Sum of electronic and thermal Free Energies= -1336.492107

Ir	0.13305	-1.1085	0.35635
C	0.05701	-0.84397	-1.75925
H	1.0553	-0.67664	-2.1725
C	-0.55868	0.27278	-1.13646
H	0.03511	1.18391	-1.07077
C	-1.62754	-2.41772	-0.15654
H	-1.37538	-3.34231	0.36561
C	-2.04493	-1.34578	0.63238
H	-2.13815	-1.5368	1.70311
C	-2.06054	0.50069	-1.11076
H	-2.25799	1.57834	-1.13645
H	-2.50954	0.09154	-2.02525
C	-2.72143	-0.09548	0.13596
H	-3.7912	-0.28715	-0.04171
H	-2.67556	0.63981	0.94886
C	-1.85289	-2.51421	-1.64472
H	-2.04157	-3.56044	-1.90967
H	-2.76212	-1.96242	-1.91134
C	-0.64748	-1.99558	-2.43277
H	0.08631	-2.80678	-2.53412
H	-0.94371	-1.72116	-3.45759
Cl	0.39581	-2.17456	2.52103
C	2.20876	-0.23923	0.78933
H	2.17754	-0.34787	1.8733
C	2.36953	-1.39472	0.0488
H	2.49615	-2.34948	0.5555
H	2.65707	-1.37123	-1.00019
C	2.5475	1.16127	0.34259
H	3.34602	1.50801	1.01651
C	2.98448	1.33781	-1.09
H	3.20864	2.39146	-1.27942
H	3.88957	0.75507	-1.28553
H	2.2082	1.0246	-1.79635
O	1.42342	2.0534	0.5267
C	0.98659	2.22123	1.77436
O	-0.18203	2.85694	1.7133
O	1.54746	1.867	2.78461
C	-0.78471	3.1109	2.9832
H	-1.71002	3.64687	2.77242
H	-0.12719	3.7204	3.60931
H	-1.00088	2.16996	3.49815

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.35324

6-Ir-C', Ester

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.342130 (Hartree/Particle)
Thermal correction to Energy= 0.363207
Thermal correction to Enthalpy= 0.364151
Thermal correction to Gibbs Free Energy= 0.291022
Sum of electronic and zero-point Energies= -1336.441415
Sum of electronic and thermal Energies= -1336.420338
Sum of electronic and thermal Enthalpies= -1336.419394
Sum of electronic and thermal Free Energies= -1336.492522

Ir	-1.0955	0.14335	0.12254
C	-1.26357	0.88452	-1.83175
H	-0.25632	0.95576	-2.2547
C	-1.63957	1.90719	-0.9143
H	-0.88729	2.67263	-0.70464
C	-2.9242	-0.76404	-0.36651
H	-2.8901	-1.81055	-0.05214
C	-3.10763	0.19688	0.67407
H	-3.20016	-0.20338	1.68779
C	-3.08323	2.32436	-0.6933
H	-3.1325	3.40422	-0.513
H	-3.66089	2.14601	-1.60972
C	-3.70021	1.574	0.49298
H	-4.79631	1.51556	0.39901
H	-3.5027	2.13605	1.41523
C	-3.36378	-0.52733	-1.803
H	-3.69784	-1.47435	-2.24186
H	-4.24157	0.13177	-1.81318
C	-2.22872	0.06067	-2.65157
H	-1.65559	-0.76088	-3.10052
H	-2.63024	0.6476	-3.49281
Cl	-0.54744	-1.44087	1.8857
C	3.74661	-0.83311	-0.82566
H	3.38164	0.09514	-1.26654
C	4.86482	-1.39271	-1.27601
H	5.43252	-0.93932	-2.0839
H	5.25438	-2.3244	-0.87069
C	2.87901	-1.39538	0.25467
H	1.87658	-1.60719	-0.14218
C	3.41704	-2.59314	0.99152
H	2.72461	-2.88379	1.78645
H	3.52158	-3.43695	0.30313
H	4.39512	-2.37796	1.43481
O	2.69657	-0.35472	1.28025
C	1.7266	0.50476	1.11085
O	1.5011	1.29529	2.13155
O	1.07281	0.62771	0.06823
C	2.1456	1.01646	3.38425
H	1.76679	1.7659	4.07766
H	3.23002	1.10144	3.28661
H	1.872	0.01282	3.72065

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1337.3494548

6-Ir-A, Ketone

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.337742 (Hartree/Particle)
Thermal correction to Energy= 0.356871
Thermal correction to Enthalpy= 0.357815
Thermal correction to Gibbs Free Energy= 0.291365
Sum of electronic and zero-point Energies= -1261.257023
Sum of electronic and thermal Energies= -1261.237895
Sum of electronic and thermal Enthalpies= -1261.236950
Sum of electronic and thermal Free Energies= -1261.303400

Ir	0.43634	-0.80527	0.03086
C	0.79166	-1.64589	-1.88346
H	1.81355	-2.03136	-1.89763
C	0.62716	-0.24214	-2.03115
H	1.54776	0.33286	-2.14877
C	-1.57162	-1.49635	-0.38184
H	-1.96175	-1.9758	0.51836
C	-1.55846	-0.07086	-0.37248
H	-1.97192	0.40106	0.5234
C	-0.6055	0.39206	-2.65162
H	-0.30092	1.25469	-3.25512
H	-1.06186	-0.31817	-3.35271
C	-1.60226	0.82707	-1.58263
H	-2.62428	0.88651	-1.98942
H	-1.34704	1.84074	-1.24469
C	-1.65261	-2.32352	-1.65486
H	-2.18385	-3.25684	-1.43793
H	-2.26959	-1.80109	-2.39865
C	-0.26969	-2.66212	-2.2313
H	0.06253	-3.62343	-1.82521
H	-0.31348	-2.78239	-3.3257
Cl	1.12086	-3.12612	0.8656
C	1.58986	0.98535	0.37574
H	1.4973	1.70695	-0.44
C	2.47764	-0.12437	0.26318
H	3.05787	-0.28219	-0.6464
H	2.93866	-0.52855	1.16504
C	1.43397	1.58644	1.74927
H	1.9416	0.9387	2.47682
C	1.97616	2.99413	1.80852
H	1.89843	3.40564	2.81904
H	3.02854	2.9926	1.50856
H	1.42289	3.64264	1.11993
O	0.05469	1.69619	2.2404
C	-0.55212	0.5745	2.55215
C	-1.71004	0.75309	3.46917
O	-0.19797	-0.5367	2.14358
H	-2.34148	-0.13605	3.45326
H	-2.28105	1.64035	3.18178
H	-1.33998	0.91762	4.48688

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1048137
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1259.830870530434
ΔG_{solv} = -0.016478

6-Ir-B, Ketone

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.337810 (Hartree/Particle)
Thermal correction to Energy= 0.357280
Thermal correction to Enthalpy= 0.358224
Thermal correction to Gibbs Free Energy= 0.290673
Sum of electronic and zero-point Energies= -1261.260829

Sum of electronic and thermal Energies= -1261.241359
Sum of electronic and thermal Enthalpies= -1261.240415
Sum of electronic and thermal Free Energies= -1261.307966

Ir	-0.19766	-0.92866	0.47575
C	-0.12888	-2.24528	-1.19541
H	0.72072	-2.92581	-1.09314
C	0.1581	-0.93449	-1.66119
H	1.20726	-0.72789	-1.87278
C	-2.34047	-1.06736	0.06489
H	-2.82767	-1.2332	1.02638
C	-1.88813	0.24356	-0.19386
H	-2.03293	0.97327	0.60745
C	-0.81304	-0.08135	-2.45518
H	-0.25296	0.52058	-3.18055
H	-1.47621	-0.72344	-3.04778
C	-1.61746	0.84775	-1.54321
H	-2.56287	1.15189	-2.01917
H	-1.0479	1.77165	-1.37452
C	-2.65552	-2.06806	-1.02888
H	-3.49321	-2.69719	-0.70863
H	-3.00385	-1.54225	-1.92642
C	-1.44983	-2.95651	-1.34753
H	-1.4429	-3.80979	-0.65706
H	-1.53058	-3.38457	-2.35955
Cl	-0.84248	-0.42884	2.76443
C	1.87593	-0.26241	1.33601
H	1.69243	-0.32028	2.40707
C	1.99277	-1.44233	0.63369
H	1.95575	-2.38722	1.17881
H	2.4445	-1.48405	-0.35626
C	2.29854	1.11062	0.8895
H	3.1969	1.34953	1.48046
C	2.57372	1.33001	-0.57671
H	2.98128	2.33397	-0.7263
H	3.30656	0.60728	-0.95022
H	1.65349	1.24133	-1.16443
O	1.2782	2.06352	1.25566
C	1.19925	2.40984	2.55469
C	0.00151	3.2694	2.79906
O	1.98913	2.04129	3.39425
H	-0.11588	4.01874	2.01207
H	0.0774	3.74586	3.77734
H	-0.88305	2.62092	2.78127

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1101721
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1259.832225914851
ΔG_{solv} = -0.0113795

6-Ir-C, Ketone

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.335490 (Hartree/Particle)
Thermal correction to Energy= 0.356057
Thermal correction to Enthalpy= 0.357002
Thermal correction to Gibbs Free Energy= 0.285418
Sum of electronic and zero-point Energies= -1261.257915
Sum of electronic and thermal Energies= -1261.237348
Sum of electronic and thermal Enthalpies= -1261.236403
Sum of electronic and thermal Free Energies= -1261.307987

Ir	-0.72166	0.79771	0.61707
C	-0.68719	0.27369	-1.42156
H	0.35633	0.22276	-1.75006
C	-1.24222	1.57761	-1.28776
H	-0.57175	2.41229	-1.51051
C	-2.4155	-0.44799	0.60954
H	-2.346	-1.12108	1.46777
C	-2.79064	0.89809	0.89986
H	-2.98849	1.12787	1.95069
C	-2.72537	1.87168	-1.43571
H	-2.85804	2.85375	-1.90387
H	-3.17749	1.14913	-2.12691
C	-3.437	1.85005	-0.07769
H	-4.50757	1.61849	-0.19497
H	-3.38926	2.85233	0.36788
C	-2.67833	-1.11936	-0.72884
H	-2.91119	-2.17778	-0.56616
H	-3.57347	-0.68226	-1.1902
C	-1.46931	-0.99536	-1.6623
H	-0.78254	-1.83359	-1.47643
H	-1.77436	-1.07693	-2.71745
Cl	-0.31561	0.54615	2.99179
C	2.58142	-1.3046	-0.84172
H	2.59862	-0.36773	-1.40277
C	2.9374	-2.43777	-1.43978
H	3.24292	-2.44963	-2.48227
H	2.93482	-3.39464	-0.92191
C	2.10333	-1.18876	0.57029
H	1.02843	-0.93241	0.57342
C	2.34069	-2.38192	1.45795
H	1.99946	-2.16099	2.47347
H	1.77411	-3.24188	1.08824
H	3.40322	-2.64632	1.48626
O	2.8192	-0.07598	1.19489
C	2.37893	1.15668	1.09522
C	3.23601	2.14449	1.80503
O	1.35822	1.5001	0.49208
H	3.23723	3.09126	1.26174
H	4.25084	1.77124	1.9481
H	2.7818	2.32161	2.78757

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1086777
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1259.831250951304
ΔG_{solv} = -0.0110629

6-Ir-A' (Ketone)

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.337853 (Hartree/Particle)
Thermal correction to Energy= 0.357315
Thermal correction to Enthalpy= 0.358260
Thermal correction to Gibbs Free Energy= 0.290561
Sum of electronic and zero-point Energies= -1261.265662
Sum of electronic and thermal Energies= -1261.246200
Sum of electronic and thermal Enthalpies= -1261.245255

Sum of electronic and thermal Free Energies= -1261.312954

Ir	0.78392	-0.5984	-0.2535
C	-0.04718	0.403	-1.93296
H	0.38508	1.4035	-2.03041
C	-1.04581	0.2508	-0.92833
H	-1.27265	1.1462	-0.34169
C	0.42684	-2.33315	-1.63024
H	1.38818	-2.849	-1.63729
C	-0.34809	-2.45924	-0.4699
H	0.0321	-3.11911	0.3117
C	-2.17867	-0.76109	-1.00053
H	-3.05315	-0.35257	-0.48031
H	-2.48775	-0.88599	-2.04679
C	-1.81513	-2.11426	-0.37048
H	-2.42513	-2.91966	-0.80847
H	-2.06334	-2.08319	0.69685
C	-0.12178	-1.90373	-2.96931
H	0.38264	-2.4671	-3.76242
H	-1.18322	-2.17244	-3.03176
C	0.07662	-0.4056	-3.1994
H	1.08803	-0.23504	-3.59339
H	-0.61962	-0.03007	-3.96609
Cl	2.42783	-1.9302	0.97219
C	1.35837	1.4097	0.42869
H	0.71654	2.16469	-0.03758
C	2.43464	0.90147	-0.30002
H	2.60797	1.22019	-1.32632
H	3.28384	0.44782	0.20771
C	1.35982	1.49873	1.93298
H	1.74555	0.57126	2.37578
C	2.14427	2.7018	2.41362
H	2.08739	2.78974	3.50299
H	3.19409	2.5991	2.12204
H	1.74753	3.62077	1.96657
O	0.00517	1.71555	2.39552
C	-0.80553	0.65707	2.50339
C	-2.17676	1.06722	2.93859
O	-0.47205	-0.48439	2.25412
H	-2.75476	0.18593	3.21972
H	-2.6783	1.57363	2.10567
H	-2.12754	1.77607	3.76905

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1133278

6-Ir-B' (Ketone)

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.336539 (Hartree/Particle)
Thermal correction to Energy= 0.356437
Thermal correction to Enthalpy= 0.357381
Thermal correction to Gibbs Free Energy= 0.288426
Sum of electronic and zero-point Energies= -1261.259000
Sum of electronic and thermal Energies= -1261.239102
Sum of electronic and thermal Enthalpies= -1261.238158
Sum of electronic and thermal Free Energies= -1261.307114

Ir	0.42167	-1.38169	0.28455
C	-1.73081	-1.296	0.70154
H	-1.79777	-1.39736	1.78692
C	-1.44362	-2.46312	-0.02749
H	-1.33465	-3.38306	0.55086
C	-0.18497	0.01496	-1.22428
H	0.49656	0.86237	-1.22487
C	0.29653	-1.18232	-1.81667
H	1.30355	-1.14472	-2.2441
C	-1.76601	-2.62477	-1.50005
H	-2.07103	-3.66022	-1.68746
H	-2.6326	-2.00535	-1.76195
C	-0.56398	-2.28249	-2.38789
H	-0.8917	-2.02358	-3.40722
H	0.06949	-3.17369	-2.48956
C	-1.64881	0.41675	-1.16243
H	-1.71671	1.50937	-1.2344
H	-2.17926	0.02651	-2.04065
C	-2.32861	-0.04166	0.13295
H	-2.23173	0.74107	0.89502
H	-3.41075	-0.18026	-0.02032
Cl	0.78875	-2.58691	2.34933
C	2.09444	0.07304	1.1023
H	1.96921	-0.21496	2.14467
C	2.60526	-0.85036	0.21355
H	2.98326	-1.8061	0.57969
H	2.94456	-0.54827	-0.77651
C	2.06608	1.56726	0.87596
H	2.58986	1.9878	1.74858
C	2.73365	2.07195	-0.38197
H	2.66316	3.16277	-0.4191
H	3.79271	1.79614	-0.37698
H	2.28394	1.67124	-1.29681
O	0.73226	2.1208	0.89438
C	0.12	2.17223	2.08979
C	-1.1687	2.9311	2.01094
O	0.58887	1.70224	3.10176
H	-0.97135	3.97511	2.27844
H	-1.87903	2.52802	2.73608
H	-1.59168	2.91612	1.00343

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1098584

6-Ir-C' (Ketone)

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.336792 (Hartree/Particle)
Thermal correction to Energy= 0.356821
Thermal correction to Enthalpy= 0.357766
Thermal correction to Gibbs Free Energy= 0.287642
Sum of electronic and zero-point Energies= -1261.258634
Sum of electronic and thermal Energies= -1261.238605
Sum of electronic and thermal Enthalpies= -1261.237661
Sum of electronic and thermal Free Energies= -1261.307785

Ir	-1.41919	-0.30051	0.59988
C	-1.03114	0.01979	-1.43931
H	-0.06672	-0.44094	-1.67888
C	-0.98475	1.26861	-0.75368
H	0.0131	1.66019	-0.52718
C	-3.40869	-0.40408	-0.09819
H	-3.87734	-1.28404	0.34982
C	-3.24156	0.72186	0.75605
H	-3.60979	0.61482	1.78004
C	-2.0887	2.30803	-0.85006
H	-1.65254	3.31298	-0.81823
H	-2.58357	2.22667	-1.82661
C	-3.10393	2.15197	0.28917
H	-4.08544	2.56148	0.00179

H	-2.76953	2.74374	1.15152
C	-3.53435	-0.28913	-1.60857
H	-4.23205	-1.0503	-1.97572
H	-3.98453	0.67855	-1.86554
C	-2.17669	-0.45817	-2.29955
H	-2.00764	-1.52418	-2.50093
H	-2.16917	0.04353	-3.28024
Cl	-1.8671	-1.51578	2.65069
C	3.33891	-0.57444	-0.75709
H	2.42002	-0.04775	-1.02193
C	4.42235	-0.43132	-1.51378
H	4.4077	0.20486	-2.39461
H	5.35984	-0.94161	-1.30292
C	3.23954	-1.44286	0.45916
H	2.46806	-2.20801	0.30065
C	4.52209	-2.07343	0.93472
H	4.34454	-2.63232	1.85751
H	4.90174	-2.76994	0.1814
H	5.28562	-1.31231	1.12696
O	2.77711	-0.60903	1.57691
C	1.49931	-0.31525	1.65113
C	1.13695	0.54793	2.80499
O	0.69754	-0.7306	0.80799
H	0.72683	1.48966	2.42254
H	1.99782	0.74672	3.44362
H	0.33533	0.05462	3.36642

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -1262.1111801

I-Z

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.444858 (Hartree/Particle)
Thermal correction to Energy= 0.477710
Thermal correction to Enthalpy= 0.478654
Thermal correction to Gibbs Free Energy= 0.381947
Sum of electronic and zero-point Energies= -3278.913443
Sum of electronic and thermal Energies= -3278.880591
Sum of electronic and thermal Enthalpies= -3278.879647
Sum of electronic and thermal Free Energies= -3278.976354

C	0.24272	-1.50584	-1.78476
C	1.1663	-0.37151	-1.45643
C	2.2646	-0.84453	-0.6889
C	2.01032	-2.4204	1.27874
C	0.76347	-1.67172	1.66837
C	-0.20304	-1.84687	0.67394
H	-0.79122	-1.19307	-1.95717
H	0.59222	-1.99189	-2.70858
H	1.22465	0.50267	-2.10124
H	1.89125	-3.47361	1.57676
H	2.91279	-2.03237	1.75128
H	0.5256	-1.48546	2.71446
C	0.45455	-2.41176	-0.57688
H	0.13775	-3.45216	-0.73056
C	1.96062	-2.27665	-0.23902
H	2.59067	-2.99605	-0.77812
C	3.65839	-0.36862	-0.85037
C	4.69615	-0.85019	-0.04025
C	3.99558	0.526	-1.87754
C	6.01012	-0.4395	-0.22345
H	4.48677	-1.55991	0.75322
C	5.30243	0.95111	-2.07257
H	3.22568	0.90206	-2.54598
C	6.29195	0.46325	-1.23497
H	6.8137	-0.81004	0.40645
H	5.55835	1.65008	-2.86436
C	-1.64956	-2.00573	0.91701
C	-2.54212	-2.28555	-0.12915
C	-2.1636	-1.99967	2.22613
C	-3.89101	-2.51516	0.10845
H	-2.1859	-2.34689	-1.15272
C	-3.50729	-2.22101	2.48169
H	-1.49742	-1.83196	3.069
C	-4.35478	-2.47139	1.41218
H	-4.58082	-2.7335	-0.70113
H	-3.90245	-2.21855	3.49302
F	-5.64791	-2.69232	1.65028
F	7.55586	0.86404	-1.41693
Ir	0.88533	0.34059	0.60814
Cl	2.73835	0.54327	2.35143
C	-1.07333	1.04622	1.41722
H	-1.60232	0.25849	1.94818
C	-0.14714	1.80422	2.11795
H	0.01471	1.60238	3.17336
H	0.24664	2.74307	1.73588
C	-1.10599	1.06451	-0.02309
O	1.52637	2.57548	-2.23298
C	1.99538	2.77335	-1.11569
C	2.93276	4.0379	-0.95899
Cl	4.32615	3.7427	0.1331
Cl	3.55381	4.55368	-2.53783
Cl	1.91188	5.35088	-0.2652
N	1.77923	2.13319	0.02064
H	2.35603	2.44532	0.79697
C	-1.16193	2.33419	-0.81721
H	-0.73089	2.2036	-1.8127
H	-2.21585	2.62048	-0.9329
H	-0.63756	3.16166	-0.33097
H	-1.71773	0.26622	-0.45058

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6546775
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.648122700460
ΔG_{solv} = -0.0150566

TS-E_1-E_2

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -45.09 cm^{-1}
Zero-point correction= 0.442999 (Hartree/Particle)
Thermal correction to Energy= 0.475911
Thermal correction to Enthalpy= 0.476855
Thermal correction to Gibbs Free Energy= 0.379475
Sum of electronic and zero-point Energies= -3278.910575
Sum of electronic and thermal Energies= -3278.877663
Sum of electronic and thermal Enthalpies= -3278.876719
Sum of electronic and thermal Free Energies= -3278.974099

C	0.04554	-3.93214	-1.14984
C	0.95675	-3.00936	-1.90869
C	2.12489	-2.77468	-1.17466
C	2.19685	-2.22287	1.26812
C	0.95153	-1.39002	1.09323

C	-0.10896	-2.23197	0.68355
H	-1.01348	-3.77791	-1.3778
H	0.29066	-4.9741	-1.40544
H	0.92297	-2.95197	-2.99381
H	2.22543	-2.63002	2.28977
H	3.13347	-1.67649	1.10913
H	0.78755	-0.47646	1.66066
C	0.43946	-3.59544	0.28944
H	0.163	-4.35788	1.02928
C	1.95794	-3.32128	0.2343
H	2.56147	-4.22546	0.38639
C	3.45688	-2.56089	-1.76927
C	4.61373	-2.86276	-1.03952
C	3.60556	-2.0855	-3.08245
C	5.87926	-2.71335	-1.59618
H	4.53567	-3.23408	-0.02055
C	4.85945	-1.92372	-3.64764
H	2.72465	-1.80263	-3.65583
C	5.98056	-2.24568	-2.89421
H	6.7788	-2.95506	-1.03774
H	4.98297	-1.54956	-4.65979
C	-1.54602	-2.05933	0.96462
C	-2.45514	-3.10569	0.73159
C	-2.03965	-0.88539	1.55892
C	-3.80377	-2.97611	1.03361
H	-2.1159	-4.055	0.32944
C	-3.38361	-0.73689	1.85677
H	-1.35932	-0.07249	1.79422
C	-4.25027	-1.78423	1.57969
H	-4.50688	-3.78444	0.85683
H	-3.76665	0.17469	2.30711
F	-5.54651	-1.64656	1.86511
F	7.19118	-2.09433	-3.4393
Ir	0.62284	-0.98177	-1.05268
Cl	0.47512	-0.28357	-3.3906
C	2.56467	1.08857	0.31535
H	2.86551	0.61442	1.25203
C	2.42004	2.42377	0.2994
C	2.42297	0.25554	-0.86676
O	-0.22937	1.59085	1.36327
C	-0.57671	1.65927	0.18908
Cl	-1.17279	4.2441	0.97039
N	-0.46	0.75204	-0.77173
H	-0.77024	1.08001	-1.68342
H	3.2211	-0.47799	-0.96507
C	-1.30623	2.98345	-0.26911
Cl	-3.04056	2.59967	-0.53428
Cl	-0.59802	3.6115	-1.7998
H	2.31165	0.84246	-1.78448
H	2.10987	2.90099	-0.63584
C	2.6349	3.30935	1.47008
H	2.93586	2.73793	2.3546
H	3.3982	4.07119	1.2682
H	1.70664	3.84592	1.70804

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6559825
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.637567228433
ΔG_{solv} = -0.0136845

TS-E_2-E_3

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -91.65 cm^{-1}

Zero-point correction= 0.442525 (Hartree/Particle)
Thermal correction to Energy= 0.475536
Thermal correction to Enthalpy= 0.476480
Thermal correction to Gibbs Free Energy= 0.378281
Sum of electronic and zero-point Energies= -3278.901358
Sum of electronic and thermal Energies= -3278.868348
Sum of electronic and thermal Enthalpies= -3278.867403
Sum of electronic and thermal Free Energies= -3278.965603

C	0.12028	-3.80027	-1.05566
C	0.99416	-2.74984	-1.67773
C	2.01941	-2.37856	-0.80349
C	1.74435	-1.98578	1.67692
C	0.45824	-1.26661	1.3621
C	-0.44474	-2.19177	0.78906
H	-0.91515	-3.76048	-1.40804
H	0.51521	-4.79754	-1.29999
H	1.0717	-2.65011	-2.75675
H	1.64863	-2.47165	2.65925
H	2.62688	-1.34186	1.72768
H	0.13643	-0.39685	1.93104
C	0.29977	-3.47168	0.42553
H	0.03346	-4.28583	1.11219
C	1.77401	-3.02073	0.55815
H	2.46525	-3.85698	0.7277
C	3.33411	-1.87097	-1.23146
C	4.43392	-1.90117	-0.36464
C	3.52007	-1.34741	-2.52073
C	5.67495	-1.41256	-0.75737
H	4.33464	-2.32021	0.63389
C	4.75072	-0.86053	-2.92894
H	2.67776	-1.29019	-3.20748
C	5.81067	-0.89424	-2.03375
H	6.53178	-1.43227	-0.0904
H	4.89833	-0.44502	-3.9216
C	-1.91205	-2.15809	0.89536
C	-2.68721	-3.26549	0.51131
C	-2.57556	-1.05543	1.4657
C	-4.06762	-3.26747	0.65165
H	-2.2159	-4.15994	0.11607
C	-3.95202	-1.04094	1.60492
H	-2.00685	-0.1951	1.81199
C	-4.68032	-2.14683	1.187
H	-4.66862	-4.12339	0.35972
H	-4.46846	-0.19168	2.04281
F	-6.00636	-2.13536	1.32209
F	6.99748	-0.41625	-2.4182
Ir	0.29975	-0.80475	-0.80915
Cl	0.00356	-0.21323	-3.16597
C	2.36096	1.37617	-1.29004
H	2.04855	1.17213	-2.31285
C	3.26851	2.33006	-1.06913
C	1.81618	0.54271	-0.17149
O	-0.72693	1.59879	1.59363
C	-1.12711	1.6787	0.43162
Cl	-3.5144	2.73286	1.14255
N	-0.92014	0.83977	-0.56717
H	-1.28497	1.14217	-1.46562
H	1.33055	1.14233	0.6061
C	-2.04299	2.92236	0.13574
Cl	-2.55296	3.11324	-1.57341
Cl	-1.16853	4.3962	0.62882
H	2.61627	-0.04235	0.28387
H	3.58992	2.53193	-0.04292
C	3.91938	3.1275	-2.14919

H	3.53331	2.84315	-3.13486
H	3.75918	4.20499	-2.01637
H	5.00662	2.97174	-2.15495

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6468396
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.631590895520
ΔG_{solv} = -0.0159637

TS-E_3-E_4

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Imaginary frequency = -60.27 cm^{-1}
Zero-point correction= 0.440794 (Hartree/Particle)
Thermal correction to Energy= 0.474233
Thermal correction to Enthalpy= 0.475177
Thermal correction to Gibbs Free Energy= 0.376048
Sum of electronic and zero-point Energies= -3278.906988
Sum of electronic and thermal Energies= -3278.873549
Sum of electronic and thermal Enthalpies= -3278.872605
Sum of electronic and thermal Free Energies= -3278.971734

C	0.24049	-3.23097	-1.58701
C	0.98676	-1.96279	-1.91583
C	1.98054	-1.73102	-0.9592
C	1.73235	-1.99113	1.51088
C	0.37959	-1.3417	1.386
C	-0.46303	-2.15833	0.59766
H	-0.78524	-3.26979	-1.96169
H	0.77583	-4.07887	-2.0414
H	1.05031	-1.58858	-2.93487
H	1.71263	-2.69127	2.35968
H	2.56586	-1.30262	1.67045
H	-0.01976	-0.6543	2.1289
C	0.37641	-3.25237	-0.06705
H	0.17841	-4.22905	0.39265
C	1.80831	-2.72516	0.18242
H	2.56591	-3.51881	0.13498
C	3.26909	-1.08003	-1.24946
C	4.41222	-1.43472	-0.52416
C	3.40263	-0.16208	-2.30084
C	5.65618	-0.89606	-0.83204
H	4.34027	-2.14878	0.29287
C	4.6341	0.39196	-2.61349
H	2.52088	0.15008	-2.85898
C	5.74429	0.0139	-1.8709
H	6.54888	-1.16572	-0.27493
H	4.74718	1.11359	-3.4176
C	-1.92736	-2.26084	0.78963
C	-2.81062	-2.5269	-0.26727
C	-2.46782	-2.04852	2.06546
C	-4.18281	-2.56977	-0.06606
H	-2.4338	-2.65928	-1.27701
C	-3.8377	-2.08697	2.28437
H	-1.80356	-1.84657	2.90095
C	-4.67473	-2.34141	1.21002
H	-4.87325	-2.76232	-0.88186
H	-4.26264	-1.91778	3.26955
F	-5.99503	-2.37543	1.41024
F	6.93321	0.55812	-2.15684
Ir	0.05648	-0.42423	-0.61861
Cl	-0.1295	0.85924	-2.67487
C	2.43204	1.19489	0.89281
H	2.53489	0.71116	1.86629
C	3.49105	1.85327	0.39015
C	1.10752	1.27326	0.30277
O	-1.56896	0.87223	2.21751
C	-2.08167	1.03314	1.11237
Cl	-4.47758	1.48029	-0.31692
N	-1.60427	0.67411	-0.06795
H	-2.11959	1.00901	-0.87651
H	1.06452	1.95564	-0.55114
C	-3.42382	1.85623	1.08625
Cl	-2.95334	3.58877	1.0141
Cl	-4.3521	1.55693	2.57207
H	0.34621	1.49769	1.05256
H	3.37482	2.36013	-0.57146
C	4.8076	1.97706	1.0665
H	4.86812	1.33022	1.94892
H	5.62839	1.7167	0.38624
H	4.98837	3.01197	1.38645

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6512577
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.633930871988
ΔG_{solv} = -0.014939

I-σ-E_3

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.442760 (Hartree/Particle)
Thermal correction to Energy= 0.476562
Thermal correction to Enthalpy= 0.477506
Thermal correction to Gibbs Free Energy= 0.376964
Sum of electronic and zero-point Energies= -3278.916427
Sum of electronic and thermal Energies= -3278.882625
Sum of electronic and thermal Enthalpies= -3278.881681
Sum of electronic and thermal Free Energies= -3278.982222

C	-0.60265	-0.81413	-1.18196
C	0.44981	0.14432	-0.68864
C	1.71853	-0.48479	-0.77813
C	2.22143	-2.79905	0.04254
C	1.29049	-2.57112	1.19867
C	-0.00543	-2.31404	0.74222
H	-1.60146	-0.63718	-0.76935
H	-0.6872	-0.73167	-2.27557
H	0.32297	1.22141	-0.77798
H	2.23731	-3.87021	-0.20834
H	3.25153	-2.49508	0.25539
H	1.5001	-2.98814	2.17967
C	0.01553	-2.14633	-0.77175
H	-0.41259	-3.02418	-1.27366
C	1.5294	-1.97312	-1.04195
H	1.81936	-2.22941	-2.06928
C	3.00193	0.18199	-1.05365
C	4.14727	-0.56447	-1.37618
C	3.0966	1.58481	-1.09649
C	5.34762	0.05385	-1.69727
H	4.10963	-1.64914	-1.40469
C	4.28878	2.21541	-1.40718
H	2.21929	2.19354	-0.89133

C	5.40137	1.43772	-1.69766
H	6.23298	-0.52033	-1.95311
H	4.36646	3.29832	-1.43951
C	-1.2302	-2.6498	1.48825
C	-2.45052	-2.81948	0.82192
C	-1.19913	-2.85245	2.8776
C	-3.60515	-3.17569	1.50964
H	-2.51023	-2.68886	-0.25575
C	-2.34229	-3.20329	3.57781
H	-0.26684	-2.71078	3.42258
C	-3.53196	-3.35973	2.87902
H	-4.55323	-3.31317	0.99815
H	-2.32673	-3.35764	4.65273
F	-4.63549	-3.70077	3.54984
F	6.55072	2.04153	-2.00402
Ir	1.09517	-0.35064	1.35503
Cl	1.98738	-0.77953	3.61197
O	0.62413	3.06136	0.42565
C	1.34585	2.76703	1.38027
C	1.91746	4.00022	2.17888
Cl	2.73771	3.59434	3.72387
Cl	3.09091	4.8225	1.10441
Cl	0.57327	5.11829	2.54925
N	1.73122	1.57228	1.78376
H	2.26944	1.56211	2.64497
C	-0.9039	1.75134	3.80698
H	-0.71276	2.65254	3.21702
C	-1.00958	0.57719	3.16053
H	-1.19974	-0.3322	3.73528
C	-0.88131	0.4545	1.71361
H	-0.88595	1.41475	1.19037
H	-1.58089	-0.25316	1.27033
C	-1.00544	1.92303	5.27665
H	-1.80296	2.6252	5.55079
H	-1.18861	0.96963	5.78336
H	-0.07241	2.3505	5.67091

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.660884
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.64294905833
ΔG_{solv} = -0.0146445

I-σ-E$_2$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.442294 (Hartree/Particle)
Thermal correction to Energy= 0.476180
Thermal correction to Enthalpy= 0.477124
Thermal correction to Gibbs Free Energy= 0.376043
Sum of electronic and zero-point Energies= -3278.915251
Sum of electronic and thermal Energies= -3278.881366
Sum of electronic and thermal Enthalpies= -3278.880422
Sum of electronic and thermal Free Energies= -3278.981503

C	0.09249	-2.46889	-1.53425
C	1.15437	-1.40143	-1.56339
C	2.18327	-1.72063	-0.66771
C	1.85873	-2.61474	1.66896
C	0.74593	-1.61835	1.83232
C	-0.26732	-1.87358	0.88393
H	-0.91026	-2.13384	-1.81147
H	0.3709	-3.26469	-2.24185
H	1.30598	-0.77881	-2.44086
H	1.63419	-3.5078	2.27141
H	2.83996	-2.25154	1.99042
H	0.53732	-1.11281	2.77179
C	0.22539	-2.94029	-0.09517
H	-0.24625	-3.90789	0.11951
C	1.7476	-2.91444	0.17921
H	2.25624	-3.83291	-0.14386
C	3.59981	-1.36856	-0.87434
C	4.61703	-2.06904	-0.21364
C	3.97074	-0.36712	-1.78619
C	5.95947	-1.79093	-0.45103
H	4.37059	-2.86302	0.48683
C	5.30251	-0.08329	-2.04059
H	3.20161	0.21726	-2.28811
C	6.28023	-0.80278	-1.36521
H	6.7515	-2.33569	0.05425
H	5.59542	0.68911	-2.74625
C	-1.70079	-1.57837	1.11189
C	-2.56389	-1.15894	0.088
C	-2.22701	-1.73197	2.40189
C	-3.90795	-0.9168	0.33504
H	-2.17897	-0.97433	-0.91181
C	-3.5703	-1.50255	2.664
H	-1.57491	-2.05483	3.20924
C	-4.38966	-1.09917	1.62193
H	-4.58027	-0.58102	-0.44886
H	-3.98802	-1.6297	3.65835
F	-5.68338	-0.87182	1.86614
F	7.56628	-0.53446	-1.60974
Ir	0.79253	-0.08811	0.21606
Cl	0.79996	1.70263	-1.4583
C	2.95107	1.79879	1.00668
H	2.28103	2.65845	1.07913
C	2.45377	0.51003	1.47388
H	3.22079	-0.26686	1.44432
C	4.19806	1.96261	0.53555
O	-0.30997	0.6592	3.52158
C	-0.54679	1.43108	2.59838
C	-1.42715	2.69397	2.94228
Cl	-1.34644	3.06554	4.67529
Cl	-0.93306	4.15636	2.02405
Cl	-3.11844	2.26569	2.50743
N	-0.22407	1.31746	1.31682
H	-0.4489	2.12224	0.73826
H	4.84544	1.08426	0.47379
H	1.9625	0.55416	2.44861
C	4.77275	3.25278	0.07898
H	5.09934	3.17492	-0.96761
H	4.04598	4.06836	0.15323
H	5.66401	3.52666	0.65788

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3280.6596376
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.643285104033
ΔG_{solv} = -0.0152398

I-σ-E$_1$

M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
Zero-point correction= 0.442142 (Hartree/Particle)
Thermal correction to Energy= 0.476009
Thermal correction to Enthalpy= 0.476953

Thermal correction to Gibbs Free Energy=	0.376570
Sum of electronic and zero-point Energies=	-3278.912739
Sum of electronic and thermal Energies=	-3278.878872
Sum of electronic and thermal Enthalpies=	-3278.877928
Sum of electronic and thermal Free Energies=	-3278.978310

B3LYP-D3/6-311+G(d,p)-SDD(Ir)-CPCM (diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = 3280.6573552
DLPNO-CCSD(T)/def2TZVPP-CPCM(diethyl ether)//M06/6-31G(d,p)-LANL2DZ (Ir)-CPCM (diethyl ether)
HF = -3275.638465467709
ΔG_{solv} = -0.0142366

C	0.13627	-3.94567	-0.91531
C	1.02513	-3.07299	-1.75847
C	2.12903	-2.64074	-1.01306
C	2.07489	-1.83544	1.35846
C	0.81493	-1.08598	1.01344
C	-0.19282	-2.02357	0.69158
H	-0.91721	-3.89356	-1.20879
H	0.4534	-4.99481	-1.01396
H	1.0413	-3.16479	-2.84177
H	2.03219	-2.13413	2.41708
H	2.99471	-1.263	1.21579
H	0.60319	-0.10001	1.41777
C	0.43941	-3.39838	0.48219
H	0.17649	-4.07865	1.30279
C	1.94167	-3.04346	0.44231
H	2.58697	-3.89262	0.70418
C	3.45814	-2.34114	-1.5732
C	4.6048	-2.46379	-0.77687
C	3.62266	-1.97508	-2.91885
C	5.87284	-2.22115	-1.29193
H	4.51792	-2.76217	0.26499
C	4.87978	-1.72139	-3.44496
H	2.7474	-1.85912	-3.55719
C	5.98881	-1.84801	-2.61985
H	6.76449	-2.31763	-0.67965
H	5.01336	-1.42828	-4.48213
C	-1.63841	-1.88674	0.94753
C	-2.50882	-2.97153	0.75197
C	-2.17497	-0.70583	1.49198
C	-3.86217	-2.88036	1.04816
H	-2.13312	-3.92079	0.38397
C	-3.5229	-0.59804	1.78791
H	-1.52832	0.14659	1.68475
C	-4.35051	-1.68748	1.5535
H	-4.5352	-3.71946	0.90002
H	-3.94055	0.31206	2.2089
F	-5.64966	-1.58721	1.84112
F	7.20219	-1.60533	-3.12438
Ir	0.46276	-1.01151	-1.19167
Cl	0.1987	-0.69286	-3.59619
C	2.97701	0.72121	-0.27377
H	3.86969	0.09155	-0.24059
C	2.83237	1.69227	0.64724
C	2.03742	0.49886	-1.35588
O	-0.36534	1.77518	0.84286
C	-0.89535	1.64059	-0.26066
Cl	-2.90096	3.27413	0.60484
N	-0.80179	0.62716	-1.10301
H	-1.25726	0.77166	-1.99986
H	2.50725	0.13705	-2.27228
C	-1.76815	2.86701	-0.71408
Cl	-2.71955	2.62369	-2.2148
Cl	-0.63127	4.22864	-0.9755
H	1.40811	1.36954	-1.55565
H	1.93035	2.30857	0.61167
C	3.8017	1.95373	1.74015
H	4.66148	1.27626	1.69095
H	4.17016	2.98706	1.71174
H	3.32091	1.83053	2.72023

Appendix 4: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 4 (Mechanistic Studies of Photoredox/Nickel Dual-Catalyzed Carbon-Carbon Bond Formations)

A4.1 Methods

A4.1.1 Computational Methods in the study of the Photoredox/Nickel Dual-Catalyzed Single-Electron Tsuji-Trost Reaction

All optimizations of intermediates and transition state structures were carried out in the gas phase without constraints using spin-unrestricted DFT using UB3LYP[231]/6-31G(d) method with the "opt=noeigen" and "guess=mix" keywords as implemented in Gaussian09. Frequency calculations were performed at the same level to determine vibrational frequencies, obtain thermal corrections to enthalpy ($H_{correction}$) and free energy ($G_{correction}$) at 298K, and to determine whether the optimized structures were transition states (if there existed only a single imaginary frequency) or intermediates (if no imaginary frequencies were found). Exhaustive conformational searches were performed for all structures to elucidate the lowest energy profiles, To refine the energies, we performed single point energy calculations on optimized geometries using implicit solvent (water;; $\varepsilon = 78.3553$) with SMD[232] as the solvation model in combination with the UM06 functional[233] and the 6-311+G(d,p) basis set. For comparison, we also computed single point energies using D3 dispersion correction of Grimme et al.with UB3LYP (i.e., UB3LYP- D3)[234] and the UM06 functionals in combination the 6-311+G(d,p) basis set in solvent (water) using the SMD solvation model. Finally, for comparison, we also performed open-shell domain-based local pair natural orbital Coupled-Cluster calculations using single and double excitations with perturbative triple excitations (DLPNO-CCSD(T)) with def2-TZVPP basis set[235] and

def2-TZVPP/C auxiliary basis set[236] were performed on the lowest energy pathways using ORCA software[237] with the "NormalPNO" and "SlowConv" keywords. The total free energies using this method was computed as followed: $G = E^{DLPNO\text{-}CCSD(T)} + G$ thermal corrections$^{UB3LYP} + \Delta G_{solvation}{}^{UB3LYP\text{-}D3}$ where $\Delta G_{solvation}{}^{UB3LYP} = E^{UB3LYP\text{-}D3/6\text{-}311+G(d,p)\text{-}SMD(water)} - E^{UB3LYP\text{-}D3/6\text{-}311+G(d,p)\text{-}gas}$ This method provides accurate energies (within 3 kJ mol^{-1}) with the computational cost comparable to DFT calculations[238] and has been used to study organometallic reaction mechanisms.[239] All structural figures were generated using CYLview[xi] and GaussView 5.[240]

A4.1.2 Computational Methods in the study of the Use of Oxabenzonorbornadiene as Electrophilic Coupling Partners under Photoredox/Nickel Dual Catalysis

All optimizations of intermediates and transition states were calculated without constraints using unrestricted using UB3LYP/6-31G(d) level of the theory in implicit solvent (acetone) using CPCM as solvation model with the "guess=mix" keyword, as implemented in Gaussian09 and Gaussian16. Frequency calculations, at the same level of theory, were used to obtain thermal corrections (at 298K) and to characterize optimized structures as transition states (only a single imaginary frequency) or intermediate (if no imaginary frequencies were found). Single point energy calculations in implicit solvent using UM06/6-311+G(d,p) were also performed on all structures. All 3-D structures were generated using CYLview.

A4.2 Supplementary Figures

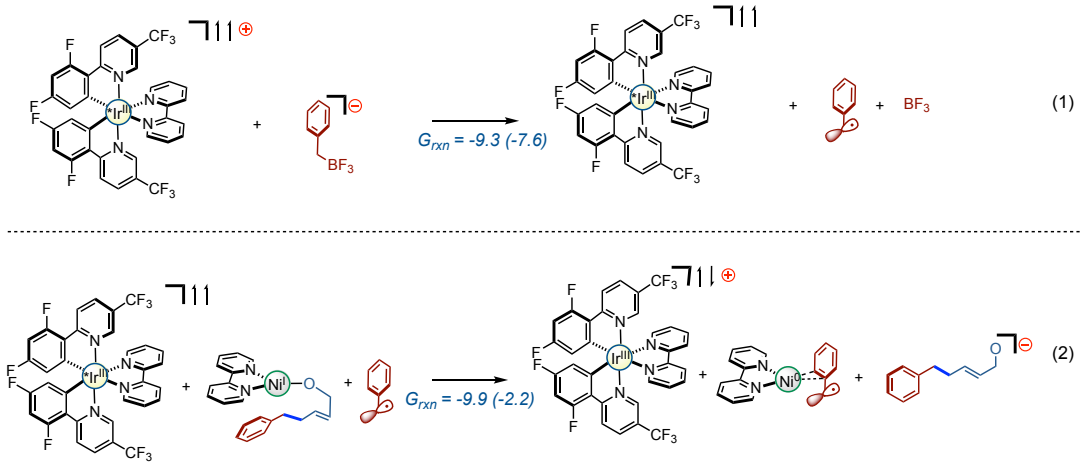


Figure A4.1 Energetics of radical formation from the photocatalyst (1) and of product formation (2). Free energies were computed computed at the UM06/6-311+G(d,p)-LANL2DZ(Ir)-SMD(water)//UB3LYP-6-31G(d) and UB3LYP-D3/6-311+G(d,p)-LANL2DZ(Ir)-SMD(water)//UB3LYP-6-31G(d) level (parethesis).

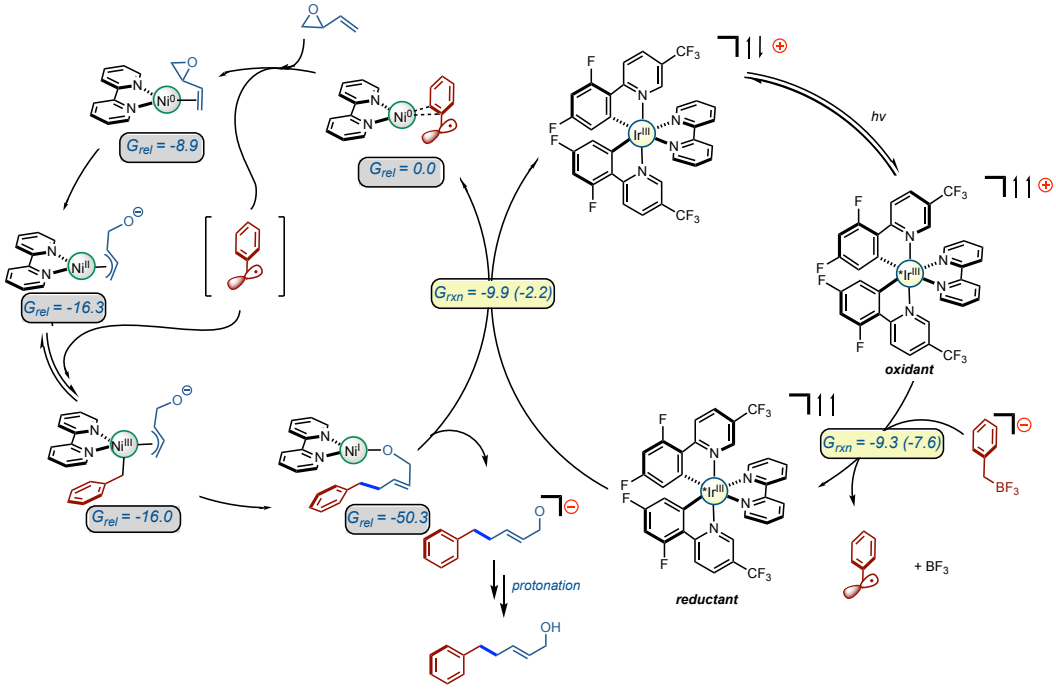


Figure A4.2 Overall computed energetics for the dual nickel/photocatalyzed cross-coupling. Listed energies are in kcal/mol computed at the UM06/6-311+G(d,p)-SMD(water)//UB3LYP-6-31G(d) level of theory. Single electron transfer events (yellow) were computed at the UM06/6-311+G(d,p)-LANL2DZ(Ir)-SMD(water)//UB3LYP-6-31G(d) and UB3LYP-D3/6-311+G(d,p)-LANL2DZ(Ir)-SMD(water)//UB3LYP-6-31G(d) level (parenthesis).

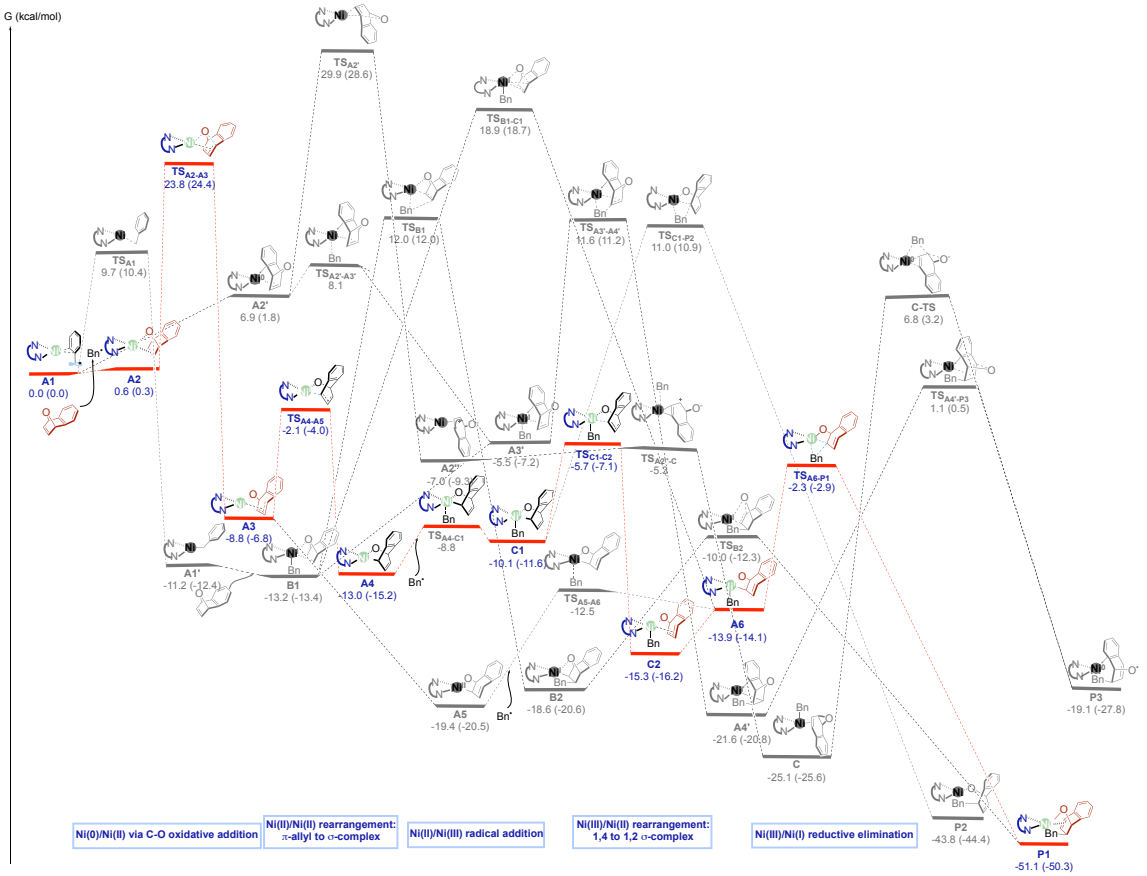


Figure A4.3 Energetics of all competing pathways. Lowest energy pathway is colored. Free energies (kcal/mol) are at the UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d) level of theory.

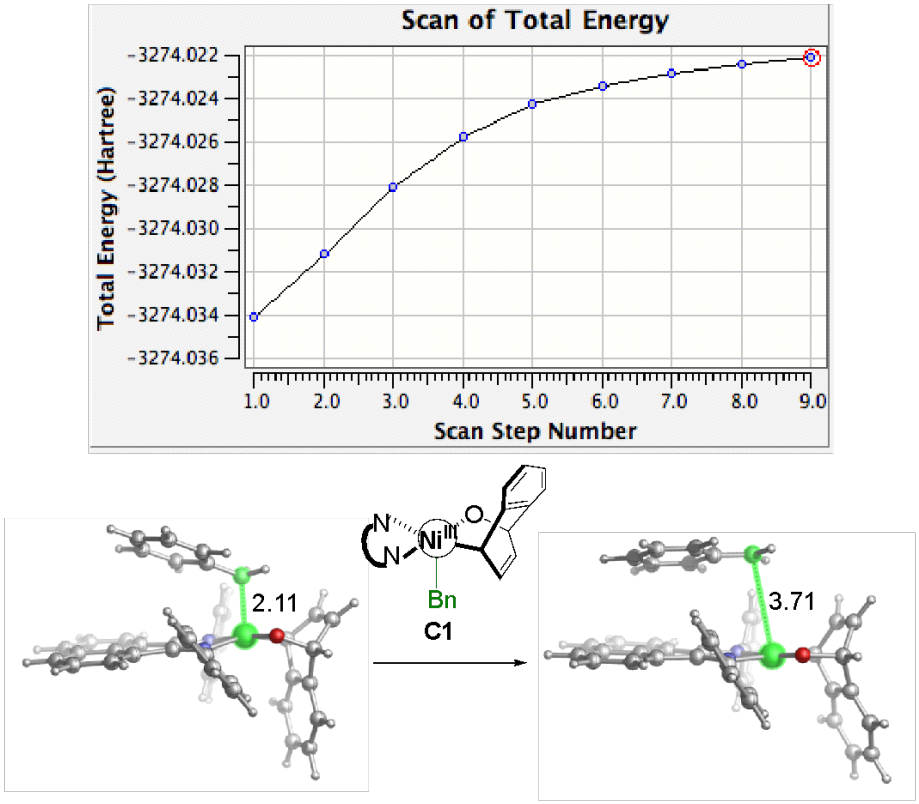


Figure A4.4 A sample of one of the relaxed scans of the total energy as a function of scan step number for the radical addition to **3** to produce **4**. The Ni-C(Bn) bond (highlighted in green) was scanned from a starting bond length of 2.11 Å to an ending point of 3.71 Å.

A4.3 Coordinates and Energies

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.276831 (Hartree/Particle)
Thermal correction to Energy= 0.293478
Thermal correction to Enthalpy= 0.294422
Thermal correction to Gibbs Free Energy= 0.231429
Sum of electronic and zero-point Energies= -2274.226213
Sum of electronic and thermal Energies= -2274.209566
Sum of electronic and thermal Enthalpies= -2274.208622
Sum of electronic and thermal Free Energies= -2274.271616
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.1583862
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.8877466
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2272.472168063574

ΔG_{solv} = -0.0056383

A-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -95.44 cm^{-1}
Zero-point correction= 0.274198 (Hartree/Particle)
Thermal correction to Energy= 0.290971
Thermal correction to Enthalpy= 0.291915
Thermal correction to Gibbs Free Energy= 0.228224
Sum of electronic and zero-point Energies= -2274.210476
Sum of electronic and thermal Energies= -2274.193704
Sum of electronic and thermal Enthalpies= -2274.192759
Sum of electronic and thermal Free Energies= -2274.256450

C	-1.45189	2.03439	0.64615
C	0.67761	2.42732	-0.32566
C	0.31175	3.71701	-0.72049
C	-0.99473	4.17848	-0.41376
C	-1.87174	3.33392	0.27313
C	-2.2916	1.05112	1.32798
C	-2.38662	-1.16384	2.17232
C	-3.72767	-1.01974	2.537
C	-4.36744	0.22467	2.29653
C	-3.64418	1.25765	1.69363
H	1.6601	2.01724	-0.53888
H	1.02148	4.34238	-1.25216
H	-1.31177	5.17443	-0.71029
H	-2.87341	3.67357	0.51576
H	-1.84616	-2.08938	2.34594
H	-4.25663	-1.84703	2.99874
H	-5.40687	0.37283	2.57569
H	-4.12059	2.21311	1.50003
N	-0.17001	1.59816	0.34673
N	-1.67275	-0.16146	1.58786
Ni	0.25102	-0.1573	1.13903
C	1.92498	-0.99434	2.11151
C	1.26732	-2.10154	2.73545
C	1.02457	-3.29735	2.05169
C	1.48479	-3.41983	0.69751
C	2.15816	-2.38884	0.06614
C	2.4592	-1.1257	0.74295
H	2.28952	-0.17869	2.73528
H	0.96138	-1.99748	3.77551
H	0.52125	-4.12749	2.53988
H	1.30811	-4.35011	0.16002
H	2.5192	-2.51546	-0.95312
C	3.20819	-0.11799	0.12261
H	3.59594	-0.25122	-0.88413
H	3.50334	0.78007	0.66057

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.1527528
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.8833272
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2272.466173902212
ΔG_{solv} = -0.014615

B

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.114993 (Hartree/Particle)
Thermal correction to Energy= 0.120659
Thermal correction to Enthalpy= 0.121603
Thermal correction to Gibbs Free Energy= 0.085325
Sum of electronic and zero-point Energies= -270.800147
Sum of electronic and thermal Energies= -270.794481
Sum of electronic and thermal Enthalpies= -270.793537
Sum of electronic and thermal Free Energies= -270.829815

C	2.74508	-1.15846	-0.78885
C	3.96616	-0.54991	-0.48172
C	4.44401	-0.53276	0.84965
C	3.67794	-1.13642	1.87431
C	2.45538	-1.74784	1.57891
C	1.94812	-1.77888	0.23416
H	2.38205	-1.16936	-1.81497
H	4.55387	-0.08618	-1.27094
H	5.39393	-0.05861	1.08397
H	4.04368	-1.12389	2.89872
H	1.8698	-2.21095	2.37103
C	0.70797	-2.39894	-0.07206
H	0.10525	-2.86798	0.70199
H	0.32508	-2.42294	-1.08953

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2274.1761005
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.9135258
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2272.490424211042

ΔG_{solv} = -0.0122301

Ni-Bn-radical

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.114993 (Hartree/Particle)
Thermal correction to Energy= 0.120659
Thermal correction to Enthalpy= 0.121603
Thermal correction to Gibbs Free Energy= 0.085325
Sum of electronic and zero-point Energies= -270.800147
Sum of electronic and thermal Energies= -270.794481
Sum of electronic and thermal Enthalpies= -270.793537
Sum of electronic and thermal Free Energies= -270.829815

C	2.74508	-1.15846	-0.78885
C	3.96616	-0.54991	-0.48172
C	4.44401	-0.53276	0.84965
C	3.67794	-1.13642	1.87431
C	2.45538	-1.74784	1.57891
C	1.94812	-1.77888	0.23416
H	2.38205	-1.16936	-1.81497
H	4.55387	-0.08618	-1.27094
H	5.39393	-0.05861	1.08397
H	4.04368	-1.12389	2.89872
H	1.8698	-2.21095	2.37103
C	0.70797	-2.39894	-0.07206
H	0.10525	-2.86798	0.70199
H	0.32508	-2.42294	-1.08953

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -270.75733
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-270.9952919
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -270.397554147875
ΔG_{solv} = -0.000751

Ni-VE-By-substrate

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.090843 (Hartree/Particle)
Thermal correction to Energy= 0.095976
Thermal correction to Enthalpy= 0.096921
Thermal correction to Gibbs Free Energy= 0.062850
Sum of electronic and zero-point Energies= -231.095575
Sum of electronic and thermal Energies= -231.090442
Sum of electronic and thermal Enthalpies= -231.089498
Sum of electronic and thermal Free Energies= -231.123568

C	1.63349	0.0152	1.78963
H	2.27435	0.84994	1.49639
C	1.2083	-0.94134	0.74956
H	1.78433	-0.3319	2.68677
H	1.04247	-1.86397	1.01291
C	1.89387	-0.84922	-0.62634
C	1.76105	-1.99599	-1.58584
H	2.85325	-0.30568	-0.56929
H	1.17447	-2.88181	-1.28537
H	2.62542	-2.2722	-2.21482
O	1.04532	-0.70447	-1.85607

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-231.0961417
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-231.2679346
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -230.802082513855
ΔG_{solv} = -0.0054462

B'

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.370239 (Hartree/Particle)
Thermal correction to Energy= 0.393161
Thermal correction to Enthalpy= 0.394106
Thermal correction to Gibbs Free Energy= 0.313482
Sum of electronic and zero-point Energies= -2505.361098
Sum of electronic and thermal Energies= -2505.338175
Sum of electronic and thermal Enthalpies= -2505.337231
Sum of electronic and thermal Free Energies= -2505.417854

C	-1.08408	1.75012	0.69367
C	1.20805	1.4324	0.92934
C	1.31986	2.51277	1.79753
C	0.17173	3.23828	2.11524
C	-1.04231	2.84826	1.55937
C	-2.32473	1.25743	0.05758
C	-3.19768	-0.16329	-1.55011
C	-4.50409	0.21548	-1.25762
C	-4.71089	1.15569	-0.24603
C	-3.60965	1.68102	0.4217
H	2.06897	0.82662	0.67327
H	2.28763	2.77115	2.21412
H	0.21964	4.09302	2.7832
H	-1.94679	3.40226	1.78355
H	-2.98412	-0.89679	-2.32327
H	-5.33434	-0.21716	-1.80642
H	-5.71495	1.47037	0.0227
H	-3.75112	2.39786	1.22303
N	0.04077	1.05826	0.37497
N	-2.13	0.34052	-0.91687
Ni	-0.11549	-0.3651	-0.978
C	1.8752	-3.05474	0.46009
C	3.08711	-3.34317	1.08223
C	3.41955	-2.74473	2.30161
C	2.51274	-1.86055	2.8886
C	1.30057	-1.57219	2.26112
C	0.94589	-2.15456	1.02571
H	1.62974	-3.54356	-0.4801
H	3.77497	-4.04587	0.61733
H	4.36351	-2.97313	2.78918
H	2.74479	-1.39979	3.84657
H	0.59517	-0.89906	2.7439
C	-0.33231	-1.82424	0.35176
H	-1.06937	-1.46494	1.08141
H	-0.74897	-2.69932	-0.15538
C	0.13302	-1.60994	-2.47576
H	-0.70148	-1.50203	-3.17391

H	0.41179	-2.64307	-2.28903
C	1.14787	-0.61584	-2.46573
H	2.17897	-0.84164	-2.19988
C	0.69765	0.72139	-2.57881
H	-0.14932	0.91912	-3.23509
C	1.65112	1.8969	-2.44166
H	2.43771	1.65923	-1.6992
H	1.11032	2.80091	-2.10134
O	1.54377	1.15542	-3.7495

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3023645
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.2104688
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.329788687910
ΔG_{solv} = -0.0193036

B'-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -319.59 cm^{-1}
Zero-point correction= 0.368655 (Hartree/Particle)
Thermal correction to Energy= 0.391384
Thermal correction to Enthalpy= 0.392328
Thermal correction to Gibbs Free Energy= 0.313674
Sum of electronic and zero-point Energies= -2505.324378
Sum of electronic and thermal Energies= -2505.301649
Sum of electronic and thermal Enthalpies= -2505.300704
Sum of electronic and thermal Free Energies= -2505.379358

C	-1.08408	1.75012	0.69367
C	1.20805	1.4324	0.92934
C	1.31986	2.51277	1.79753
C	0.17173	3.23828	2.11524
C	-1.04231	2.84826	1.55937
C	-2.32473	1.25743	0.05758
C	-3.19768	-0.16329	-1.55011
C	-4.50409	0.21548	-1.25762
C	-4.71089	1.15569	-0.24603
C	-3.60965	1.68102	0.4217
H	2.06897	0.82662	0.67327
H	2.28763	2.77115	2.21412
H	0.21964	4.09302	2.7832
H	-1.94679	3.40226	1.78355
H	-2.98412	-0.89679	-2.32327
H	-5.33434	-0.21716	-1.80642
H	-5.71495	1.47037	0.0227
H	-3.75112	2.39786	1.22303
N	0.04077	1.05826	0.37497
N	-2.13	0.34052	-0.91687
Ni	-0.11549	-0.3651	-0.978
C	1.8752	-3.05474	0.46009
C	3.08711	-3.34317	1.08223
C	3.41955	-2.74473	2.30161
C	2.51274	-1.86055	2.8886
C	1.30057	-1.57219	2.26112
C	0.94589	-2.15456	1.02571
H	1.62974	-3.54356	-0.4801
H	3.77497	-4.04587	0.61733
H	4.36351	-2.97313	2.78918
H	2.74479	-1.39979	3.84657
H	0.59517	-0.89906	2.7439
C	-0.33231	-1.82424	0.35176
H	-1.06937	-1.46494	1.08141
H	-0.74897	-2.69932	-0.15538
C	0.13302	-1.60994	-2.47576
H	-0.70148	-1.50203	-3.17391
H	0.41179	-2.64307	-2.28903
C	1.14787	-0.61584	-2.46573
H	2.17897	-0.84164	-2.19988
C	0.69765	0.72139	-2.57881
H	-0.14932	0.91912	-3.23509
C	1.65112	1.8969	-2.44166
H	2.43771	1.65923	-1.6992
H	1.11032	2.80091	-2.10134
O	1.8641	1.36807	-3.99328

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = - 2505.2857689
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.2003958
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.279192796534
ΔG_{solv} = -0.0390393

A''

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.252481 (Hartree/Particle)
Thermal correction to Energy= 0.268299
Thermal correction to Enthalpy= 0.269244
Thermal correction to Gibbs Free Energy= 0.207211
Sum of electronic and zero-point Energies= -2234.523418
Sum of electronic and thermal Energies= -2234.507600
Sum of electronic and thermal Enthalpies= -2234.506656
Sum of electronic and thermal Free Energies= -2234.568688

C	-2.09139	2.31433	0.86226
C	-0.60045	2.29548	2.65039
C	-1.34907	3.2387	3.34487
C	-2.51948	3.72874	2.76326
C	-2.89366	3.25707	1.50751
C	-2.36718	1.74219	-0.47025
C	-1.59	0.23902	-2.07149
C	-2.62395	0.56782	-2.94186
C	-3.56447	1.51936	-2.54539
C	-3.42795	2.11877	-1.29569
H	0.30859	1.87258	3.06297
H	-1.01858	3.57672	4.32156
H	-3.13207	4.46249	3.27829
H	-3.80343	3.61582	1.03871
H	-0.81183	-0.46833	-2.33986
H	-2.68287	0.08483	-3.91175
H	-4.38439	1.79863	-3.20026
H	-4.13605	2.87402	-0.97226
N	-0.94936	1.83577	1.43434
N	-1.46337	0.79615	-0.85248
Ni	-0.13439	0.41052	0.46111
C	1.16771	-0.16166	2.17333
H	1.78899	0.70341	1.93011
C	0.53731	-0.90572	1.06587
H	1.44649	-0.66908	2.95621
H	0.37552	-1.85849	1.18485

C	0.99399	-0.57334	-0.36681
C	0.6564	-1.5233	-1.47899
H	1.97313	-0.06313	-0.37557
H	0.75491	-1.18219	-2.52445
H	-0.19424	-2.2159	-1.35341
O	1.79401	-2.7243	-1.61709

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5095924
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2235.1741033
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2232.882939502140
ΔG_{solv} = -0.0206952

A''-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -329.39 cm^{-1}
Zero-point correction= 0.251353 (Hartree/Particle)
Thermal correction to Energy= 0.266957
Thermal correction to Enthalpy= 0.267901
Thermal correction to Gibbs Free Energy= 0.207241
Sum of electronic and zero-point Energies= -2234.525252
Sum of electronic and thermal Energies= -2234.509648
Sum of electronic and thermal Enthalpies= -2234.508704
Sum of electronic and thermal Free Energies= -2234.569364

C	-2.21805	2.2067	1.01322
C	-0.8602	2.24573	2.90975
C	-1.85308	2.85778	3.66243
C	-3.08162	3.13915	3.06051
C	-3.26027	2.80848	1.72103
C	-2.26557	1.84905	-0.4142
C	-1.02128	0.94125	-2.16952
C	-2.06512	1.16928	-3.06505
C	-3.2467	1.7485	-2.60533
C	-3.34417	2.10529	-1.26234
H	0.10485	2.00186	3.33588
H	-1.66162	3.10734	4.70086
H	-3.88259	3.61019	3.62197
H	-4.20318	3.01742	1.2281
H	-0.03147	0.56791	-2.4532
H	-1.93935	0.90042	-4.1089
H	-4.07648	1.9356	-3.28106
H	-4.2424	2.58264	-0.88617
N	-1.02411	1.91274	1.61144
N	-1.12845	1.24983	-0.86255
Ni	0.12817	0.87645	0.57706
C	1.17951	-0.03141	1.83021
H	2.04927	0.49458	2.23892
C	1.36142	-0.67741	0.53589
H	0.659	-0.60703	2.5993
H	0.86863	-1.61779	0.2884
C	2.28411	-0.14783	-0.37521
C	2.61845	-0.66706	-1.7188
H	2.77675	0.79031	-0.12996
H	3.04322	0.11678	-2.38177
H	1.76236	-1.1248	-2.25478
O	3.35321	-1.31789	-0.75022

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5046845
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2235.1763672
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2232.854547783025
ΔG_{solv} = -0.039931

B''

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.251237 (Hartree/Particle)
Thermal correction to Energy= 0.267198
Thermal correction to Enthalpy= 0.268142
Thermal correction to Gibbs Free Energy= 0.207218
Sum of electronic and zero-point Energies= -2234.499830
Sum of electronic and thermal Energies= -2234.483869
Sum of electronic and thermal Enthalpies= -2234.482924
Sum of electronic and thermal Free Energies= -2234.543848

C	-2.09139	2.31433	0.86226
C	-0.60045	2.29548	2.65039
C	-1.34907	3.2387	3.34487
C	-2.51948	3.72874	2.76326
C	-2.89366	3.25707	1.50751
C	-2.36718	1.74219	-0.47025
C	-1.59	0.23902	-2.07149
C	-2.62395	0.56782	-2.94186
C	-3.56447	1.51936	-2.54539
C	-3.42795	2.11877	-1.29569
H	0.30859	1.87258	3.06297
H	-1.01858	3.57672	4.32156
H	-3.13207	4.46249	3.27829
H	-3.80343	3.61582	1.03871
H	-0.81183	-0.46833	-2.33986
H	-2.68287	0.08483	-3.91175
H	-4.38439	1.79863	-3.20026
H	-4.13605	2.87402	-0.97226
N	-0.94936	1.83577	1.43434
N	-1.46337	0.79615	-0.85248
Ni	-0.13439	0.41052	0.46111
C	0.64814	-1.55952	1.45703
H	1.1168	-1.12328	2.34221
C	0.81569	-0.87001	0.16319
H	0.59959	-2.53195	1.44665
H	0.81451	-1.40784	-0.64849
C	1.84279	0.27536	0.09394
C	2.30199	0.76325	-1.24936
H	2.57003	0.22277	0.92308
H	2.83311	1.72887	-1.31668
H	1.66266	0.58597	-2.13189
O	3.57617	-0.13594	-1.81814

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5213308
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = - 2235.1929384
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2232.8431
ΔG_{solv} = -0.0624885

B''-C-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -118.30 cm^{-1}
Zero-point correction= 0.366489 (Hartree/Particle)
Thermal correction to Energy= 0.389629
Thermal correction to Enthalpy= 0.390573
Thermal correction to Gibbs Free Energy= 0.309400
Sum of electronic and zero-point Energies= -2505.299540
Sum of electronic and thermal Energies= -2505.276400
Sum of electronic and thermal Enthalpies= -2505.275456
Sum of electronic and thermal Free Energies= -2505.356629

C	-1.6496	1.2818	1.34746
C	0.6055	1.81183	1.79102
C	0.26003	2.60437	2.89104
C	-1.10348	2.7151	3.24415
C	-2.05844	2.04413	2.46607
C	-2.5476	0.57738	0.44555
C	-2.6721	-0.94304	-1.35147
C	-4.07159	-0.88506	-1.37573
C	-4.72984	-0.05014	-0.44806
C	-3.95693	0.68734	0.46427
H	1.64164	1.68806	1.49557
H	1.03494	3.11664	3.45248
H	-1.4086	3.30577	4.10355
H	-3.11074	2.10083	2.72524
H	-2.13205	-1.57032	-2.04963
H	-4.62223	-1.47773	-2.09914
H	-5.81371	0.02789	-0.44136
H	-4.43693	1.3528	1.17458
N	-0.31562	1.15801	1.01642
N	-1.90476	-0.2391	-0.46238
Ni	0.01751	-0.13324	-0.34789
C	1.56911	-3.00405	1.49008
C	2.95027	-3.02211	1.61029
C	3.61524	-2.01623	2.32751
C	2.87324	-0.98619	2.92492
C	1.49182	-0.95578	2.80895
C	0.79031	-1.96584	2.08432
H	1.05923	-3.78806	0.93559
H	3.52074	-3.82184	1.14543
H	4.69728	-2.03556	2.41998
H	3.38443	-0.20695	3.48482
H	0.92196	-0.15344	3.27132
C	-0.61159	-1.94001	1.96292
H	-1.19995	-1.14607	2.41279
H	-1.14303	-2.71192	1.41599
C	1.9537	-0.27448	-0.22614
H	2.40663	0.58352	-0.72956
H	2.41666	-0.52918	0.72549
C	1.43789	-1.33452	-1.01819
H	1.41227	-2.35578	-0.63945
C	0.64903	-0.99034	-2.12941
H	0.9012	-0.06924	-2.66265
C	0.05869	-2.0586	-3.03744
H	-0.83786	-1.65833	-3.56619
H	-0.2854	-2.91871	-2.41372
O	1.1063	-2.31999	-3.85428

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2944336
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.2038158
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.253379015522
ΔG_{solv} = -0.0613693

C

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.368972 (Hartree/Particle)
Thermal correction to Energy= 0.391340
Thermal correction to Enthalpy= 0.392284
Thermal correction to Gibbs Free Energy= 0.316297
Sum of electronic and zero-point Energies= -2505.338240
Sum of electronic and thermal Energies= -2505.315872
Sum of electronic and thermal Enthalpies= -2505.314928
Sum of electronic and thermal Free Energies= -2505.390915

C	-1.52959	-0.2832	2.37299
C	0.66317	0.22089	2.98422
C	0.26326	0.6746	4.23412
C	-1.09331	0.63081	4.5604
C	-1.99563	0.15047	3.61794
C	-2.38927	-0.76001	1.2763
C	-2.42354	-1.34748	-0.98999
C	-3.81004	-1.52569	-0.93487
C	-4.48983	-1.33293	0.26276
C	-3.76889	-0.93058	1.38643
H	1.70519	0.22769	2.68906
H	1.00324	1.05034	4.93263
H	-1.44332	0.97224	5.52985
H	-3.05566	0.12324	3.8418
H	-1.82853	-1.35462	-1.94374
H	-4.33707	-1.81067	-1.84006
H	-5.56482	-1.47727	0.32793
H	-4.27553	-0.7549	2.3289
N	-0.20238	-0.25756	2.06901
N	-1.72559	-0.99121	0.10966
Ni	0.23847	-0.93697	0.33881
C	1.67633	1.50578	-2.73846
C	2.84579	2.028	-3.27364
C	3.62099	2.94076	-2.54419
C	3.21083	3.33156	-1.26172
C	2.04348	2.81837	-0.71381
C	1.24056	1.89302	-1.43653
H	1.06449	0.78834	-3.28509
H	3.1614	1.72688	-4.26954
H	4.53515	3.34542	-2.97039
H	3.80754	4.04302	-0.69574
H	1.72245	3.13122	0.27806
C	0.03438	1.35819	-0.9123
H	-0.40418	1.79883	-0.02053
H	-0.58769	0.76477	-1.57417
C	2.01628	-1.61358	0.74633
H	2.78574	-0.88668	0.47812
H	2.16834	-2.07883	1.72067
C	1.43097	-2.39603	-0.29719
H	1.03997	-3.39597	-0.10548
C	1.05503	-1.69432	-1.44099
H	1.63983	-0.81184	-1.69559
C	0.15883	-2.14958	-2.5765
H	-0.45509	-3.01103	-2.18333
H	0.81979	-2.6249	-3.34577
O	-0.57159	-1.09859	-3.03637

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3019133
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.2165871
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.305941489868
ΔG_{solv} = -0.0344223

P_L

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.372785 (Hartree/Particle)
Thermal correction to Energy= 0.395870
Thermal correction to Enthalpy= 0.396814
Thermal correction to Gibbs Free Energy= 0.313731
Sum of electronic and zero-point Energies= -2505.410880
Sum of electronic and thermal Energies= -2505.387795
Sum of electronic and thermal Enthalpies= -2505.386851
Sum of electronic and thermal Free Energies= -2505.469934

C	-3.28798	0.69913	0.35567
C	-1.16957	0.00449	1.11144
C	-1.61602	-0.10808	2.40753
C	-2.96357	0.20076	2.70018
C	-3.78778	0.60128	1.66201
C	-4.06488	1.09337	-0.80647
C	-3.94302	1.43252	-3.12511
C	-5.27897	1.79434	-3.19524
C	-6.03125	1.80196	-2.00734
C	-5.42591	1.4509	-0.81182
H	-0.14174	-0.22577	0.84886
H	-0.93096	-0.43071	3.18486
H	-3.34539	0.12329	3.71305
H	-4.82893	0.83974	1.85454
H	-3.29515	1.39766	-3.99607
H	-5.72353	2.06298	-4.14756
H	-7.08123	2.08033	-2.02368
H	-5.99583	1.45223	0.11118
N	-1.95981	0.405	0.07329
N	-3.34871	1.09122	-1.96925
Ni	-1.47546	0.57395	-1.72361
C	4.32524	0.11979	2.60261
C	4.98306	-0.41393	3.7086
C	5.16384	-1.79537	3.81703
C	4.67972	-2.62793	2.80987
C	4.01826	-2.0875	1.70303
C	3.82921	-0.7057	1.58072
H	4.19279	1.19742	2.52527
H	5.35865	0.24816	4.48476
H	5.67891	-2.21542	4.67684
H	4.81574	-3.70424	2.87985
H	3.65257	-2.75756	0.93098
C	3.10101	-0.0677	0.408
H	2.15091	0.35661	0.76544
H	3.68554	0.79635	0.06206
C	2.81071	-0.9796	-0.79727
H	2.1725	-1.82074	-0.49802
H	3.76114	-1.41612	-1.14112
C	2.16186	-0.2407	-1.93665
H	2.68558	0.65354	-2.28362
C	1.03111	-0.59687	-2.56021
H	0.50009	-1.49888	-2.24204
C	0.40375	0.14923	-3.71332
H	0.37852	-0.51522	-4.59707
H	1.05237	1.00112	-3.98582
O	-0.8974	0.58068	-3.41635

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3541091
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.2673435
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.370430155434
ΔG_{solv} = -0.0228725

P_B

UB3LYP/6-31g(d)-gas
Zero-point correction= 0.372712 (Hartree/Particle)
Thermal correction to Energy= 0.395587
Thermal correction to Enthalpy= 0.396532
Thermal correction to Gibbs Free Energy= 0.315690
Sum of electronic and zero-point Energies= -2505.407982
Sum of electronic and thermal Energies= -2505.385106
Sum of electronic and thermal Enthalpies= -2505.384162
Sum of electronic and thermal Free Energies= -2505.465003

C	-2.41018	2.09416	0.98134
C	-0.09	2.17185	1.33364
C	-0.23051	3.07095	2.36716
C	-1.52122	3.51683	2.7207
C	-2.60513	3.01675	2.01818
C	-3.4742	1.49055	0.19483
C	-3.89665	-0.035	-1.53483
C	-5.26562	0.15896	-1.44199
C	-5.74773	1.06623	-0.48293
C	-4.85168	1.73491	0.33606
H	0.88945	1.80428	1.04487
H	0.65011	3.42211	2.89514
H	-1.66351	4.23099	3.52539
H	-3.61165	3.33352	2.27147
H	-3.4462	-0.70864	-2.25771
H	-5.93953	-0.37715	-2.10171
H	-6.81446	1.24453	-0.38165
H	-5.21028	2.43969	1.07855
N	-1.13976	1.67576	0.61941
N	-3.02286	0.60308	-0.73711
Ni	-1.06424	0.50169	-0.8477
C	3.45124	-0.36794	1.19085
C	4.15827	-0.9004	2.27103
C	3.85671	-2.1775	2.7428
C	2.84408	-2.91445	2.12387
C	2.13957	-2.37647	1.04798
C	2.42784	-1.09091	0.56417
H	3.70171	0.62575	0.82384
H	4.94722	-0.31663	2.73859
H	4.40536	-2.59662	3.58204
H	2.60094	-3.91194	2.48125
H	1.3504	-2.95983	0.58061
C	1.62848	-0.49347	-0.57212
H	0.59864	-0.33189	-0.19755
H	2.02851	0.4982	-0.84001
C	3.29349	-2.70162	-2.98112

H	2.72396	-3.62272	-2.87313
H	4.24954	-2.78009	-3.49182
C	2.84	-1.53912	-2.51171
H	3.44924	-0.64245	-2.64622
C	1.50648	-1.33015	-1.84771
H	1.08403	-2.3102	-1.58617
C	0.51284	-0.67457	-2.86298
H	0.43051	-1.37577	-3.70942
H	0.99454	0.23825	-3.26706
O	-0.75773	-0.4035	-2.36115

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3533175
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.2656535
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.372425835385
ΔG_{solv} = -0.0221931

C-TS$_B$

UB3LYP/6-31g(d)-gas
Imaginary frequency = -229.10 cm^{-1}
Zero-point correction= 0.369235 (Hartree/Particle)
Thermal correction to Energy= 0.391133
Thermal correction to Enthalpy= 0.392077
Thermal correction to Gibbs Free Energy= 0.317630
Sum of electronic and zero-point Energies= -2505.303251
Sum of electronic and thermal Energies= -2505.281353
Sum of electronic and thermal Enthalpies= -2505.280409
Sum of electronic and thermal Free Energies= -2505.354856

C	-2.42248	1.29717	1.28299
C	-0.74205	2.83838	0.79219
C	-1.17536	3.6922	1.80077
C	-2.27472	3.31918	2.57813
C	-2.90506	2.10663	2.31821
C	-3.0098	-0.00289	0.89711
C	-2.82347	-1.84296	-0.50009
C	-3.94979	-2.44874	0.04583
C	-4.63322	-1.77807	1.06156
C	-4.15819	-0.54446	1.49058
H	0.10881	3.04021	0.14631
H	-0.65703	4.62993	1.9733
H	-2.63439	3.96122	3.37697
H	-3.75519	1.79629	2.91556
H	-2.26142	-2.32612	-1.29386
H	-4.27943	-3.41649	-0.31768
H	-5.52195	-2.20962	1.51267
H	-4.67711	-0.00622	2.27559
N	-1.35508	1.66711	0.53837
N	-2.35576	-0.65286	-0.09711
Ni	-0.73209	0.46974	-0.93473
C	0.71124	-0.36628	-2.34619
H	1.27783	-1.26669	-2.57809
C	-0.6519	-0.32698	-2.82883
H	-1.13914	-1.29055	-2.98511
C	-1.4373	0.82503	-2.91038
H	-0.99629	1.80771	-3.0314
C	0.73307	-1.07707	-0.27135
H	1.36769	-1.87508	-0.66447
C	0.42133	-1.3514	1.14457
C	0.10659	-2.65276	1.58219
C	0.43527	-0.32517	2.10671
C	-0.16649	-2.91424	2.922
H	0.04502	-3.44979	0.84642
C	0.16198	-0.5857	3.44963
H	0.6829	0.68852	1.7965
C	-0.13812	-1.88326	3.8663
H	-0.40826	-3.92806	3.23236
H	0.18908	0.22686	4.17196
H	-0.34954	-2.08982	4.91221
H	1.24062	-0.12182	-0.41524
C	1.45577	0.95783	-2.23765
H	-2.47208	0.71387	-3.22633
H	1.51421	1.41437	-3.2036
O	2.69285	0.73781	-1.77201
H	0.9326	1.60728	-1.56727

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2794819
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.1862011
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.286377222440
ΔG_{solv} = -0.0366925

CH-TS$_B$

UB3LYP/6-31g(d)-gas
Imaginary frequency = -348.32 cm^{-1}
Zero-point correction= 0.424888 (Hartree/Particle)
Thermal correction to Energy= 0.451155
Thermal correction to Enthalpy= 0.452100
Thermal correction to Gibbs Free Energy= 0.365281
Sum of electronic and zero-point Energies= -2621.033104
Sum of electronic and thermal Energies= -2621.006837
Sum of electronic and thermal Enthalpies= -2621.005893
Sum of electronic and thermal Free Energies= -2621.092711

C	-0.82961	1.94453	1.64199
C	1.29757	2.77275	1.20205
C	1.22882	3.63829	2.29222
C	0.08009	3.64579	3.07632
C	-0.96459	2.78253	2.75006
C	-1.87408	0.9869	1.20161
C	-2.42957	-0.67735	-0.32054
C	-3.68697	-0.85522	0.24536
C	-4.04097	-0.06219	1.33454
C	-3.12467	0.86818	1.81586
H	2.16266	2.72675	0.55497
H	2.0688	4.2911	2.50308
H	-0.00715	4.30966	3.9313
H	-1.86452	2.76634	3.35405
H	-2.10849	-1.26954	-1.17115
H	-4.3655	-1.59731	-0.16186
H	-5.01532	-0.16323	1.80301
H	-3.38498	1.49947	2.65716
N	0.28811	1.9493	0.87837
N	-1.53882	0.21711	0.13816
Ni	0.24251	0.708	-0.71581
C	1.4421	-0.25802	-2.27185
H	1.67408	-1.27777	-2.57048
C	0.11912	0.17135	-2.67413

H	-0.58201	-0.62343	-2.9321
C	-0.35372	1.4863	-2.56958
H	0.32097	2.33353	-2.62301
C	1.7393	-0.84824	-0.1736
H	2.7823	-0.58143	-0.30842
C	1.47856	-2.30476	-0.14991
C	2.34968	-3.20828	-0.79034
C	0.35758	-2.84613	0.50885
C	2.11295	-4.5819	-0.77385
H	3.23506	-2.82238	-1.29118
C	0.11769	-4.21907	0.52642
H	-0.32464	-2.17749	1.02845
C	0.99284	-5.09673	-0.11789
H	2.80973	-5.25317	-1.2697
H	-0.75214	-4.60685	1.05162
H	0.80838	-6.16742	-0.10235
H	1.41649	-0.40052	0.77103
C	2.50616	0.81155	-2.29862
O	2.10117	1.68633	-1.27629
H	-1.38763	1.68791	-2.84052
H	2.51146	1.31288	-3.28034
H	3.51704	0.40237	-2.13708
H	4.57391	3.71551	-1.07058
C	3.65336	4.35414	-1.05648
O	2.61851	3.91522	-1.84418
H	4.00005	5.36201	-1.36589
H	2.36024	2.80252	-1.56068
H	3.41776	4.47063	0.04056

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2621.007
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2621.9977
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2618.9044
ΔG_{solv} = -0.0229495

C-TS$_L$

UB3LYP/6-31g(d)-gas
Imaginary frequency = -293.16 cm^{-1}
Zero-point correction= 0.368710 (Hartree/Particle)
Thermal correction to Energy= 0.390876
Thermal correction to Enthalpy= 0.391820
Thermal correction to Gibbs Free Energy= 0.316349
Sum of electronic and zero-point Energies= -2505.302047
Sum of electronic and thermal Energies= -2505.279881
Sum of electronic and thermal Enthalpies= -2505.278937
Sum of electronic and thermal Free Energies= -2505.354409

C	-1.5686	2.18377	1.56507
C	0.48993	3.16267	1.12464
C	0.24254	4.21694	1.99655
C	-0.97821	4.24194	2.6723
C	-1.89019	3.214	2.45568
C	-2.45577	1.03657	1.26535
C	-2.79101	-0.78066	-0.17297
C	-3.99554	-1.0848	0.46584
C	-4.4183	-0.31677	1.5476
C	-3.64613	0.77361	1.9441
H	1.42902	3.09501	0.58206
H	0.98586	4.99473	2.13694
H	-1.21627	5.04881	3.35906
H	-2.84452	3.21489	2.96958
H	-2.42244	-1.27389	-1.11724
H	-4.59119	-1.91573	0.10044
H	-5.34461	-0.54507	2.06815
H	-3.9669	1.39915	2.76996
N	-0.38662	2.17274	0.90088
N	-2.02951	0.24881	0.25039
Ni	-0.19004	0.6344	-0.41963
C	1.59975	0.86222	-1.53699
H	1.61552	1.9527	-1.44818
H	2.60094	0.49015	-1.74143
C	0.50411	0.2676	-2.30966
H	0.54351	-0.80218	-2.52213
C	-0.71548	0.86697	-2.56437
H	-0.81131	1.95671	-2.60589
C	-1.84257	-0.02524	-3.10219
H	-1.89372	0.22259	-4.20024
C	1.80391	-0.08757	0.1788
H	2.69434	0.47818	0.45657
H	-2.79166	0.44454	-2.70441
O	-1.66998	-1.32226	-2.81474
C	1.04653	-0.51513	1.40651
C	1.2531	0.0947	2.65814
C	0.19528	-1.64314	1.35905
C	0.60039	-0.36669	3.79975
H	1.93922	0.93537	2.73278
C	-0.46137	-2.09845	2.49761
H	0.04266	-2.15173	0.40924
C	-0.2679	-1.45926	3.7263
H	0.78171	0.12025	4.75502
H	-1.11869	-2.9614	2.42837
H	-0.77126	-1.82063	4.61886
H	2.0981	-0.97851	-0.37641

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.287780
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.1928851
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.284994203000
ΔG_{solv} = -0.0445728

CH-TS$_L$

UB3LYP/6-31g(d)-gas
Imaginary frequency = -287.04 cm^{-1}
Zero-point correction= 0.423290 (Hartree/Particle)
Thermal correction to Energy= 0.449618
Thermal correction to Enthalpy= 0.450562
Thermal correction to Gibbs Free Energy= 0.365002
Sum of electronic and zero-point Energies= -2620.999177
Sum of electronic and thermal Energies= -2620.972849
Sum of electronic and thermal Enthalpies= -2620.971905
Sum of electronic and thermal Free Energies= -2621.057465

C	-0.7467	1.87713	0.88217
C	1.30271	2.79721	0.30286
C	1.09197	3.9204	1.09392
C	-0.10202	4.00889	1.8107
C	-1.02787	2.97753	1.70112
C	-1.67356	0.74229	0.68273

C	-2.00786	-1.25839	-0.48594
C	-3.26643	-1.4135	0.10074
C	-3.72785	-0.46078	1.004
C	-2.92541	0.64174	1.29295
H	2.21954	2.68646	-0.26828
H	1.8444	4.70059	1.14287
H	-0.30958	4.86713	2.44287
H	-1.96248	3.02845	2.24741
H	-1.59112	-1.93222	-1.27596
H	-3.87313	-2.27225	-0.16897
H	-4.70465	-0.55881	1.47012
H	-3.27511	1.40581	1.97809
N	0.41838	1.79304	0.19053
N	-1.22708	-0.20407	-0.17647
Ni	0.63481	0.04174	-0.88489
C	2.27372	0.4421	-2.17851
H	2.10262	1.52138	-2.19932
H	3.31074	0.22226	-2.41555
C	1.26077	-0.39369	-2.80483
H	1.45318	-1.45955	-2.92274
C	-0.03166	0.00455	-3.04031
H	-0.27693	1.06374	-3.16456
C	-1.07361	-1.07397	-3.37052
H	-1.16439	-1.05431	-4.49359
C	2.66877	-0.31479	-0.29355
H	3.16367	0.52236	0.19969
H	-2.05762	-0.61964	-3.04034
C	1.82646	-1.13329	0.62883
C	1.578	-0.73255	1.96286
C	1.34201	-2.39476	0.21334
C	0.84006	-1.53503	2.82364
H	1.97683	0.2165	2.31342
C	0.58807	-3.18757	1.0802
H	1.54273	-2.74972	-0.79271
C	0.33178	-2.76496	2.38383
H	0.66817	-1.2101	3.847
H	0.2088	-4.14304	0.72906
H	-0.24546	-3.39005	3.05967
H	3.40644	-0.95616	-0.76933
H	0.7184	-6.56556	-1.47765
O	-0.0874	-4.79406	-2.26315
O	-0.8563	-2.42246	-2.86325
C	0.5812	-5.97316	-2.42125
H	-0.6177	-3.30446	-3.23375
H	0.0905	-6.69176	-3.12195
H	1.6238	-5.85936	-2.82855

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2620.9982
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2621.9847
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2618.8747
ΔG_{solv} = -0.0340259

B''-TSL

UB3LYP/6-31g(d)-gas
Imaginary frequency = -636.59 cm^{-1}
Zero-point correction= 0.365804 (Hartree/Particle)
Thermal correction to Energy= 0.388564
Thermal correction to Enthalpy= 0.389508
Thermal correction to Gibbs Free Energy= 0.310314
Sum of electronic and zero-point Energies= -2505.299320
Sum of electronic and thermal Energies= -2505.276559
Sum of electronic and thermal Enthalpies= -2505.275615
Sum of electronic and thermal Free Energies= -2505.354809

C	-0.92081	0.98226	2.85884
C	0.67014	2.31217	1.794
C	0.47953	3.35274	2.69422
C	-0.45476	3.1855	3.71796
C	-1.15798	1.98782	3.79956
C	-1.5887	-0.3339	2.85009
C	-1.72129	-2.37911	1.70945
C	-2.60446	-2.87359	2.6738
C	-2.98004	-2.07177	3.74791
C	-2.46364	-0.77945	3.84019
H	1.38905	2.39112	0.98607
H	1.05273	4.26801	2.59223
H	-0.63389	3.97557	4.44093
H	-1.89076	1.83878	4.58437
H	-1.33493	-2.98137	0.84436
H	-2.98485	-3.8845	2.56672
H	-3.65853	-2.44172	4.51178
H	-2.72919	-0.1412	4.6758
N	-0.00759	1.15114	1.86035
N	-1.23443	-1.12306	1.80007
Ni	0.04227	-0.29963	0.59114
C	1.83921	-0.03604	-0.58031
H	1.571	0.90726	-1.04641
H	2.68603	-0.02865	0.09911
C	1.08032	-1.2273	-0.79853
H	1.43511	-2.2025	-0.46333
C	-0.23453	-1.18673	-1.25843
H	-0.58624	-0.31939	-1.83027
C	-1.03659	-2.48073	-1.36483
H	-1.07585	-2.68547	-2.47363
C	3.20106	-0.11228	-2.04303
H	3.36256	-1.17159	-1.87679
H	-2.10453	-2.16932	-1.14588
O	-0.57116	-3.48718	-0.62193
C	2.52945	0.31832	-3.23213
C	1.74914	-0.58196	-4.00078
C	2.58448	1.66945	-3.65929
C	1.06791	-0.15095	-5.13345
H	1.68558	-1.62149	-3.69098
C	1.90408	2.09253	-4.79435
H	3.18104	2.37834	-3.08843
C	1.1401	1.18622	-5.5396
H	0.47627	-0.86082	-5.70572
H	1.96966	3.13213	-5.10621
H	0.60908	1.51847	-6.4274
H	3.91701	0.55573	-1.57185

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2737072
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.1837374
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.267387295916
ΔG_{solv} = -0.0452782

BH-TSL

UB3LYP/6-31g(d)-gas
Imaginary frequency = 619.59 cm^{-1}

Zero-point correction= 0.420604 (Hartree/Particle)
Thermal correction to Energy= 0.447585
Thermal correction to Enthalpy= 0.448530
Thermal correction to Gibbs Free Energy= 0.359079
Sum of electronic and zero-point Energies= -2620.993664
Sum of electronic and thermal Energies= -2620.966683
Sum of electronic and thermal Enthalpies= -2620.965739
Sum of electronic and thermal Free Energies= -2621.055190

C	-1.126	1.59829	3.24424
C	0.63832	2.93524	2.49797
C	0.3049	3.95845	3.37295
C	-0.80369	3.78481	4.21287
C	-1.51951	2.5956	4.14501
C	-1.77827	0.29144	3.10729
C	-1.69937	-1.75898	1.97797
C	-2.71252	-2.28077	2.78111
C	-3.28573	-1.47021	3.76335
C	-2.80447	-0.17511	3.93525
H	1.48883	3.02669	1.83108
H	0.899	4.86555	3.39524
H	-1.09945	4.56601	4.90799
H	-2.38231	2.44077	4.78374
H	-1.1858	-2.35783	1.22191
H	-3.03466	-3.30608	2.63023
H	-4.08284	-1.84731	4.39869
H	-3.21062	0.45783	4.71629
N	-0.04941	1.77845	2.41615
N	-1.25948	-0.49182	2.1152
Ni	0.13765	0.37266	1.09642
C	1.84503	1.0602	-0.07536
H	1.32233	1.94318	-0.43164
H	2.70009	1.21842	0.57513
C	1.3538	-0.2518	-0.32865
H	1.94524	-1.12602	-0.06533
C	0.03523	-0.44104	-0.75688
H	-0.46248	0.38259	-1.28232
C	-0.51307	-1.80804	-1.06598
H	-0.3117	-2.02233	-2.13257
C	3.27408	1.47438	-1.86464
H	3.93114	0.64801	-1.60712
H	-1.62055	-1.78199	-0.97876
O	0.0685	-2.7562	-0.22666
C	2.469	1.38377	-3.04951
C	2.23277	0.12992	-3.67333
C	1.84585	2.52873	-3.61163
C	1.42337	0.03148	-4.80104
H	2.69707	-0.76437	-3.26041
C	1.03989	2.42532	-4.74045
H	2.01541	3.50305	-3.15265
C	0.82275	1.17618	-5.34294
H	1.25962	-0.94158	-5.26115
H	0.57977	3.31852	-5.15929
H	0.19206	1.09798	-6.2251
H	3.59126	2.45445	-1.51331
H	0.07136	-3.66199	-0.73709
H	-0.84	-6.70154	-0.85571
C	-1.0556	-5.64312	-1.1517
O	0.07536	-4.92419	-1.44835
H	-1.7696	-5.7243	-2.01473
H	-1.65254	-5.21138	-0.31179

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2620.986
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2621.9764
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2618.8572
ΔG_{solv} = -0.0368533

B-TSB

UB3LYP/6-31g(d)-gas
Imaginary frequency = -469.64 cm^{-1}
Zero-point correction= 0.367811 (Hartree/Particle)
Thermal correction to Energy= 0.390034
Thermal correction to Enthalpy= 0.390978
Thermal correction to Gibbs Free Energy= 0.313856
Sum of electronic and zero-point Energies= -2505.299873
Sum of electronic and thermal Energies= -2505.277651
Sum of electronic and thermal Enthalpies= -2505.276707
Sum of electronic and thermal Free Energies= -2505.353829

C	-1.80936	0.7111	2.99187
C	-1.90017	1.86364	0.95515
C	-2.54453	2.93768	1.57502
C	-2.8104	2.89256	2.94046
C	-2.43832	1.75954	3.66263
C	-1.44326	-0.57421	3.61927
C	-0.64935	-2.72612	3.19952
C	-0.75578	-3.07952	4.53942
C	-1.22673	-2.12901	5.44609
C	-1.5761	-0.86538	4.97888
H	-1.68401	1.84452	-0.13999
H	-2.82344	3.79752	0.97445
H	-3.30753	3.71876	3.44117
H	-2.65075	1.69117	4.72384
H	-0.29552	-3.42657	2.45206
H	-0.47626	-4.07793	4.85854
H	-1.32186	-2.36744	6.50117
H	-1.94382	-0.11193	5.66614
N	-1.53086	0.77298	1.66148
N	-0.97799	-1.50488	2.74006
Ni	-0.76297	-0.87133	0.95418
C	0.41297	-0.30447	-1.02147
H	1.39382	-0.63414	-0.66391
C	-0.65951	-1.22253	-0.95821
H	-1.58519	-0.92645	-1.44929
C	-0.52708	-2.42792	-0.19993
H	0.45938	-2.89375	-0.13545
C	0.21831	1.20021	-1.2196
H	1.12319	1.57262	-1.76076
C	0.66427	-0.70089	-3.35107
H	-0.28173	-0.171	-3.38089
H	0.41698	1.60604	-0.17461
O	-0.95872	1.53941	-1.74422
C	1.83659	-0.04723	-3.82354
C	1.81382	1.35087	-4.08341
C	3.05041	-0.74892	-4.04597
C	2.94891	1.99907	-4.55637
H	0.88872	1.89324	-3.90404
C	4.17758	-0.09106	-4.51736
H	3.07832	-1.81968	-3.85271
C	4.13389	1.28652	-4.77636

H	2.91443	3.06715	-4.75599
H	5.09646	-0.64603	-4.69033
H	5.01747	1.79841	-5.14845
H	0.6398	-1.7848	-3.29719
H	-1.34407	-3.14984	-0.23024

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2692424
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.1777816
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.270786690197
ΔG_{solv} = -0.0372232

BH-TSB

UB3LYP/6-31g(d)-gas
Imaginary frequency = -456.51 cm^{-1}
Zero-point correction= 0.421862 (Hartree/Particle)
Thermal correction to Energy= 0.448464
Thermal correction to Enthalpy= 0.449408
Thermal correction to Gibbs Free Energy= 0.360831
Sum of electronic and zero-point Energies= -2620.994637
Sum of electronic and thermal Energies= -2620.968035
Sum of electronic and thermal Enthalpies= -2620.967091
Sum of electronic and thermal Free Energies= -2621.055668

C	-1.03211	0.71352	3.51861
C	-1.29912	2.15956	1.70403
C	-1.59765	3.22426	2.55114
C	-1.59239	3.01604	3.93116
C	-1.31743	1.74346	4.41893
C	-0.81484	-0.686	3.90093
C	-0.57314	-2.85944	3.08736
C	-0.47287	-3.37895	4.37158
C	-0.54198	-2.50231	5.45979
C	-0.71554	-1.14498	5.21738
H	-1.32425	2.26207	0.62119
H	-1.83566	4.193	2.1253
H	-1.81797	3.82676	4.61795
H	-1.34507	1.54921	5.48556
H	-0.52799	-3.49926	2.21429
H	-0.3434	-4.44657	4.51266
H	-0.46177	-2.87087	6.47766
H	-0.76822	-0.44593	6.04429
N	-0.99552	0.93287	2.17142
N	-0.73596	-1.54429	2.83928
Ni	-0.67977	-0.67589	1.14115
C	0.38881	-0.08032	-0.86912
H	1.32963	-0.46756	-0.48146
C	-0.77566	-0.88654	-0.80638
H	-1.69612	-0.49324	-1.26716
C	-0.70172	-2.14405	-0.139
H	0.24317	-2.6962	-0.14489
C	0.35626	1.39941	-1.18947
H	0.98097	1.5834	-2.07754
C	1.12435	-0.94987	-2.92079
H	0.1719	-0.72452	-3.39399
H	0.82482	1.96238	-0.36987
O	-0.93852	1.92235	-1.3454
C	2.2998	-0.24884	-3.32791
C	2.21495	0.89401	-4.16818
C	3.58696	-0.64497	-2.88115
C	3.35701	1.59583	-4.53752
H	1.24071	1.20467	-4.53862
C	4.7219	0.06157	-3.25324
H	3.67568	-1.52073	-2.24217
C	4.61513	1.18693	-4.08176
H	3.26978	2.46283	-5.18757
H	5.69835	-0.2629	-2.90337
H	5.50666	1.73577	-4.37311
H	1.21116	-1.94205	-2.48533
H	-1.58152	-2.78461	-0.16251
H	-1.41267	1.49889	-2.11828
H	-3.56323	-1.33813	-2.97248
C	-3.79634	-0.24442	-3.03711
O	-2.74082	0.52754	-2.63024
H	-4.10729	-0.06473	-4.0946
H	-4.71146	-0.10813	-2.41146

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2620.9837
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2621.9729
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2618.8588
ΔG_{solv} = -0.031814

Bn-rad

UB3LYP-D3/6-31G(d)-CPCM (acetone)
Zero-point correction= 0.115032 (Hartree/Particle)
Thermal correction to Energy= 0.120680
Thermal correction to Enthalpy= 0.121624
Thermal correction to Gibbs Free Energy= 0.085373
Sum of electronic and zero-point Energies= -270.810084
Sum of electronic and thermal Energies= -270.804435
Sum of electronic and thermal Enthalpies= -270.803491
Sum of electronic and thermal Free Energies= -270.839742

C	-0.19151	2.31831	-0.12954
C	-0.0756	0.91773	-0.05128
H	-1.1635	2.80147	-0.1301
H	0.68793	2.95148	-0.19146
C	-1.22965	0.08019	0.03011
C	-1.10935	-1.29946	0.10706
C	0.15723	-1.905	0.10643
C	1.30778	-1.10449	0.0273
C	1.20057	0.27626	-0.05004
H	2.09557	0.89072	-0.11103
H	2.2904	-1.56915	0.02648
H	-2.21344	0.54321	0.03113
H	-2.00282	-1.91544	0.16824
H	0.24642	-2.98582	0.16669

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -270.7595418

UB3LYP/6-31G(d)
Zero-point correction= 0.114953 (Hartree/Particle)
Thermal correction to Energy= 0.120623
Thermal correction to Enthalpy= 0.121567
Thermal correction to Gibbs Free Energy= 0.085283

Sum of electronic and zero-point Energies= -270.800183
Sum of electronic and thermal Energies= -270.794513
Sum of electronic and thermal Enthalpies= -270.793569
Sum of electronic and thermal Free Energies= -270.829853

C	-0.72142	1.94	-0.20557
C	-0.60579	0.54034	-0.12744
H	-1.69218	2.42499	-0.2062
H	0.1569	2.57429	-0.26728
C	-1.75825	-0.29723	-0.04608
C	-1.63836	-1.67572	0.03091
C	-0.37295	-2.28072	0.03034
C	0.77646	-1.48084	-0.04877
C	0.66883	-0.10135	-0.12617
H	1.56341	0.51372	-0.18726
H	1.75933	-1.94528	-0.04961
H	-2.74185	0.16624	-0.04511
H	-2.53204	-2.29161	0.09205
H	-0.28365	-3.36161	0.09063

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -270.7596381

Epoxynaphthalene

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.152151 (Hartree/Particle)
Thermal correction to Energy= 0.159311
Thermal correction to Enthalpy= 0.160255
Thermal correction to Gibbs Free Energy= 0.120356
Sum of electronic and zero-point Energies= -460.898119
Sum of electronic and thermal Energies= -460.890959
Sum of electronic and thermal Enthalpies= -460.890015
Sum of electronic and thermal Free Energies= -460.929914

C	-2.26044	0.48792	-0.50091
C	-2.15229	-0.84276	-0.50485
C	-1.21164	-1.18016	0.6701
C	0.18929	-0.69105	0.27004
C	0.07551	0.71096	0.27385
C	-1.38567	0.96577	0.67622
C	1.37488	-1.31421	-0.06388
C	2.47662	-0.49718	-0.39523
C	2.36393	0.89184	-0.39137
C	1.14507	1.51884	-0.05602
O	-1.5737	-0.13219	1.60832
H	-1.29313	-2.16763	1.12297
H	-2.54305	-1.56155	-1.21424
H	-2.76247	1.13839	-1.20621
H	1.46773	-2.39709	-0.0691
H	3.42574	-0.95921	-0.65328
H	3.22614	1.50216	-0.6463
H	1.06234	2.60256	-0.05486
H	-1.62488	1.92458	1.13477

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -460.8174752

UB3LYP/6-31G(d)
Zero-point correction= 0.152238 (Hartree/Particle)
Thermal correction to Energy= 0.159385
Thermal correction to Enthalpy= 0.160329
Thermal correction to Gibbs Free Energy= 0.120459
Sum of electronic and zero-point Energies= -460.878668
Sum of electronic and thermal Energies= -460.871521
Sum of electronic and thermal Enthalpies= -460.870577
Sum of electronic and thermal Free Energies= -460.910447

C	-2.76194	2.45498	-0.48562
C	-2.65404	1.12522	-0.48936
C	-1.71016	0.79113	0.68469
C	-0.30755	1.27722	0.27984
C	-0.42122	2.67869	0.2837
C	-1.8836	2.93026	0.69065
C	0.87959	0.65617	-0.05174
C	1.98152	1.47178	-0.38009
C	1.86904	2.85919	-0.37605
C	0.65027	3.48475	-0.04356
O	-2.06938	1.836	1.61773
H	-1.79383	-0.19371	1.14386
H	-3.04905	0.40938	-1.19996
H	-3.26767	3.10171	-1.1923
H	0.97676	-0.42687	-0.05527
H	2.93166	1.00964	-0.63465
H	2.73227	3.46978	-0.62736
H	0.57181	4.5693	-0.04061
H	-2.12467	3.88616	1.15528

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -460.8176345

A1

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.451580 (Hartree/Particle)
Thermal correction to Energy= 0.478534
Thermal correction to Enthalpy= 0.479478
Thermal correction to Gibbs Free Energy= 0.392404
Sum of electronic and zero-point Energies= -2812.455363
Sum of electronic and thermal Energies= -2812.428409
Sum of electronic and thermal Enthalpies= -2812.427465
Sum of electronic and thermal Free Energies= -2812.514539

H	-5.64425	-6.61001	-0.28489
C	-5.55429	-5.5613	-0.55325
H	-7.68342	-5.20417	-0.54906
H	-3.39699	-5.59155	-0.62754
C	-6.69845	-4.77185	-0.70409
C	-4.2933	-4.98805	-0.74355
C	-6.58554	-3.42358	-1.04396
C	-4.17545	-3.64118	-1.08582
H	-7.47093	-2.80448	-1.1556
H	-6.70014	-3.61958	-3.68601
C	-5.3208	-2.84714	-1.2486
H	-3.20085	-3.18776	-1.23659
H	-7.89769	-3.78918	-5.83938
C	-6.90657	-2.71562	-4.2474
C	-7.59647	-2.80562	-5.48934
N	-5.1836	-1.47552	-1.55572
C	-6.51892	-1.46979	-3.78602
C	-5.79431	-0.94129	-2.62256

C	-7.89431	-1.69474	-6.25926
Ni	-4.40396	-0.0861	-0.47776
H	-8.42309	-1.8057	-7.20228
C	-6.82442	-0.33112	-4.59143
C	-7.49862	-0.39757	-5.81899
C	-5.67425	0.48097	-2.77204
N	-4.95085	1.12035	-1.84579
C	-6.33394	0.88029	-4.01995
H	-6.95719	2.83283	-1.45895
C	-7.70016	0.83752	-6.50263
H	-8.22089	0.84557	-7.45657
C	-4.86296	2.53244	-1.85118
C	-6.00102	3.32275	-1.62008
C	-6.53625	2.06135	-4.71127
C	-7.22722	2.01756	-5.95497
H	-6.18475	3.0123	-4.32718
C	-3.62227	3.15352	-2.04608
C	-5.89834	4.71317	-1.60344
H	-6.78558	5.31516	-1.42617
H	-2.7456	2.53618	-2.20687
H	-7.38411	2.95031	-6.48969
C	-3.52488	4.54631	-2.02608
C	-4.65974	5.33118	-1.80787
H	-2.55808	5.01728	-2.18266
H	-4.58109	6.41455	-1.79301
C	-4.2026	0.08608	1.45667
C	-3.59613	1.21004	0.841
C	-3.66277	-1.16066	1.05685
H	-5.13644	0.15998	2.0086
C	-2.25484	-1.23169	0.66529
C	-1.52664	-0.10983	0.43809
C	-2.14767	1.21076	0.53706
H	-4.06724	2.1826	0.95739
H	-1.80304	-2.21372	0.55851
C	-1.45206	2.35292	0.33395
H	-0.39795	2.33144	0.0708
H	-1.92544	3.32638	0.41083
H	-0.46961	-0.16911	0.19268
H	-4.16079	-2.08013	1.34574

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -2812.1910061

UB3LYP/6-31G(d)-gas
Zero-point correction= 0.451028
(Hartree/Particle)
Thermal correction to Energy= 0.478172
Thermal correction to Enthalpy= 0.479116
Thermal correction to Gibbs Free Energy= 0.390946
Sum of electronic and zero-point Energies= -2812.375439
Sum of electronic and thermal Energies= -2812.348296
Sum of electronic and thermal Enthalpies= -2812.347352
Sum of electronic and thermal Free Energies= -2812.435521

H	-5.66463	-6.62693	-0.34802
C	-5.57518	-5.57322	-0.59709
H	-7.67758	-5.16157	-0.33964
H	-3.44495	-5.65974	-0.925
C	-6.70417	-4.75043	-0.59499
C	-4.32968	-5.02811	-0.91713
C	-6.59123	-3.39648	-0.91087
C	-4.21127	-3.67483	-1.23402
H	-7.46551	-2.7517	-0.90208
H	-6.68106	-3.61839	-3.66944
C	-5.34228	-2.84468	-1.24041
H	-3.24722	-3.24623	-1.49108
H	-7.85338	-3.80102	-5.83445
C	-6.88036	-2.71745	-4.23873
C	-7.55481	-2.8153	-5.4872
N	-5.20993	-1.46345	-1.5263
C	-6.49573	-1.46904	-3.78264
C	-5.7898	-0.93329	-2.61116
C	-7.84047	-1.71035	-6.26809
Ni	-4.43557	-0.07376	-0.44135
H	-8.35769	-1.8294	-7.21701
C	-6.79024	-0.33594	-4.59833
C	-7.44986	-0.41065	-5.83322
C	-5.6723	0.48914	-2.76316
N	-4.98637	1.13748	-1.81425
C	-6.31154	0.87932	-4.02577
H	-6.95217	2.86312	-1.29268
C	-7.64534	0.81984	-6.52513
H	-8.15337	0.82332	-7.4864
C	-4.89416	2.55278	-1.84028
C	-6.01046	3.34852	-1.53374
C	-6.51013	2.0556	-4.72611
C	-7.18391	2.00299	-5.97763
H	-6.16627	3.01056	-4.34472
C	-3.67375	3.17469	-2.13898
C	-5.90805	4.73909	-1.54108
H	-6.77992	5.34293	-1.30244
H	-2.81156	2.55703	-2.36653
H	-7.33645	2.93267	-6.51959
C	-3.57831	4.56759	-2.14711
C	-4.69209	5.35493	-1.8503
H	-2.62814	5.03712	-2.38851
H	-4.61396	6.43867	-1.85611
C	-4.20275	0.08399	1.48735
C	-3.59376	1.20885	0.87707
C	-3.67333	-1.16243	1.07291
H	-5.13299	0.15892	2.04482
C	-2.26343	-1.23738	0.68846
C	-1.53045	-0.11818	0.47288
C	-2.14468	1.20425	0.5762
H	-4.05497	2.18365	1.01144
H	-1.81341	-2.22084	0.58163
C	-1.43955	2.34239	0.38694
H	-0.38267	2.31461	0.1362
H	-1.90114	3.32044	0.47607
H	-0.47165	-0.17943	0.23506
H	-4.17311	-2.08052	1.36363

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -2812.1912833

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UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.486973
(Hartree/Particle)
Thermal correction to Energy= 0.515790
Thermal correction to Enthalpy= 0.516734
Thermal correction to Gibbs Free Energy= 0.425513
Sum of electronic and zero-point Energies= -3002.555716
Sum of electronic and thermal Energies= -3002.526899
Sum of electronic and thermal Enthalpies= -3002.525955
Sum of electronic and thermal Free Energies= -3002.617175

H	2.68078	-5.11595	7.21987
C	2.7961	-4.04375	7.09016
H	3.30857	-4.18058	4.99702
H	2.2998	-3.57363	9.13759
C	3.14598	-3.51757	5.84256
C	2.58612	-3.17693	8.16717
C	3.28868	-2.14112	5.67408
C	2.72929	-1.79907	8.00505
H	3.55671	-1.71882	4.71007
H	5.16277	-1.33768	8.83745
C	3.09674	-1.2662	6.75681
H	2.55263	-1.12398	8.83707
H	6.88357	-0.91519	10.55571
C	5.44081	-0.31484	9.06343
C	6.43243	-0.06451	10.05252
N	3.1946	0.11874	6.53126
C	4.85326	0.75812	8.41684
C	3.86176	0.94009	7.34221
C	6.83761	1.21477	10.39131
Ni	2.18052	1.15455	5.19411
H	7.59941	1.36614	11.15158
C	5.28416	2.07102	8.76578
C	6.26416	2.34096	9.73317
C	3.7299	2.35703	7.08652
N	2.92049	2.71974	6.08258
C	4.63839	3.07669	7.98676
H	3.34789	3.90876	3.77298
C	6.60113	3.71123	9.9363
H	7.35112	3.97718	10.67645
C	2.65423	4.07623	5.79767
C	2.90555	4.57317	4.50917
C	4.99822	4.39676	8.19847
C	5.98159	4.6932	9.18323
H	4.54841	5.20591	7.63514
C	2.07646	4.92607	6.75613
C	2.60342	5.89729	4.19183
H	2.81206	6.26929	3.19219
H	1.86965	4.53741	7.74916
H	6.25268	5.73335	9.34211
C	1.77574	6.24944	6.43275
C	2.0382	6.74303	5.15105
H	1.32894	6.8951	7.18428
H	1.80039	7.77318	4.90171
H	1.10961	-1.61622	4.14159
H	-0.24674	-2.44702	1.60304
C	0.77497	-0.64698	3.77845
H	2.6478	0.17172	2.71263
C	-0.73445	-1.48631	1.74506
C	1.85369	0.38661	3.4203
C	-0.3318	-0.61341	2.74069
O	0.13394	0.1112	4.87498
H	-2.15039	-1.76649	0.13794
C	-1.80525	-1.09566	0.91994
C	1.2115	1.64954	3.5904
C	-0.96521	0.62988	2.91951
C	-0.20999	1.29469	4.05516
C	-2.4333	0.13881	1.09702
H	1.42656	2.55521	3.03389
C	-2.01213	1.02522	2.10546
H	-0.73616	2.02944	4.66256
H	-3.2617	0.41748	0.45146
H	-2.50209	1.9859	2.23964

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.2465471

UB3LYP/6-31G(d)

Zero-point correction= 0.486604
(Hartree/Particle)
Thermal correction to Energy= 0.515542
Thermal correction to Enthalpy= 0.516486
Thermal correction to Gibbs Free Energy= 0.424602
Sum of electronic and zero-point Energies= -3002.470629
Sum of electronic and thermal Energies= -3002.441691
Sum of electronic and thermal Enthalpies= -3002.440746
Sum of electronic and thermal Free Energies= -3002.532631

H	2.76337	-5.13914	7.2775
C	2.86995	-4.06824	7.12922
H	3.52968	-4.24609	5.08283
H	2.22433	-3.55781	9.12339
C	3.29533	-3.56523	5.89728
C	2.57293	-3.17987	8.16558
C	3.42488	-2.19097	5.70254
C	2.70627	-1.80462	7.9794
H	3.75739	-1.79201	4.74874
H	5.19941	-1.34136	8.82715
C	3.14639	-1.29241	6.74615
H	2.45573	-1.11429	8.77939
H	6.89243	-0.89999	10.56706
C	5.46509	-0.31529	9.05461
C	6.43977	-0.0543	10.05616
N	3.2336	0.09388	6.50318
C	4.87728	0.7508	8.39739
C	3.89408	0.92212	7.31153
C	6.82748	1.2282	10.39851
Ni	2.2145	1.13105	5.15979
H	7.57726	1.38588	11.16998
C	5.29065	2.06757	8.75058
C	6.253	2.34816	9.73252
C	3.75302	2.3382	7.05412
N	2.94341	2.69616	6.0486
C	4.64317	3.06653	7.96547
H	3.58788	3.99994	3.8333
C	6.56846	3.72184	9.94226
H	7.30499	3.99777	10.69282
C	2.67067	4.05839	5.77562
C	3.04329	4.61601	4.54297
C	4.98075	4.39065	8.18673
C	5.94597	4.69692	9.18476
H	4.52785	5.19585	7.61966
C	1.96785	4.85452	6.69553
C	2.73392	5.94284	4.24469
H	3.03812	6.36121	3.28857
H	1.66312	4.42034	7.64362
H	6.20113	5.74033	9.35056
C	1.65941	6.17999	6.39042
C	2.04153	6.73231	5.16543
H	1.11236	6.78139	7.11219
H	1.79815	7.76452	4.92959
H	0.96722	-1.61497	4.21103
H	-0.43397	-2.46472	1.69478
C	0.68873	-0.64138	3.81026
H	2.59916	0.0442	2.70961
C	-0.86553	-1.47257	1.80197
C	1.82474	0.31857	3.41929
C	-0.4133	-0.58769	2.76513
O	0.08873	0.18653	4.87313
H	-2.29732	-1.73811	0.20747
C	-1.91453	-1.05745	0.96327

C	1.25086	1.62029	3.54864
C	-0.97865	0.69279	2.89767
C	-0.18996	1.35352	4.01572
C	-2.47478	0.21308	1.09435
H	1.51656	2.49055	2.95788
C	-2.00487	1.11086	2.06874
H	-0.68347	2.13203	4.59707
H	-3.28921	0.51139	0.43958
H	-2.44651	2.09956	2.16605

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF=-3002.246814

TS_{1-2}

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -559.50 cm^{-1}
Zero-point correction= 0.484802 (Hartree/Particle)
Thermal correction to Energy= 0.513255
Thermal correction to Enthalpy= 0.514199
Thermal correction to Gibbs Free Energy= 0.424311
Sum of electronic and zero-point Energies= -3002.515277
Sum of electronic and thermal Energies= -3002.486824
Sum of electronic and thermal Enthalpies= -3002.485880
Sum of electronic and thermal Free Energies= -3002.575768

H	2.59478	-5.12732	7.61219
C	2.66757	-4.06009	7.42267
H	3.03266	-4.29945	5.30711
H	2.31664	-3.50078	9.47798
C	2.90284	-3.59754	6.12808
C	2.51355	-3.14661	8.46943
C	2.99848	-2.22915	5.88267
C	2.6021	-1.77527	8.22657
H	3.21726	-1.8538	4.8916
H	5.18557	-1.36065	8.82914
C	2.85624	-1.28911	6.93149
H	2.48476	-1.06081	9.03491
H	7.07567	-0.8964	10.35169
C	5.49744	-0.33341	8.98403
C	6.58559	-0.05767	9.86418
N	2.99481	0.06531	6.59749
C	4.85862	0.72931	8.36588
C	3.75734	0.92501	7.40888
C	7.0303	1.2263	10.1216
Ni	1.83032	1.10205	5.55041
H	7.86783	1.39561	10.80424
C	5.34779	2.04132	8.62871
C	6.39759	2.33683	9.48405
C	3.62869	2.24925	7.13281
N	2.51743	2.61066	6.3349
C	4.60959	3.02413	7.88328
H	4.42641	3.65307	4.69093
C	6.74483	3.72568	9.63034
H	7.55983	4.01396	10.29805
C	2.56487	3.89633	5.72558
C	3.6053	4.33444	4.89463
C	4.9588	4.35195	8.0462
C	6.02818	4.67823	8.93117
H	4.44491	5.14447	7.5122
C	1.49692	4.77397	5.989
C	3.57978	5.61222	4.33689
H	4.38959	5.93215	3.68671
H	0.69943	4.42881	6.64546
H	6.29505	5.72498	9.05089
C	1.4725	6.05262	5.43663
C	2.51329	6.47642	4.60637
H	0.64133	6.71837	5.65238
H	2.49308	7.47093	4.1698
H	1.99742	-0.73122	3.23518
H	0.34406	-1.36873	0.89249
C	1.14705	-0.04642	3.41363
H	2.10396	2.0132	2.9498
C	-0.43694	-0.9506	1.5162
C	1.46861	1.43452	3.61
C	-0.14698	-0.29414	2.68613
O	0.58722	-0.26846	4.83977
H	-2.05458	-1.60719	0.24359
C	-1.79393	-1.08451	1.16687
C	0.47354	1.92121	4.4708
C	-1.17639	0.20086	3.48768
C	-0.39712	0.63615	4.76342
C	-2.80742	-0.59772	1.9791
H	0.08135	2.95808	4.51586
C	-2.50698	0.06995	3.18302
H	-0.84373	0.51699	5.78686
H	-3.84444	-0.7393	1.69402
H	-3.2895	0.43956	3.83607

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.1962612

UB3LYP/6-31G(d)
Imaginary frequency = -470.17 cm^{-1}
Zero-point correction= 0.483141 (Hartree/Particle)
Thermal correction to Energy= 0.512271
Thermal correction to Enthalpy= 0.513215
Thermal correction to Gibbs Free Energy= 0.420565
Sum of electronic and zero-point Energies= -3002.437114
Sum of electronic and thermal Energies= -3002.407984
Sum of electronic and thermal Enthalpies= -3002.407040
Sum of electronic and thermal Free Energies= -3002.499690

H	3.3614	-5.2301	7.06155
C	3.38527	-4.15293	6.92189
H	4.58428	-4.24354	5.13072
H	2.18331	-3.73188	8.6637
C	4.06822	-3.59817	5.83703
C	2.72726	-3.31108	7.82183
C	4.09573	-2.21625	5.65177
C	2.75446	-1.92795	7.64496
H	4.62972	-1.77903	4.81294
H	5.2217	-1.34959	8.79452
C	3.44761	-1.36488	6.56007
H	2.2321	-1.27082	8.33399
H	6.71763	-0.87274	10.70275
C	5.42446	-0.31875	9.06243
C	6.28504	-0.03715	10.15891
N	3.4345	0.03156	6.33436
C	4.86549	0.73658	8.36529
C	3.98388	0.88581	7.19562
C	6.58985	1.25373	10.55032
Ni	2.3711	1.00901	4.99487
H	7.25601	1.42707	11.39199
C	5.18413	2.06222	8.77501
C	6.03894	2.36275	9.84621

C	3.79176	2.29584	6.94836
N	3.07498	2.62398	5.86515
C	4.56312	3.04661	7.95028
H	3.33518	3.90063	3.57639
C	6.27911	3.74365	10.10184
H	6.93151	4.03601	10.92092
C	2.64308	3.94229	5.61119
C	2.80906	4.48565	4.32559
C	4.82889	4.3782	8.21868
C	5.69001	4.70545	9.30204
H	4.39619	5.17591	7.62561
C	1.96453	4.70238	6.58136
C	2.33163	5.76093	4.02613
H	2.48233	6.16861	3.02967
H	1.80202	4.2764	7.56673
H	5.88763	5.75528	9.50238
C	1.48694	5.97536	6.27425
C	1.66909	6.5143	4.99804
H	0.95931	6.54502	7.0351
H	1.29394	7.50624	4.76259
H	0.59654	-1.53638	4.84597
H	-1.61631	-2.40546	3.3639
C	0.52814	-0.59236	4.2955
H	2.4807	-0.97142	3.08414
C	-1.68085	-1.36439	3.05692
C	1.79968	-0.23881	3.50427
C	-0.7003	-0.45807	3.41949
O	0.43815	0.53989	5.18106
H	-3.57009	-1.60752	2.03836
C	-2.78507	-0.90913	2.316
C	1.68552	1.10683	3.08438
C	-0.79991	0.89493	3.03967
C	0.39309	1.67495	3.41459
C	-2.89674	0.43443	1.95904
H	2.3838	1.6318	2.44045
C	-1.9019	1.35295	2.32398
H	0.30232	2.75032	3.55789
H	-3.76295	0.77528	1.39858
H	-1.98418	2.39807	2.03558

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.2057211

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UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.487495
(Hartree/Particle)
Thermal correction to Energy= 0.516302
Thermal correction to Enthalpy= 0.517247
Thermal correction to Gibbs Free Energy= 0.427626
Sum of electronic and zero-point Energies= -3002.578789
Sum of electronic and thermal Energies= -3002.549981
Sum of electronic and thermal Enthalpies= -3002.549037
Sum of electronic and thermal Free Energies= -3002.638657

H	6.41149	2.04210	1.52722
C	5.36793	1.78939	1.36310
H	4.61532	3.53217	2.39179
H	5.80701	-0.01498	0.26296
C	4.35912	2.62535	1.85107
C	5.02739	0.63379	0.65287
C	3.01678	2.30513	1.64358
C	3.68933	0.30797	0.43254
H	2.22629	2.94968	2.01660
H	2.52891	0.94788	3.83917
C	2.68200	1.13640	0.94632
H	3.38811	-0.56634	-0.13751
H	1.93670	0.60090	6.21401
C	1.51516	0.66502	4.09673
C	1.16724	0.46408	5.45991
N	1.32789	0.80395	0.68448
C	0.54121	0.49605	3.12973
C	0.48036	0.57146	1.66207
C	-0.10977	0.10213	5.85406
Ni	0.53826	0.36938	-1.04715
H	-0.33614	-0.04414	6.90675
C	-0.77016	0.11804	3.53975
C	-1.13200	-0.09069	4.88213
C	-0.87098	0.21457	1.24619
N	-1.05357	0.12752	-0.05686
C	-1.66774	-0.06442	2.44687
H	-3.33528	1.49706	0.23777
C	-2.47567	-0.49462	5.12461
H	-2.80855	-0.66644	6.14459
C	-2.32349	-0.20820	-0.60153
C	-3.43785	0.61225	-0.38333
C	-2.96320	-0.46850	2.71443
C	-3.34959	-0.67608	4.06623
H	-3.68519	-0.62525	1.92183
C	-2.42965	-1.33488	-1.42463
C	-4.66136	0.28611	-0.96959
H	-5.52295	0.92585	-0.80090
H	-1.54425	-1.93233	-1.61254
H	-4.36955	-0.98992	4.26799
C	-3.65770	-1.65756	-2.00048
C	-4.77691	-0.85111	-1.77466
H	-3.73485	-2.53427	-2.63705
H	-5.73039	-1.10095	-2.23081
H	3.03306	-1.07525	-2.96974
H	2.16228	-2.64086	-4.72652
C	2.02216	-0.72273	-2.70290
H	2.94965	1.23575	-2.02636
C	1.21249	-2.11045	-4.70048
C	2.03082	0.78353	-2.38643
C	1.03906	-1.05855	-3.80522
O	1.55394	-1.30585	-1.50358
H	0.30315	-3.32881	-6.23486
C	0.16375	-2.50326	-5.54184
C	0.89430	1.56257	-2.62371
C	-0.19026	-0.36518	-3.76643
C	-0.28669	0.80433	-2.87772
C	-1.06627	-1.84267	-5.47680
H	0.86783	2.62647	-2.40394
C	-1.24287	-0.77468	-4.59257
H	-1.24657	1.31398	-2.84195
H	-1.88552	-2.15165	-6.12069
H	-2.19407	-0.25028	-4.54859

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3002.260087

UB3LYP/6-31G(d)
Zero-point correction= 0.485227
(Hartree/Particle)
Thermal correction to Energy= 0.514850
Thermal correction to Enthalpy= 0.515794
Thermal correction to Gibbs Free Energy= 0.422855
Sum of electronic and zero-point Energies= -3002.489582

Sum of electronic and thermal Energies= -3002.459960
Sum of electronic and thermal Enthalpies= -3002.459015
Sum of electronic and thermal Free Energies= -3002.551954

H	6.42505	2.0624	1.565
C	5.3835	1.79958	1.40206
H	4.61631	3.61519	2.28039
H	5.83401	-0.08561	0.45516
C	4.36777	2.66892	1.80653
C	5.05002	0.595	0.77732
C	3.02895	2.33564	1.5981
C	3.71526	0.25372	0.56027
H	2.23629	3.01364	1.9022
H	2.50912	1.00928	3.87036
C	2.69381	1.11805	0.98543
H	3.43517	-0.67073	0.06323
H	1.91247	0.72509	6.24973
C	1.4966	0.72232	4.12992
C	1.14652	0.55581	5.49768
N	1.34602	0.77583	0.7177
C	0.5308	0.51137	3.16274
C	0.47256	0.54738	1.6918
C	-0.12383	0.18516	5.89899
Ni	0.56374	0.30572	-1.02925
H	-0.35028	0.06425	6.95548
C	-0.77468	0.12688	3.58428
C	-1.1387	-0.05097	4.92835
C	-0.86099	0.17113	1.28265
N	-1.06578	0.05954	-0.03041
C	-1.65883	-0.09606	2.48785
H	-3.33371	1.46934	0.21591
C	-2.47719	-0.46995	5.17601
H	-2.81426	-0.62159	6.19842
C	-2.33717	-0.27555	-0.56162
C	-3.44704	0.56317	-0.37263
C	-2.94844	-0.51496	2.76304
C	-3.33915	-0.69349	4.11811
H	-3.66437	-0.70884	1.97275
C	-2.4699	-1.43023	-1.34608
C	-4.67717	0.23509	-0.94274
H	-5.52977	0.89249	-0.79249
H	-1.60028	-2.06081	-1.50325
H	-4.3552	-1.02086	4.32174
C	-3.7047	-1.75213	-1.90892
C	-4.81273	-0.92534	-1.70895
H	-3.79765	-2.65292	-2.50955
H	-5.77195	-1.17836	-2.15214
H	2.99903	-1.17191	-3.01413
H	2.10659	-2.66173	-4.81373
C	2.00291	-0.76795	-2.77286
H	2.99826	1.14191	-2.04886
C	1.18212	-2.08844	-4.80744
C	2.07291	0.72803	-2.43671
C	1.02905	-1.04671	-3.89893
O	1.48429	-1.3119	-1.58032
H	0.27363	-3.2357	-6.39343
C	0.14595	-2.41833	-5.68849
C	0.94804	1.53193	-2.63609
C	-0.1734	-0.30343	-3.88509
C	-0.24577	0.86586	-3.01252
C	-1.05696	-1.709	-5.6508
H	0.93895	2.57859	-2.34164
C	-1.21862	-0.6557	-4.75058
H	-1.18492	1.41092	-2.97151
H	-1.86552	-1.97036	-6.32827
H	-2.14676	-0.0897	-4.72978

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.2600632

$TS_{2\text{-}3}$

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -105.06 cm^{-1}
Zero-point correction= 0.485316 (Hartree/Particle)
Thermal correction to Energy= 0.514043
Thermal correction to Enthalpy= 0.514987
Thermal correction to Gibbs Free Energy= 0.425801
Sum of electronic and zero-point Energies= -3002.579121
Sum of electronic and thermal Energies= -3002.550394
Sum of electronic and thermal Enthalpies= -3002.549450
Sum of electronic and thermal Free Energies= -3002.638636

H	6.39045	2.589	1.67357
C	5.38355	2.21732	1.50612
H	4.49867	3.43186	3.05653
H	5.95143	0.91903	-0.12179
C	4.32169	2.68592	2.28628
C	5.13485	1.27971	0.49841
C	3.02682	2.21428	2.07466
C	3.84386	0.80427	0.27546
H	2.19985	2.59849	2.66346
H	2.52082	0.55519	4.02604
C	2.78041	1.25084	1.07966
H	3.61823	0.08832	-0.51012
H	1.79259	0.00068	6.31709
C	1.48396	0.29151	4.19917
C	1.05752	-0.0288	5.51785
N	1.48409	0.78622	0.7917
C	0.55943	0.26231	3.17047
C	0.57578	0.47757	1.71151
C	-0.25169	-0.36653	5.81493
Ni	0.71884	0.50992	-1.0173
H	-0.53998	-0.59737	6.83697
C	-0.7805	-0.11195	3.48301
C	-1.22591	-0.42163	4.77726
C	-0.74744	0.19527	1.20787
N	-0.93819	0.30961	-0.11055
C	-1.61529	-0.16352	2.32876
H	-2.86486	1.94902	-0.92162
C	-2.60084	-0.77334	4.9105
H	-2.99956	-1.01907	5.89107
C	-2.18974	-0.07503	-0.66789
C	-3.10985	0.90097	-1.06722
C	-2.94503	-0.51116	2.48767
C	-3.42067	-0.80772	3.79493
H	-3.62278	-0.56708	1.64323
C	-2.48808	-1.43111	-0.85226
C	-4.32649	0.52005	-1.63685
H	-5.03876	1.28211	-1.94046
H	-1.75924	-2.17665	-0.54862
H	-4.46582	-1.07902	3.91369
C	-3.70554	-1.80645	-1.41999
C	-4.62836	-0.83335	-1.81362
H	-3.92974	-2.85999	-1.56125
H	-5.57455	-1.12724	-2.25868
H	3.05465	-1.06044	-3.40563

H	1.79445	-2.78823	-4.76049
C	2.13945	-0.55725	-3.06378
H	3.23751	1.4298	-3.32054
C	0.8805	-2.22789	-4.5758
C	2.2678	0.95787	-3.19741
C	0.92878	-1.05281	-3.83462
O	1.8999	-0.83995	-1.69203
H	-0.38146	-3.61564	-5.64638
C	-0.34675	-2.69793	-5.0652
C	1.1222	1.67335	-3.02296
C	-0.25742	-0.32476	-3.58917
C	-0.11824	0.92935	-2.84461
C	-1.52593	-1.99764	-4.79322
H	1.11923	2.75614	-2.94031
C	-1.4849	-0.81337	-4.053
H	-1.02688	1.50583	-2.68991
H	-2.47824	-2.37189	-5.15912
H	-2.39862	-0.26702	-3.83543

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF= -3002.2536594

UB3LYP/6-31G(d)
Imaginary frequency = -112.14 cm^{-1}
Zero-point correction= 0.486178
(Hartree/Particle)
Thermal correction to Energy= 0.514568
Thermal correction to Enthalpy= 0.515513
Thermal correction to Gibbs Free Energy= 0.426319
Sum of electronic and zero-point Energies= -3002.478010
Sum of electronic and thermal Energies= -3002.449620
Sum of electronic and thermal Enthalpies= -3002.448676
Sum of electronic and thermal Free Energies= -3002.537869

H	6.23271	2.04155	1.61543
C	5.20326	1.73544	1.45007
H	4.36268	3.36533	2.58948
H	5.73012	0.03905	0.22768
C	4.15439	2.47544	2.00108
C	4.91884	0.61117	0.67046
C	2.83283	2.08362	1.7912
C	3.60151	0.21655	0.4409
H	2.01418	2.66496	2.2058
H	2.39966	0.60304	3.95018
C	2.55181	0.94102	1.02445
H	3.34513	-0.61913	-0.20258
H	1.77621	0.23745	6.31279
C	1.36937	0.37404	4.19655
C	1.00357	0.1642	5.55251
N	1.20969	0.55192	0.77332
C	0.39319	0.2845	3.221
C	0.34683	0.37867	1.74835
C	-0.29456	-0.12623	5.93345
Ni	0.34967	0.2364	-0.97499
H	-0.53372	-0.27805	6.98311
C	-0.93842	-0.02835	3.61852
C	-1.32115	-0.23733	4.95493
C	-1.02236	0.1234	1.32881
N	-1.22779	0.12779	0.02019
C	-1.83813	-0.13816	2.51677
H	-3.23167	1.88096	-0.04391
C	-2.68988	-0.55736	5.18429
H	-3.03999	-0.72719	6.19928
C	-2.55436	-0.12	-0.45396
C	-3.50786	0.90494	-0.43257
C	-3.15961	-0.45808	2.77302
C	-3.56621	-0.66044	4.11944
H	-3.88582	-0.55835	1.97471
C	-2.88896	-1.37669	-0.97014
C	-4.79727	0.66428	-0.91003
H	-5.53276	1.46409	-0.89264
H	-2.13188	-2.15359	-1.00668
H	-4.60609	-0.91047	4.31123
C	-4.18197	-1.6103	-1.43901
C	-5.14013	-0.5939	-1.40958
H	-4.43757	-2.58991	-1.8334
H	-6.1441	-0.7787	-1.78106
H	3.1067	-0.57188	-3.17192
H	2.49894	-2.2492	-4.97614
C	2.05692	-0.3726	-2.90434
H	2.60513	1.85116	-2.77132
C	1.45337	-1.98255	-4.83495
C	1.78933	1.13503	-2.822
C	1.10912	-1.01228	-3.90067
O	1.74442	-0.90495	-1.64034
H	0.72702	-3.38747	-6.30509
C	0.45608	-2.62877	-5.57511
C	0.48041	1.50851	-2.74314
C	-0.24414	-0.66456	-3.70564
C	-0.51154	0.43073	-2.75198
C	-0.88617	-2.30584	-5.3672
H	0.18302	2.54375	-2.59374
C	-1.23757	-1.32636	-4.43372
H	-1.55222	0.73854	-2.67865
H	-1.66157	-2.80898	-5.93974
H	-2.28211	-1.06119	-4.28483

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF=-3002.2528487

3

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.487473
(Hartree/Particle)
Thermal correction to Energy= 0.516349
Thermal correction to Enthalpy= 0.517293
Thermal correction to Gibbs Free Energy= 0.426332
Sum of electronic and zero-point Energies= -3002.585269
Sum of electronic and thermal Energies= -3002.556393
Sum of electronic and thermal Enthalpies= -3002.555449
Sum of electronic and thermal Free Energies= -3002.646409

H	6.52019	1.05681	1.46016
C	5.45192	0.94787	1.29646
H	5.66429	-0.72808	-0.04737
H	4.92145	2.61054	2.56835
C	4.97051	-0.05593	0.44971
C	4.55501	1.81851	1.92155
C	3.60183	-0.19273	0.22566
C	3.18199	1.67717	1.71632
H	3.21036	-0.94061	-0.45268
H	2.57921	0.17782	3.77241
C	2.70458	0.65965	0.88037
H	2.47696	2.35077	2.19442
H	1.96433	-0.33099	6.11236
C	1.53831	0.01487	4.02471
C	1.17708	-0.27583	5.36662

N	1.31425	0.50747	0.63988
C	0.54022	0.08834	3.06999
C	0.47828	0.31639	1.61872
C	-0.13679	-0.48501	5.75324
Ni	0.37987	0.62836	-1.10073
H	-0.37182	-0.70006	6.79199
C	-0.80913	-0.13955	3.46938
C	-1.18626	-0.42477	4.79458
C	-0.93151	0.20175	1.20708
N	-1.15985	0.31254	-0.07547
C	-1.74006	-0.07606	2.39194
H	-3.00244	2.22182	-0.29434
C	-2.57475	-0.63336	5.0293
H	-2.91974	-0.85297	6.03585
C	-2.51413	0.14035	-0.51114
C	-3.37153	1.24073	-0.5771
C	-3.08274	-0.28801	2.6489
C	-3.4812	-0.56239	3.98386
H	-3.82541	-0.24989	1.86065
C	-2.9555	-1.13143	-0.8848
C	-4.68829	1.0598	-1.00459
H	-5.35791	1.91363	-1.05214
H	-2.26486	-1.96757	-0.84142
H	-4.53555	-0.72645	4.1849
C	-4.27312	-1.30337	-1.3121
C	-5.14237	-0.21042	-1.3703
H	-4.61841	-2.29229	-1.59926
H	-6.16684	-0.34676	-1.70378
H	3.05947	1.06816	-3.65854
H	3.12375	-1.24207	-4.77524
C	2.01269	0.96356	-3.34302
H	1.57296	2.98224	-4.32136
C	2.07778	-1.36397	-4.49951
C	1.14947	2.11522	-3.82306
C	1.41034	-0.33554	-3.84561
O	1.95954	0.91964	-1.90878
H	1.92745	-3.37289	-5.28748
C	1.40557	-2.56256	-4.78472
C	-0.14105	1.98693	-3.47118
C	0.05461	-0.47607	-3.47649
C	-0.56032	0.71378	-2.81953
C	0.06881	-2.7153	-4.40763
H	-0.88221	2.76656	-3.63648
C	-0.60871	-1.67436	-3.75931
H	-1.63999	0.62485	-2.7083
H	-0.45476	-3.64233	-4.62948
H	-1.65587	-1.78658	-3.48637

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3002.2720406

UB3LYP/6-31G(d)
Zero-point correction= 0.486487 (Hartree/Particle)
Thermal correction to Energy= 0.515465
Thermal correction to Enthalpy= 0.516409
Thermal correction to Gibbs Free Energy= 0.424916
Sum of electronic and zero-point Energies= -3002.493647
Sum of electronic and thermal Energies= -3002.464669
Sum of electronic and thermal Enthalpies= -3002.463725
Sum of electronic and thermal Free Energies= -3002.555218

H	6.51895	1.09822	1.4501
C	5.45277	0.95717	1.29529
H	5.69944	-0.74115	-0.01167
H	4.88375	2.63853	2.52331
C	4.99166	-0.07563	0.47526
C	4.53535	1.8181	1.9013
C	3.62669	-0.25372	0.26168
C	3.16657	1.6379	1.70377
H	3.25998	-1.03311	-0.39568
H	2.57123	0.10866	3.79604
C	2.70369	0.58887	0.89574
H	2.45025	2.31605	2.15869
H	1.95813	-0.30613	6.15452
C	1.52709	-0.01711	4.05805
C	1.16697	-0.25307	5.41178
N	1.31898	0.40322	0.66269
C	0.52709	0.05242	3.10575
C	0.46048	0.24039	1.64271
C	-0.14797	-0.41082	5.81229
Ni	0.36265	0.49921	-1.09534
H	-0.38196	-0.58373	6.85986
C	-0.82226	-0.12677	3.52232
C	-1.20044	-0.35333	4.85633
C	-0.93185	0.14332	1.24351
N	-1.17825	0.23209	-0.0655
C	-1.74859	-0.07242	2.43705
H	-2.9198	2.22474	-0.37855
C	-2.5938	-0.51125	5.10624
H	-2.94284	-0.68515	6.1209
C	-2.54254	0.11118	-0.47986
C	-3.34545	1.25076	-0.60163
C	-3.09588	-0.23277	2.71461
C	-3.49712	-0.44739	4.06043
H	-3.8466	-0.20044	1.9337
C	-3.07318	-1.14886	-0.77991
C	-4.67506	1.12638	-1.00744
H	-5.29296	2.01558	-1.099
H	-2.43605	-2.02421	-0.69523
H	-4.55663	-0.57065	4.26774
C	-4.40349	-1.26658	-1.18512
C	-5.20906	-0.13111	-1.29741
H	-4.80909	-2.24816	-1.41493
H	-6.24339	-0.22462	-1.61607
H	3.02832	1.15136	-3.59895
H	3.22682	-1.07146	-4.90481
C	1.98343	0.96341	-3.3256
H	1.43829	3.01341	-4.17243
C	2.18705	-1.26585	-4.6493
C	1.06052	2.0963	-3.73155
C	1.46405	-0.33186	-3.91934
O	1.90578	0.81779	-1.89706
H	2.13719	-3.20025	-5.61043
C	1.57423	-2.46351	-5.043
C	-0.22225	1.87288	-3.40922
C	0.11854	-0.57064	-3.57665
C	-0.55777	0.5366	-2.83429
C	0.24562	-2.71271	-4.69744
H	-1.00893	2.61235	-3.54107
C	-0.48464	-1.76838	-3.966
H	-1.62547	0.37154	-2.70527
H	-0.23036	-3.64026	-5.00628
H	-1.52789	-1.95539	-3.71958

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.2687635

$TS_{A4\text{-}C1}$

UB3LYP/6-31G(d)
Imaginary frequency = -243.96 cm^{-1}
Zero-point correction= 0.602637
(Hartree/Particle)
Thermal correction to Energy= 0.638340
Thermal correction to Enthalpy= 0.639284
Thermal correction to Gibbs Free Energy= 0.532110
Sum of electronic and zero-point Energies= -3273.292399
Sum of electronic and thermal Energies= -3273.256696
Sum of electronic and thermal Enthalpies= -3273.255752
Sum of electronic and thermal Free Energies= -3273.362925

H	6.41879	0.84283	2.33065
C	5.38271	0.64318	2.07149
H	5.83824	-1.12838	0.92814
H	4.61635	2.37341	3.10936
C	5.0555	-0.46396	1.28401
C	4.37215	1.49941	2.51137
C	3.73172	-0.71835	0.93384
C	3.04115	1.2418	2.18076
H	3.46947	-1.55299	0.29584
H	2.30786	-0.19976	4.27873
C	2.71278	0.12324	1.40098
H	2.25428	1.91064	2.51721
H	1.48815	-0.57418	6.58021
C	1.25639	-0.40686	4.43971
C	0.77777	-0.62087	5.75955
N	1.36948	-0.14281	1.02835
C	0.35933	-0.46353	3.38873
C	0.4334	-0.33713	1.91986
C	-0.55394	-0.87936	6.03185
Ni	0.60186	-0.18774	-0.83853
H	-0.88122	-1.03087	7.05749
C	-1.00663	-0.74747	3.6732
C	-1.50145	-0.95325	4.97324
C	-0.90394	-0.57587	1.38229
N	-1.01488	-0.58328	0.06671
C	-1.81828	-0.81744	2.50307
H	-1.88774	-3.04734	-0.36346
C	-2.89484	-1.22149	5.08936
H	-3.33123	-1.38472	6.07151
C	-2.29612	-0.93905	-0.47097
C	-2.61753	-2.29149	-0.63692
C	-3.16852	-1.08159	2.65019
C	-3.68839	-1.27656	3.95771
H	-3.83301	-1.14287	1.7965
C	-3.21618	0.04975	-0.83207
C	-3.86222	-2.65158	-1.15498
H	-4.10668	-3.70298	-1.28034
H	-2.95699	1.09511	-0.70102
H	-4.75	-1.48167	4.06442
C	-4.4596	-0.32043	-1.34848
C	-4.78799	-1.66796	-1.51051
H	-5.17297	0.45157	-1.6244
H	-5.75593	-1.94995	-1.91535
H	3.59489	-0.21995	-3.06237
H	3.84572	-2.71151	-3.6762
C	2.51529	-0.30808	-2.88935
H	2.18947	1.424	-4.34588
C	2.77305	-2.81601	-3.52446
C	1.71218	0.67415	-3.72237
C	2.01019	-1.70975	-3.17585
O	2.25476	-0.04769	-1.50373
H	2.75132	-4.93725	-3.93856
C	2.15721	-4.06714	-3.6707
C	0.38884	0.56263	-3.53496
C	0.61994	-1.82659	-2.97372
C	-0.08816	-0.54516	-2.65822
C	0.78313	-4.19286	-3.46674
H	-0.33558	1.24183	-3.98022
C	0.0122	-3.07548	-3.12217
H	-1.17204	-0.6452	-2.63978
H	0.30294	-5.16089	-3.58914
H	-1.06333	-3.17325	-2.99469
C	0.48409	2.38589	-0.58582
C	-0.68916	2.95933	-0.0204
C	-1.74082	3.45236	-0.84392
C	-2.88331	4.01846	-0.29536
C	-3.03606	4.10756	1.09596
C	-2.01887	3.62766	1.92862
C	-0.86807	3.06788	1.3864
H	-1.62785	3.39214	-1.92396
H	-3.93157	4.55091	1.52222
H	-3.66263	4.40032	-0.95076
H	-0.07823	2.71513	2.04442
H	-2.12479	3.69781	3.00845
H	0.64573	2.44352	-1.65569
H	1.37541	2.28236	0.02056

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0438493
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UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.606614
(Hartree/Particle)
Thermal correction to Energy= 0.641910
Thermal correction to Enthalpy= 0.642855
Thermal correction to Gibbs Free Energy= 0.538678
Sum of electronic and zero-point Energies= -3273.432607
Sum of electronic and thermal Energies= -3273.397311
Sum of electronic and thermal Enthalpies= -3273.396366
Sum of electronic and thermal Free Energies= -3273.500543

H	6.50013	0.29423	0.98835
C	5.42441	0.22222	0.854
H	5.55536	-1.20241	-0.76418
H	4.96584	1.64222	2.41397
C	4.89243	-0.61896	-0.13072
C	4.56385	0.97585	1.6554
C	3.51469	-0.70675	-0.31341
C	3.18087	0.88384	1.48533
H	3.09028	-1.33056	-1.09197
H	2.51844	-0.66434	3.39697
C	2.64825	0.02912	0.51001
H	2.5082	1.47668	2.09362
H	1.90423	-1.22048	5.72003
C	1.47274	-0.79587	3.64697
C	1.11148	-1.11559	4.9849
N	1.25791	-0.07875	0.29044
C	0.47473	-0.6548	2.6997
C	0.40308	-0.34575	1.25862
C	-0.2041	-1.28553	5.38009
Ni	0.26729	0.40917	-1.39814
H	-0.44012	-1.51659	6.41539
C	-0.87502	-0.85961	3.11032

C	-1.25564	-1.16037	4.42796
C	-0.98708	-0.42726	0.85737
N	-1.26427	-0.23966	-0.42732
C	-1.8012	-0.72888	2.03561
H	-3.18513	1.53334	-1.14047
C	-2.65201	-1.31104	4.66937
H	-3.00149	-1.53982	5.67253
C	-2.58828	-0.52025	-0.87097
C	-3.48632	0.49576	-1.21961
C	-3.15078	-0.88054	2.29915
C	-3.55703	-1.16701	3.63135
H	-3.89734	-0.78849	1.51883
C	-2.99216	-1.8605	-0.96626
C	-4.77328	0.1717	-1.65493
H	-5.46333	0.96844	-1.91775
H	-2.28656	-2.63958	-0.6953
H	-4.61808	-1.28256	3.83309
C	-4.27862	-2.17838	-1.39923
C	-5.17483	-1.16286	-1.74605
H	-4.5796	-3.22001	-1.4667
H	-6.17673	-1.41002	-2.08451
H	3.09359	0.54683	-3.80623
H	3.38772	-1.97865	-4.09929
C	2.03124	0.46431	-3.54328
H	1.5887	2.13984	-5.03042
C	2.32424	-2.09006	-3.89954
C	1.15975	1.37975	-4.38431
C	1.54114	-0.96613	-3.67465
O	1.87375	0.84555	-2.17506
H	2.35666	-4.24836	-4.01364
C	1.74325	-3.36689	-3.84733
C	-0.15473	1.25259	-4.13753
C	0.15959	-1.09729	-3.40404
C	-0.57535	0.18023	-3.20858
C	0.38064	-3.50475	-3.56971
H	-0.90577	1.92385	-4.54644
C	-0.4139	-2.37411	-3.35024
H	-1.65186	0.07053	-3.10055
H	-0.06865	-4.49367	-3.53277
H	-1.47689	-2.47897	-3.15275
C	-0.32198	2.32666	-1.23136
C	-0.12476	2.78623	0.14492
C	-1.11008	2.6026	1.13861
C	-0.89644	3.01889	2.45137
C	0.30419	3.64032	2.80575
C	1.28807	3.84583	1.83031
C	1.08088	3.41423	0.52356
H	-2.04948	2.12797	0.87475
H	0.47224	3.96445	3.82902
H	-1.66779	2.85474	3.19912
H	1.85587	3.55444	-0.22527
H	2.2234	4.33174	2.09558
H	-1.3567	2.34875	-1.56665
H	0.34427	2.78917	-1.95523

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0528301

UB3LYP/6-31G(d)
Zero-point correction= 0.605605
(Hartree/Particle)
Thermal correction to Energy= 0.641221
Thermal correction to Enthalpy= 0.642165
Thermal correction to Gibbs Free Energy= 0.536526
Sum of electronic and zero-point Energies= -3273.304319
Sum of electronic and thermal Energies= -3273.268704
Sum of electronic and thermal Enthalpies= -3273.267760
Sum of electronic and thermal Free Energies= -3273.373399

H	6.37698	0.48359	1.36542
C	5.31444	0.37077	1.16723
H	5.59055	-1.11543	-0.37233
H	4.71482	1.8402	2.62902
C	4.87151	-0.52616	0.19098
C	4.38207	1.1284	1.87765
C	3.51179	-0.66701	-0.07555
C	3.017	0.98393	1.62581
H	3.16191	-1.34694	-0.84371
H	2.47737	-0.87878	3.39937
C	2.57193	0.07341	0.65595
H	2.2912	1.582	2.16653
H	1.90655	-1.67638	5.66505
C	1.43886	-1.06362	3.64741
C	1.10233	-1.52007	4.95118
N	1.19223	-0.08411	0.37661
C	0.4259	-0.85855	2.72879
C	0.33427	-0.43023	1.31824
C	-0.20241	-1.76173	5.33995
Ni	0.21495	0.38935	-1.33513
H	-0.41879	-2.10099	6.34998
C	-0.91239	-1.13253	3.13044
C	-1.26857	-1.57046	4.416
C	-1.05461	-0.5044	0.92078
N	-1.34388	-0.22567	-0.35037
C	-1.85225	-0.92227	2.07878
H	-3.27058	1.61673	-0.82017
C	-2.65666	-1.78187	4.65536
H	-2.98955	-2.11771	5.63431
C	-2.67729	-0.45535	-0.80041
C	-3.57743	0.59622	-1.02023
C	-3.19416	-1.13575	2.34463
C	-3.57587	-1.56161	3.64552
H	-3.95669	-0.99034	1.58822
C	-3.10085	-1.77309	-1.0379
C	-4.87223	0.33321	-1.47308
H	-5.55877	1.15992	-1.63506
H	-2.40277	-2.58577	-0.86293
H	-4.63158	-1.72543	3.84454
C	-4.39557	-2.03053	-1.4865
C	-5.2872	-0.97808	-1.70858
H	-4.70733	-3.05651	-1.66361
H	-6.29497	-1.17877	-2.06099
H	3.07926	0.51851	-3.70183
H	3.41537	-2.00098	-4.11429
C	2.01387	0.40348	-3.46586
H	1.55825	2.05057	-4.98477
C	2.3546	-2.13562	-3.91271
C	1.13676	1.29498	-4.32832
C	1.55796	-1.03536	-3.6285
O	1.82623	0.77093	-2.1005
H	2.41471	-4.28373	-4.14264
C	1.79063	-3.42009	-3.92787
C	-0.1769	1.13657	-4.10387
C	0.17966	-1.19651	-3.36681
C	-0.5797	0.07047	-3.15548
C	0.4317	-3.58856	-3.66116
H	-0.93826	1.77597	-4.54498
C	-0.37631	-2.48049	-3.38348
H	-1.65473	-0.06481	-3.05645

H	-0.00647	-4.5832	-3.68192
H	-1.44137	-2.61102	-3.21127
C	-0.33717	2.31009	-1.28327
C	0.00514	2.95575	-0.00926
C	-0.88474	2.97371	1.08477
C	-0.56585	3.65036	2.25986
C	0.65182	4.32729	2.37356
C	1.55094	4.3135	1.30223
C	1.23723	3.62883	0.1319
H	-1.8402	2.46256	1.00335
H	0.89637	4.86255	3.28732
H	-1.27126	3.6566	3.08694
H	1.94086	3.60717	-0.69546
H	2.50058	4.8364	1.38211
H	-1.40418	2.30487	-1.49798
H	0.24096	2.6876	-2.12057

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0501358

TS_{4-5}

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -65.21 cm^{-1}
Zero-point correction= 0.605435
(Hartree/Particle)
Thermal correction to Energy= 0.640267
Thermal correction to Enthalpy= 0.641211
Thermal correction to Gibbs Free Energy= 0.538757
Sum of electronic and zero-point Energies= -3273.425758
Sum of electronic and thermal Energies= -3273.390926
Sum of electronic and thermal Enthalpies= -3273.389982
Sum of electronic and thermal Free Energies= -3273.492435

H	5.46262	-1.99519	1.20195
C	4.49393	-1.5483	0.99684
H	4.08823	-2.80614	-0.71283
H	4.61385	-0.1397	2.62831
C	3.7218	-2.0041	-0.07783
C	4.01691	-0.50871	1.79885
C	2.48679	-1.42345	-0.35338
C	2.76997	0.06503	1.54233
H	1.89435	-1.74625	-1.20067
H	1.24061	-0.94776	3.29369
C	1.99572	-0.40074	0.47087
H	2.39863	0.87774	2.15502
H	0.17634	-1.19116	5.50539
C	0.22468	-0.59877	3.43014
C	-0.39355	-0.73446	4.70174
N	0.74345	0.16271	0.13627
C	-0.48958	-0.01611	2.39873
C	-0.23639	0.30581	0.98281
C	-1.68222	-0.29403	4.95073
Ni	0.2598	1.04642	-1.65522
H	-2.11521	-0.40042	5.94159
C	-1.82696	0.40243	2.65144
C	-2.44863	0.29935	3.90937
C	-1.48061	0.87287	0.42807
N	-1.48002	1.18876	-0.84477
C	-2.47317	0.94348	1.50466
H	-2.02514	3.51763	-2.06445
C	-3.77739	0.79967	4.00662
H	-4.30061	0.74924	4.95754
C	-2.70042	1.55776	-1.48124
C	-2.84074	2.80604	-2.09754
C	-3.76384	1.42455	1.62996
C	-4.39925	1.34871	2.89754
H	-4.29589	1.85199	0.78861
C	-3.74335	0.62294	-1.5553
C	-4.03155	3.12834	-2.74997
H	-4.13628	4.10385	-3.21594
H	-3.61176	-0.35321	-1.09883
H	-5.41176	1.7299	2.99102
C	-4.92824	0.9506	-2.21295
C	-5.0793	2.20617	-2.80834
H	-5.73062	0.22033	-2.26479
H	-6.00217	2.45992	-3.32129
H	3.14948	0.31278	-3.94809
H	3.10034	-2.23979	-4.06482
C	2.08053	0.39435	-3.711
H	1.92009	2.01424	-5.30818
C	2.02841	-2.19242	-3.88342
C	1.3733	1.36534	-4.63097
C	1.39945	-0.95651	-3.78261
O	1.95288	0.84024	-2.34893
H	1.78104	-4.33714	-3.78167
C	1.28785	-3.371	-3.71398
C	0.04176	1.43959	-4.42294
C	0.01013	-0.87989	-3.53508
C	-0.56904	0.47842	-3.49292
C	-0.0819	-3.30058	-3.43606
H	-0.59127	2.19043	-4.89038
C	-0.72203	-2.06072	-3.34848
H	-1.65317	0.50954	-3.43171
H	-0.65486	-4.21402	-3.29773
H	-1.79086	-2.00521	-3.1516
C	0.69978	2.99129	-1.11927
C	0.59064	3.33498	0.29923
C	-0.63706	3.69414	0.89588
C	-0.73301	3.96226	2.26161
C	0.39687	3.87961	3.07733
C	1.62922	3.53746	2.50521
C	1.72133	3.26792	1.14305
H	-1.52735	3.75798	0.27752
H	0.32278	4.07987	4.14255
H	-1.69776	4.22219	2.68945
H	2.67948	2.98981	0.71126
H	2.5192	3.47767	3.12704
H	0.01495	3.54781	-1.76274
H	1.71894	3.04341	-1.49825

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0457883

UB3LYP/6-31G(d)
Imaginary frequency = -70.73 cm^{-1}
Zero-point correction= 0.603820
(Hartree/Particle)
Thermal correction to Energy= 0.639136
Thermal correction to Enthalpy= 0.640080
Thermal correction to Gibbs Free Energy= 0.535338
Sum of electronic and zero-point Energies= -3273.296591
Sum of electronic and thermal Energies= -3273.261275
Sum of electronic and thermal Enthalpies= -3273.260331
Sum of electronic and thermal Free Energies= -3273.365073

H	5.39931	-1.75727	1.66124
C	4.42905	-1.361	1.37409

H	4.18949	-2.70478	-0.29748
H	4.38843	0.12643	2.93683
C	3.74926	-1.89251	0.27455
C	3.86024	-0.30777	2.09173
C	2.51399	-1.37843	-0.11094
C	2.61219	0.19967	1.72807
H	1.99783	-1.76644	-0.98043
H	1.06333	-1.09758	3.32491
C	1.92612	-0.34464	0.63202
H	2.17635	1.03036	2.27221
H	-0.0874	-1.52167	5.46647
C	0.03385	-0.78143	3.44184
C	-0.6337	-1.019	4.67319
N	0.66883	0.16255	0.21929
C	-0.64812	-0.14135	2.42331
C	-0.35034	0.26181	1.03212
C	-1.94001	-0.62473	4.89668
Ni	0.20849	1.0026	-1.60032
H	-2.41173	-0.81314	5.85787
C	-2.00181	0.2342	2.64948
C	-2.67465	0.02647	3.86707
C	-1.57817	0.83162	0.46585
N	-1.5509	1.19678	-0.79971
C	-2.60988	0.83703	1.51153
H	-2.17937	3.65884	-1.70147
C	-4.01989	0.48498	3.93812
H	-4.58444	0.35441	4.85794
C	-2.76353	1.60187	-1.43578
C	-2.95091	2.91819	-1.87556
C	-3.91913	1.27443	1.61417
C	-4.6067	1.09374	2.84321
H	-4.43046	1.74424	0.78235
C	-3.76864	0.65033	-1.67286
C	-4.13398	3.27882	-2.52326
H	-4.26884	4.30586	-2.85143
H	-3.61233	-0.37397	-1.34758
H	-5.63354	1.44132	2.91602
C	-4.94584	1.01716	-2.32304
C	-5.13549	2.33392	-2.74924
H	-5.71345	0.26909	-2.50196
H	-6.05212	2.6182	-3.25797
H	3.08997	0.32529	-3.90346
H	3.14535	-2.21702	-4.17658
C	2.0204	0.34644	-3.65724
H	1.77573	2.01737	-5.193
C	2.07263	-2.22612	-3.99327
C	1.2644	1.32627	-4.52996
C	1.39496	-1.02765	-3.8003
O	1.88779	0.70722	-2.27875
H	1.90842	-4.3784	-4.08685
C	1.3778	-3.44158	-3.93656
C	-0.06918	1.33018	-4.32271
C	0.00268	-1.02686	-3.55975
C	-0.63418	0.29748	-3.44152
C	0.00448	-3.44891	-3.67691
H	-0.73528	2.06479	-4.77018
C	-0.68261	-2.24756	-3.48795
H	-1.71738	0.28452	-3.36026
H	-0.53498	-4.39183	-3.63304
H	-1.75682	-2.25477	-3.31267
C	0.6968	2.95049	-1.21422
C	0.81318	3.4177	0.17118
C	-0.30018	3.83887	0.93019
C	-0.1537	4.31639	2.23201
C	1.11041	4.3847	2.82026
C	2.22838	3.96963	2.0882
C	2.08102	3.488	0.79094
H	-1.29028	3.80975	0.48444
H	1.22556	4.76144	3.8331
H	-1.03075	4.64013	2.7871
H	2.95439	3.16872	0.22837
H	3.22001	4.02794	2.53084
H	-0.08154	3.4624	-1.78369
H	1.64429	2.96361	-1.74686

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0419592

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UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.606765
(Hartree/Particle)
Thermal correction to Energy= 0.642030
Thermal correction to Enthalpy= 0.642974
Thermal correction to Gibbs Free Energy= 0.539815
Sum of electronic and zero-point Energies= -3273.439318
Sum of electronic and thermal Energies= -3273.404052
Sum of electronic and thermal Enthalpies= -3273.403108
Sum of electronic and thermal Free Energies= -3273.506267

H	5.78899	-2.20127	1.45636
C	4.78088	-1.85781	1.2428
H	4.81252	-2.49309	-0.82236
H	4.45435	-1.05343	3.22062
C	4.23411	-2.02241	-0.03258
C	4.02888	-1.22264	2.23553
C	2.94589	-1.57292	-0.31164
C	2.73323	-0.78592	1.96846
H	2.5394	-1.66742	-1.3066
H	1.08613	-2.20605	3.28988
C	2.16516	-0.9863	0.69685
H	2.18014	-0.24847	2.72685
H	-0.07713	-2.64788	5.41219
C	0.1283	-1.73354	3.46912
C	-0.54702	-1.98527	4.69173
N	0.87986	-0.51239	0.35172
C	-0.4524	-0.88628	2.54053
C	-0.1182	-0.40474	1.1845
C	-1.76508	-1.40323	4.9989
Ni	0.47629	0.45118	-1.41741
H	-2.24149	-1.60118	5.95507
C	-1.73512	-0.34308	2.83667
C	-2.40553	-0.55157	4.05784
C	-1.29595	0.35259	0.69004
N	-1.22884	0.81055	-0.52587
C	-2.28555	0.4189	1.77093
H	-1.19917	3.03545	-1.94289
C	-3.65891	0.10178	4.21684
H	-4.21118	-0.0188	5.14468
C	-2.33767	1.3669	-1.20799
C	-2.16291	2.54065	-1.95239
C	-3.50458	1.04574	1.95554
C	-4.17363	0.88414	3.19641
H	-3.9595	1.64516	1.17626
C	-3.56439	0.68669	-1.25613
C	-3.22135	3.05517	-2.69969
H	-3.08112	3.97218	-3.26436
H	-3.67991	-0.24601	-0.71386
H	-5.12917	1.38023	3.33713

C	-4.61308	1.19973	-2.01682
C	-4.44849	2.38817	-2.73556
H	-5.55727	0.66439	-2.05546
H	-5.26785	2.78444	-3.32788
H	2.06886	-0.03483	-4.80077
H	3.28916	-2.24833	-4.60043
C	1.34718	-0.2693	-4.0068
H	-0.29936	0.50773	-5.37587
C	2.52993	-2.56826	-3.8895
C	-0.07759	-0.02553	-4.45613
C	1.48374	-1.70967	-3.564
O	1.63021	0.572	-2.86685
H	3.43195	-4.50076	-3.54008
C	2.6127	-3.83212	-3.28933
C	-1.01613	-0.4029	-3.56341
C	0.50088	-2.10576	-2.62933
C	-0.56719	-1.12827	-2.36101
C	1.64472	-4.22609	-2.35918
H	-2.06859	-0.15913	-3.67647
C	0.59243	-3.36748	-2.0288
H	-1.35395	-1.48561	-1.69831
H	1.70906	-5.20521	-1.89129
H	-0.16027	-3.6746	-1.30574
C	1.34802	2.18094	-0.74767
C	1.1787	2.55167	0.66648
C	-0.01914	3.11615	1.15675
C	-0.18482	3.42076	2.5068
C	0.84571	3.17296	3.4185
C	2.04845	2.63124	2.95398
C	2.2096	2.32742	1.60292
H	-0.83336	3.30993	0.46438
H	0.7159	3.40295	4.47248
H	-1.12599	3.84371	2.84923
H	3.14791	1.90333	1.25656
H	2.86437	2.44159	3.6474
H	0.90156	2.90865	-1.43148
H	2.39518	2.02267	-1.01282

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0612788

UB3LYP/6-31G(d)
Zero-point correction= 0.604732
(Hartree/Particle)
Thermal correction to Energy= 0.640711
Thermal correction to Enthalpy= 0.641655
Thermal correction to Gibbs Free Energy= 0.535235
Sum of electronic and zero-point Energies= -3273.304298
Sum of electronic and thermal Energies= -3273.268319
Sum of electronic and thermal Enthalpies= -3273.267375
Sum of electronic and thermal Free Energies= -3273.373795

H	5.57865	-2.58743	1.70395
C	4.61065	-2.16413	1.44967
H	4.35388	-3.377	-0.31824
H	4.58658	-0.79403	3.11756
C	3.92473	-2.60674	0.31618
C	4.05223	-1.16149	2.2452
C	2.69354	-2.05446	-0.02801
C	2.8085	-0.61844	1.92384
H	2.17074	-2.38193	-0.91591
H	1.22729	-1.92482	3.44996
C	2.11589	-1.07471	0.7906
H	2.38454	0.17713	2.52605
H	0.07615	-2.38572	5.58232
C	0.22046	-1.5531	3.59604
C	-0.44638	-1.81081	4.82294
N	0.86869	-0.51666	0.41051
C	-0.4307	-0.82136	2.61963
C	-0.12292	-0.37648	1.24264
C	-1.72193	-1.34572	5.08495
Ni	0.45582	0.45267	-1.36757
H	-2.19311	-1.55048	6.04299
C	-1.75622	-0.37585	2.8812
C	-2.4254	-0.59958	4.0999
C	-1.32907	0.30203	0.72048
N	-1.28725	0.72968	-0.51427
C	-2.3441	0.31445	1.78469
H	-1.62456	3.14842	-1.60499
C	-3.73584	-0.05956	4.2159
H	-4.29413	-0.19854	5.13828
C	-2.45876	1.21192	-1.166
C	-2.48505	2.49973	-1.71825
C	-3.61909	0.83211	1.93167
C	-4.29822	0.63952	3.16259
H	-4.11019	1.37288	1.13134
C	-3.56708	0.36715	-1.33707
C	-3.61589	2.94331	-2.40398
H	-3.62759	3.9478	-2.81776
H	-3.53787	-0.63812	-0.92823
H	-5.29835	1.04972	3.27095
C	-4.68855	0.81409	-2.03424
C	-4.7202	2.10491	-2.56679
H	-5.53657	0.14768	-2.16617
H	-5.59459	2.45099	-3.11036
H	2.80277	0.05871	-4.20975
H	3.56896	-2.35998	-4.37351
C	1.90388	-0.18771	-3.6276
H	0.72449	1.17343	-5.03591
C	2.64039	-2.65735	-3.89022
C	0.66223	0.44089	-4.23613
C	1.70361	-1.68867	-3.54366
O	2.07163	0.27497	-2.29306
H	3.12806	-4.76132	-3.88202
C	2.39655	-4.00617	-3.60512
C	-0.50462	0.06861	-3.66076
C	0.4984	-2.06261	-2.90711
C	-0.45482	-0.98001	-2.62696
C	1.21343	-4.38035	-2.96029
H	-1.45689	0.52165	-3.92295
C	0.26871	-3.41326	-2.61017
H	-1.41588	-1.30499	-2.2339
H	1.02198	-5.42762	-2.73949
H	-0.65902	-3.70793	-2.12285
C	1.14511	2.30628	-0.81212
C	1.13455	2.74145	0.59197
C	-0.01788	3.24444	1.23434
C	0.01482	3.68166	2.55837
C	1.20107	3.62672	3.29144
C	2.35706	3.13256	2.67813
C	2.3219	2.69446	1.35707
H	-0.94837	3.31498	0.67783
H	1.22821	3.97052	4.32204
H	-0.8911	4.07052	3.01739
H	3.22762	2.32015	0.88706
H	3.29308	3.09789	3.23115
H	0.51533	2.92982	-1.45492
H	2.1475	2.24143	-1.22828

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0571884

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UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.606735 (Hartree/Particle)
Thermal correction to Energy= 0.642346
Thermal correction to Enthalpy= 0.643290
Thermal correction to Gibbs Free Energy= 0.537082
Sum of electronic and zero-point Energies= -3273.437049
Sum of electronic and thermal Energies= -3273.401438
Sum of electronic and thermal Enthalpies= -3273.400494
Sum of electronic and thermal Free Energies= -3273.506701

H	6.12956	-0.15814	1.99608
C	5.05197	-0.21141	1.8697
H	5.12007	-1.96612	0.61473
H	4.65858	1.54318	3.06535
C	4.48362	-1.22718	1.09407
C	4.22588	0.7419	2.47248
C	3.10213	-1.29566	0.92287
C	2.84205	0.6752	2.31245
H	2.64979	-2.06095	0.30284
H	1.99193	-0.6822	4.47474
C	2.26776	-0.35641	1.54864
H	2.19623	1.41611	2.77417
H	1.29801	-0.67263	6.84875
C	0.94729	-0.53018	4.72143
C	0.54151	-0.51915	6.08451
N	0.88238	-0.40971	1.31167
C	-0.0079	-0.3342	3.74098
C	-0.02328	-0.28945	2.27135
C	-0.77274	-0.309	6.4664
Ni	0.05268	-0.04387	-0.47334
H	-1.04112	-0.29388	7.51935
C	-1.36162	-0.14356	4.14019
C	-1.78074	-0.10929	5.47941
C	-1.38945	-0.10181	1.83782
N	-1.59712	-0.02072	0.52345
C	-2.24131	0.01678	3.02887
H	-2.57598	1.88429	-1.06316
C	-3.1674	0.12678	5.70649
H	-3.54709	0.16535	6.72394
C	-2.91212	0.04707	0.0019
C	-3.28577	1.09464	-0.85012
C	-3.58069	0.25378	3.28344
C	-4.02358	0.30886	4.634
H	-4.29753	0.3899	2.48238
C	-3.83161	-0.9807	0.27112
C	-4.56424	1.12468	-1.40779
H	-4.84184	1.94691	-2.06135
H	-3.52933	-1.80245	0.9131
H	-5.07735	0.49363	4.82208
C	-5.10849	-0.94403	-0.28684
C	-5.48137	0.10858	-1.12881
H	-5.80969	-1.74526	-0.07076
H	-6.47489	0.13258	-1.56675
H	1.21299	0.6202	-3.27048
H	3.08177	-0.55744	-4.364
C	0.91988	-0.29176	-2.73677
H	-1.15473	0.57747	-2.64814
C	2.54088	-1.49488	-4.2518
C	-0.54439	-0.2621	-2.31873
C	1.36658	-1.51458	-3.5021
O	1.54137	-0.32597	-1.44041
H	3.95017	-2.63494	-5.42557
C	3.032	-2.66331	-4.84517
C	-1.21084	-1.55828	-2.23688
C	0.65009	-2.72478	-3.35237
C	-0.62921	-2.71282	-2.65717
C	2.33797	-3.86606	-4.68419
H	-2.21856	-1.58869	-1.83523
C	1.15342	-3.89404	-3.94773
H	-1.15848	-3.65762	-2.55354
H	2.71484	-4.7786	-5.13823
H	0.60356	-4.82601	-3.83649
C	0.29423	1.94543	-0.36828
C	0.79511	2.61474	-1.57656
C	2.18059	2.7191	-1.81176
C	2.66805	3.32443	-2.96596
C	1.78102	3.84073	-3.91901
C	0.40388	3.7541	-3.69794
C	-0.08162	3.14842	-2.5391
H	2.86736	2.30192	-1.08092
H	2.16141	4.30884	-4.82271
H	3.74043	3.39392	-3.12856
H	-1.15459	3.08852	-2.37508
H	-0.29207	4.15866	-4.42801
H	1.01051	1.98489	0.45362
H	-0.68084	2.30825	-0.04658

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0553005

UB3LYP/6-31G(d)
Zero-point correction= 0.605643 (Hartree/Particle)
Thermal correction to Energy= 0.641601
Thermal correction to Enthalpy= 0.642545
Thermal correction to Gibbs Free Energy= 0.533982
Sum of electronic and zero-point Energies= -3273.317447
Sum of electronic and thermal Energies= -3273.281489
Sum of electronic and thermal Enthalpies= -3273.280545
Sum of electronic and thermal Free Energies= -3273.389108

H	6.12002	-0.31879	2.42648
C	5.04672	-0.31992	2.25695
H	5.08826	-2.02842	0.94079
H	4.68185	1.41123	3.49366
C	4.46613	-1.27989	1.42424
C	4.23925	0.648	2.85854
C	3.09191	-1.28272	1.19537
C	2.86177	0.64739	2.64283
H	2.63847	-2.00551	0.52791
H	1.93143	-0.7992	4.7135
C	2.27164	-0.33122	1.82244
H	2.234	1.40513	3.10301
H	1.19457	-0.91601	7.0687
C	0.88477	-0.64257	4.94819
C	0.45441	-0.70449	6.30172
N	0.88895	-0.32394	1.54678
C	-0.04714	-0.37407	3.96247
C	-0.03462	-0.24591	2.49323
C	-0.86136	-0.49458	6.67203
Ni	0.07153	0.02916	-0.27098
H	-1.14814	-0.53632	7.7199

C	-1.40447	-0.18943	4.34923
C	-1.84736	-0.22373	5.68083
C	-1.39343	-0.0365	2.04881
N	-1.59523	0.07841	0.73211
C	-2.26244	0.03651	3.23245
H	-2.67534	2.10048	-0.64847
C	-3.23439	0.01716	5.89734
H	-3.6324	0.00642	6.90895
C	-2.91914	0.15077	0.22628
C	-3.35041	1.26395	-0.50845
C	-3.60346	0.2758	3.47964
C	-4.06844	0.26664	4.8229
H	-4.30694	0.46372	2.67711
C	-3.80763	-0.92332	0.41229
C	-4.64271	1.30817	-1.0331
H	-4.96163	2.18298	-1.59361
H	-3.4696	-1.79498	0.96484
H	-5.12336	0.45556	5.00297
C	-5.09776	-0.87337	-0.11287
C	-5.52297	0.24291	-0.83813
H	-5.76995	-1.7139	0.03884
H	-6.52738	0.27892	-1.25022
H	1.27849	0.50098	-3.10848
H	3.18286	-0.76839	-4.03603
C	0.96813	-0.36486	-2.51074
H	-1.09388	0.5353	-2.49512
C	2.61685	-1.68656	-3.89527
C	-0.50204	-0.29677	-2.1155
C	1.42083	-1.64318	-3.18204
O	1.56365	-0.30135	-1.20504
H	4.03397	-2.90955	-4.96885
C	3.09859	-2.89144	-4.41568
C	-1.19078	-1.57738	-1.98893
C	0.67645	-2.83017	-2.99813
C	-0.62067	-2.7585	-2.34465
C	2.37483	-4.06999	-4.22063
H	-2.2125	-1.57625	-1.62212
C	1.17044	-4.03672	-3.52063
H	-1.17462	-3.68664	-2.21828
H	2.74461	-5.01094	-4.61973
H	0.59583	-4.95001	-3.3809
C	0.37329	2.00242	-0.28097
C	0.72065	2.70966	-1.52631
C	2.06342	2.80922	-1.94427
C	2.40812	3.5203	-3.08982
C	1.41951	4.14439	-3.8576
C	0.08316	4.05129	-3.46431
C	-0.25937	3.3427	-2.31376
H	2.82993	2.30816	-1.36022
H	1.68943	4.69852	-4.75262
H	3.45126	3.58896	-3.38794
H	-1.30222	3.28957	-2.01005
H	-0.69291	4.53573	-4.05139
H	1.19633	2.01808	0.43407
H	-0.54114	2.38154	0.17439

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0536435

$TS_{6\text{-}P1}$

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -327.98 cm^{-1}
Zero-point correction= 0.606533
(Hartree/Particle)
Thermal correction to Energy= 0.641551
Thermal correction to Enthalpy= 0.642495
Thermal correction to Gibbs Free Energy= 0.537777
Sum of electronic and zero-point Energies= -3273.407151
Sum of electronic and thermal Energies= -3273.372133
Sum of electronic and thermal Enthalpies= -3273.371188
Sum of electronic and thermal Free Energies= -3273.475906

H	6.03944	-0.9906	2.00519
C	4.98232	-0.80909	1.83191
H	4.75964	-2.43662	0.42828
H	4.8847	0.88472	3.16768
C	4.26357	-1.62129	0.94838
C	4.33385	0.24299	2.48519
C	2.90814	-1.38954	0.72094
C	2.97694	0.48061	2.25883
H	2.34591	-2.00469	0.02939
H	2.01	-1.13527	4.16495
C	2.25216	-0.34404	1.38535
H	2.46547	1.29758	2.76007
H	1.33214	-1.65484	6.48485
C	0.97231	-1.01157	4.45321
C	0.57495	-1.30475	5.78873
N	0.8778	-0.11292	1.14846
C	0.01862	-0.56413	3.55699
C	-0.01533	-0.17351	2.14134
C	-0.72856	-1.15364	6.22902
Ni	0.07965	0.43999	-0.51186
H	-0.98947	-1.38091	7.2593
C	-1.3259	-0.42779	4.01593
C	-1.73633	-0.69915	5.32825
C	-1.36059	0.15423	1.79099
N	-1.58074	0.52503	0.52312
C	-2.20523	0.01332	2.98267
H	-2.71488	2.88271	0.01001
C	-3.11747	-0.49324	5.61802
H	-3.49202	-0.68585	6.6199
C	-2.92164	0.74456	0.10905
C	-3.3883	2.04364	-0.13395
C	-3.5388	0.20813	3.29514
C	-3.97468	-0.04957	4.62566
H	-4.25451	0.54622	2.55422
C	-3.79865	-0.3401	-0.05077
C	-4.70825	2.25259	-0.53843
H	-5.05917	3.26468	-0.72002
H	-3.43703	-1.34221	0.16032
H	-5.02376	0.10537	4.86212
C	-5.11729	-0.12738	-0.45274
C	-5.57628	1.16976	-0.7004
H	-5.78643	-0.97523	-0.57048
H	-6.60268	1.33504	-1.01501
H	1.62636	0.4233	-3.41442
H	3.67988	-0.9559	-3.51317
C	1.25628	-0.18971	-2.58268
H	-0.77007	0.25254	-3.38906
C	3.10782	-1.80397	-3.14322
C	-0.27021	-0.11319	-2.49695
C	1.80046	-1.60105	-2.70275
O	1.6808	0.36205	-1.34523
H	4.71111	-3.2166	-3.44246
C	3.69145	-3.07325	-3.09567
C	-0.95684	-1.29596	-1.93272
C	1.04807	-2.69638	-2.22231
C	-0.33776	-2.49452	-1.82078
C	2.95828	-4.15606	-2.5997

H	-2.01692	-1.20453	-1.72669
C	1.64447	-3.96831	-2.17271
H	-0.89307	-3.35596	-1.45694
H	3.40686	-5.14464	-2.55452
H	1.06752	-4.81092	-1.79845
C	-0.62657	1.86049	-1.89135
C	0.13926	2.59908	-2.92584
C	1.38839	3.16869	-2.62555
C	2.1017	3.87051	-3.59456
C	1.58108	4.01594	-4.88553
C	0.33868	3.45867	-5.19576
C	-0.37468	2.75586	-4.223
H	1.80131	3.03123	-1.63137
H	2.1391	4.5621	-5.64112
H	3.06675	4.30379	-3.34552
H	-1.34671	2.33301	-4.46781
H	-0.07779	3.57305	-6.1929
H	-0.49797	2.35176	-0.91835
H	-1.69065	1.79569	-2.10068

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0380837

UB3LYP/6-31G(d)
Imaginary frequency = -331.13 cm^{-1}
Zero-point correction= 0.605298
(Hartree/Particle)
Thermal correction to Energy= 0.640675
Thermal correction to Enthalpy= 0.641619
Thermal correction to Gibbs Free Energy= 0.535220
Sum of electronic and zero-point Energies= -3273.287785
Sum of electronic and thermal Energies= -3273.252407
Sum of electronic and thermal Enthalpies= -3273.251463
Sum of electronic and thermal Free Energies= -3273.3578

H	6.07691	-0.60513	2.22838
C	5.01494	-0.50989	2.01801
H	4.94313	-2.24537	0.73812
H	4.76755	1.2688	3.21596
C	4.3777	-1.43043	1.1824
C	4.28007	0.53983	2.57348
C	3.01756	-1.31056	0.90311
C	2.91803	0.66339	2.30085
H	2.52071	-2.01405	0.24593
H	2.01177	-1.06496	4.24429
C	2.27245	-0.27002	1.47448
H	2.34236	1.48148	2.7248
H	1.3326	-1.52095	6.57585
C	0.97196	-0.94248	4.52554
C	0.57407	-1.1993	5.86708
N	0.88823	-0.144	1.20082
C	0.0169	-0.53276	3.61344
C	-0.0152	-0.18972	2.18339
C	-0.73109	-1.04797	6.29787
Ni	0.10025	0.31311	-0.495
H	-0.99215	-1.24672	7.33446
C	-1.32916	-0.39715	4.06241
C	-1.74033	-0.63214	5.38173
C	-1.36343	0.10966	1.81695
N	-1.58093	0.43864	0.5336
C	-2.2096	0.0009	3.01238
H	-2.71199	2.80754	0.04239
C	-3.12329	-0.43202	5.6623
H	-3.49933	-0.59695	6.66901
C	-2.91849	0.66728	0.11135
C	-3.38256	1.97027	-0.12576
C	-3.54557	0.19131	3.31976
C	-3.9814	-0.02853	4.65579
H	-4.26616	0.50014	2.57089
C	-3.80301	-0.40858	-0.07539
C	-4.69489	2.18976	-0.54851
H	-5.03854	3.20611	-0.7224
H	-3.4514	-1.41598	0.12798
H	-5.03287	0.12367	4.88513
C	-5.11398	-0.18543	-0.49652
C	-5.56489	1.11457	-0.73799
H	-5.7847	-1.02959	-0.63419
H	-6.58553	1.28767	-1.0676
H	1.71295	0.3453	-3.36072
H	3.67569	-1.12393	-3.57795
C	1.29226	-0.30103	-2.5789
H	-0.69493	0.27094	-3.40813
C	3.05686	-1.96678	-3.27874
C	-0.23112	-0.1572	-2.52165
C	1.77055	-1.72657	-2.79718
O	1.70485	0.15141	-1.30185
H	4.56019	-3.43936	-3.75054
C	3.55735	-3.26803	-3.36837
C	-0.97469	-1.33783	-2.02599
C	0.96052	-2.81578	-2.40683
C	-0.41101	-2.56785	-1.98537
C	2.76516	-4.3465	-2.96642
H	-2.03416	-1.21931	-1.8248
C	1.47539	-4.12006	-2.49119
H	-1.00969	-3.42368	-1.68004
H	3.14939	-5.36113	-3.03042
H	0.85026	-4.95795	-2.18984
C	-0.5122	1.80874	-1.84397
C	0.23705	2.56889	-2.8786
C	1.53972	3.04234	-2.64169
C	2.20649	3.79778	-3.60316
C	1.58962	4.09602	-4.82191
C	0.29821	3.63094	-5.07185
C	-0.36884	2.87336	-4.10866
H	2.03289	2.78505	-1.70943
H	2.11244	4.68688	-5.56928
H	3.21344	4.15409	-3.40214
H	-1.38235	2.52771	-4.30343
H	-0.19328	3.86089	-6.01359
H	-0.33168	2.26115	-0.85989
H	-1.58405	1.79804	-2.02406

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0364023

P1

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.609716
(Hartree/Particle)
Thermal correction to Energy= 0.644574
Thermal correction to Enthalpy= 0.645518
Thermal correction to Gibbs Free Energy= 0.541004
Sum of electronic and zero-point Energies= -3273.484123
Sum of electronic and thermal Energies= -3273.449266
Sum of electronic and thermal Enthalpies= -3273.448322
Sum of electronic and thermal Free Energies= -3273.552836

H	5.599	1.85278	1.41602
C	4.60831	1.40783	1.38938
H	5.31369	-0.52716	0.74411
H	3.59688	3.21185	2.00963
C	4.44628	0.07074	1.01096
C	3.48537	2.16892	1.72557
C	3.17688	-0.50448	0.97001
C	2.21312	1.59948	1.68214
H	3.04013	-1.53505	0.66411
H	2.05415	0.57511	4.22777
C	2.04874	0.25394	1.3129
H	1.3347	2.19007	1.9253
H	1.51942	0.91375	6.61965
C	1.03463	0.43441	4.56901
C	0.71823	0.62979	5.94306
N	0.75565	-0.3088	1.23431
C	0.02265	0.07552	3.6975
C	-0.09042	-0.23553	2.26748
C	-0.56391	0.4753	6.44269
Ni	-0.18202	-0.78618	-0.39415
H	-0.76386	0.63737	7.4985
C	-1.29407	-0.0888	4.22303
C	-1.62789	0.09853	5.5715
C	-1.45018	-0.57524	1.98383
N	-1.73278	-0.91061	0.72057
C	-2.22977	-0.48311	3.22134
H	-3.56689	0.94967	0.25254
C	-2.99317	-0.11637	5.92285
H	-3.31074	0.01653	6.95367
C	-3.09466	-1.14251	0.37764
C	-3.95457	-0.05992	0.15057
C	-3.54599	-0.6893	3.59236
C	-3.90796	-0.49708	4.95549
H	-4.29978	-0.99223	2.87407
C	-3.57825	-2.45134	0.25396
C	-5.29012	-0.28603	-0.18606
H	-5.95182	0.55837	-0.35752
H	-2.8995	-3.28122	0.42819
H	-4.94359	-0.65924	5.24088
C	-4.91472	-2.6729	-0.08274
C	-5.77389	-1.59216	-0.30182
H	-5.28469	-3.69044	-0.17193
H	-6.81321	-1.76718	-0.56443
H	2.18907	0.00509	-3.04695
H	2.64999	-1.9267	-4.57211
C	1.24604	-0.39905	-2.6587
H	-0.1573	0.85171	-3.7888
C	1.68903	-2.35008	-4.2882
C	0.11494	0.64146	-2.74219
C	0.87039	-1.66435	-3.398
O	1.40129	-0.70575	-1.28173
H	1.92213	-4.12079	-5.50234
C	1.2806	-3.58693	-4.8064
C	-1.05887	-0.02692	-2.04077
C	-0.37157	-2.21355	-3.0208
C	-1.22074	-1.4092	-2.13582
C	0.0566	-4.13988	-4.42058
H	-1.90198	0.58788	-1.72967
C	-0.77044	-3.45601	-3.52434
H	-2.15916	-1.85457	-1.82194
H	-0.25487	-5.10243	-4.81681
H	-1.72935	-3.8763	-3.22998
C	0.48186	1.97334	-2.03918
C	1.75177	2.61323	-2.54777
C	2.97745	2.31707	-1.93101
C	4.1646	2.88643	-2.39422
C	4.14584	3.7604	-3.48526
C	2.93131	4.05835	-4.10954
C	1.74417	3.4884	-3.64187
H	2.99039	1.63035	-1.08998
H	5.06889	4.20736	-3.84518
H	5.10249	2.64938	-1.89801
H	0.80041	3.7295	-4.12695
H	2.90705	4.73862	-4.95715
H	0.59442	1.76589	-0.97072
H	-0.36577	2.66095	-2.15104

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.1169254

UB3LYP/6-31G(d)
Zero-point correction= 0.608532 (Hartree/Particle)
Thermal correction to Energy= 0.643688
Thermal correction to Enthalpy= 0.644632
Thermal correction to Gibbs Free Energy= 0.537621
Sum of electronic and zero-point Energies= -3273.371668
Sum of electronic and thermal Energies= -3273.336512
Sum of electronic and thermal Enthalpies= -3273.335568
Sum of electronic and thermal Free Energies= -3273.442579

H	5.9786	0.39896	2.25813
C	4.91423	0.2527	2.09478
H	5.16619	-1.59364	1.0077
H	4.34022	2.07275	3.10296
C	4.45686	-0.86602	1.39343
C	3.99488	1.18918	2.57208
C	3.09421	-1.05424	1.1745
C	2.62874	1.00241	2.36137
H	2.73137	-1.90749	0.61284
H	2.04184	-0.34555	4.60217
C	2.16618	-0.13166	1.67665
H	1.91095	1.73561	2.71801
H	1.439	-0.46854	6.9934
C	0.99523	-0.3892	4.88091
C	0.64033	-0.45716	6.25649
N	0.7828	-0.33488	1.45275
C	-0.00966	-0.37219	3.93078
C	-0.0922	-0.33473	2.46122
C	-0.6737	-0.50188	6.68473
Ni	-0.11507	-0.33754	-0.26358
H	-0.90254	-0.54536	7.74671
C	-1.36106	-0.43839	4.38188
C	-1.73342	-0.49534	5.7327
C	-1.47365	-0.40076	2.08636
N	-1.73682	-0.38588	0.7725
C	-2.2924	-0.45252	3.3014
H	-3.33807	1.60046	0.0222
C	-3.13108	-0.5469	6.00594
H	-3.47791	-0.58854	7.0355
C	-3.09	-0.50906	0.34795
C	-3.81741	0.62716	-0.03424
C	-3.64261	-0.50252	3.60045
C	-4.04129	-0.54566	4.96462
H	-4.39978	-0.51253	2.82436
C	-3.70881	-1.76713	0.28926
C	-5.14132	0.50675	-0.45992
H	-5.69586	1.39626	-0.74686
H	-3.14422	-2.64454	0.59269

H	-5.10389	-0.58417	5.18946
C	-5.03216	-1.88333	-0.13864
C	-5.75272	-0.74764	-0.51465
H	-5.50006	-2.86352	-0.17714
H	-6.78237	-0.83955	-0.84874
H	2.31854	0.43651	-2.88027
H	3.23208	-1.65991	-3.91022
C	1.41704	-0.03945	-2.47359
H	-0.07693	0.57543	-3.95605
C	2.32169	-2.1765	-3.61461
C	0.13772	0.71586	-2.88294
C	1.32599	-1.48229	-2.93878
O	1.47493	-0.00752	-1.06062
H	2.9434	-4.07726	-4.42773
C	2.15951	-3.53833	-3.90193
C	-0.95429	0.03286	-2.07394
C	0.14856	-2.15304	-2.54743
C	-0.89668	-1.35134	-1.89565
C	1.00013	-4.20587	-3.50506
H	-1.90469	0.54316	-1.93566
C	-0.00562	-3.5148	-2.82446
H	-1.78248	-1.87798	-1.55105
H	0.87759	-5.26328	-3.72355
H	-0.91637	-4.02849	-2.52402
C	0.21096	2.23276	-2.59259
C	1.20649	2.97498	-3.4578
C	2.50191	3.24438	-2.99414
C	3.42704	3.91155	-3.79944
C	3.07106	4.32268	-5.08486
C	1.78341	4.06263	-5.55858
C	0.8623	3.39582	-4.75036
H	2.78275	2.92616	-1.99284
H	3.7893	4.84498	-5.71151
H	4.42562	4.11267	-3.4197
H	-0.14167	3.20385	-5.1245
H	1.49432	4.38387	-6.55619
H	0.46588	2.36275	-1.53575
H	-0.79105	2.65898	-2.73926

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.1166006

TS_{A1}

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -109.17 cm^{-1}
Zero-point correction= 0.448660 (Hartree/Particle)
Thermal correction to Energy= 0.475473
Thermal correction to Enthalpy= 0.476417
Thermal correction to Gibbs Free Energy= 0.390294
Sum of electronic and zero-point Energies= -2812.434100
Sum of electronic and thermal Energies= -2812.407287
Sum of electronic and thermal Enthalpies= -2812.406343
Sum of electronic and thermal Free Energies= -2812.492466

H	-5.23564	-6.98025	-0.20467
C	-5.21467	-5.92959	-0.47943
H	-7.29572	-5.86137	-1.04780
H	-3.13641	-5.65519	0.04161
C	-6.36849	-5.30104	-0.95870
C	-4.03827	-5.18489	-0.34179
C	-6.34996	-3.95219	-1.31190
C	-4.01233	-3.83698	-0.69041
H	-7.25617	-3.46391	-1.65513
H	-6.41257	-3.81432	-3.89943
C	-5.16150	-3.20423	-1.20292
H	-3.10493	-3.25070	-0.57421
H	-7.63838	-3.81584	-6.03608
C	-6.70491	-2.86603	-4.33514
C	-7.41327	-2.86033	-5.57003
N	-5.08687	-1.83334	-1.48216
C	-6.41027	-1.66053	-3.71995
C	-5.70671	-1.22351	-2.50450
C	-7.82992	-1.69371	-6.18557
Ni	-4.23039	-0.53606	-0.32864
H	-8.38049	-1.73100	-7.12187
C	-6.81328	-0.46223	-4.38431
C	-7.52762	-0.43344	-5.59103
C	-5.64411	0.21833	-2.51720
N	-4.98055	0.82276	-1.52937
C	-6.38910	0.70522	-3.68821
H	-5.86412	2.49963	0.31222
C	-7.86824	0.85407	-6.09974
H	-8.42729	0.93475	-7.02838
C	-4.78491	2.21938	-1.52505
C	-5.27877	2.98969	-0.46074
C	-6.73660	1.94077	-4.20463
C	-7.48639	1.99338	-5.41305
H	-6.44482	2.86397	-3.71735
C	-4.02296	2.84845	-2.52492
C	-5.03292	4.36279	-0.40848
H	-5.42866	4.94647	0.41839
H	-3.62723	2.24749	-3.33841
H	-7.75579	2.96816	-5.81038
C	-3.78117	4.22074	-2.46877
C	-4.28502	4.98535	-1.41140
H	-3.19101	4.69288	-3.24973
H	-4.09208	6.05338	-1.36773
C	-4.01536	-0.27600	2.12386
C	-3.38431	0.51799	1.13083
C	-3.45543	-1.48100	2.55001
H	-4.92201	0.09727	2.59084
C	-2.20581	-1.89971	2.02624
C	-1.58171	-1.17981	1.02954
C	-2.17229	0.02307	0.49561
H	-3.65755	1.56369	1.01770
H	-1.74854	-2.81177	2.39965
C	-1.59507	0.71691	-0.57911
H	-0.70113	0.34304	-1.06739
H	-2.03608	1.63550	-0.94891
H	-0.64055	-1.52220	0.60764
H	-3.96186	-2.08301	3.29767

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -2812.172376

UB3LYP/6-31G(d)
Imaginary frequency = -121.43 cm^{-1}
Zero-point correction= 0.447323 (Hartree/Particle)
Thermal correction to Energy= 0.474684
Thermal correction to Enthalpy= 0.475628
Thermal correction to Gibbs Free Energy= 0.387234
Sum of electronic and zero-point Energies= -2812.353207
Sum of electronic and thermal Energies= -2812.325847

Sum of electronic and thermal Enthalpies= -2812.324903
Sum of electronic and thermal Free Energies= -2812.413296

H	-5.18906	-6.99449	-0.34629
C	-5.15143	-5.93671	-0.5911
H	-7.29033	-5.73259	-0.78774
H	-3.00297	-5.80368	-0.44512
C	-6.32889	-5.22806	-0.84441
C	-3.92699	-5.26643	-0.64394
C	-6.28682	-3.87078	-1.15803
C	-3.87762	-3.90842	-0.95148
H	-7.20543	-3.31943	-1.33353
H	-6.41538	-3.81798	-3.78585
C	-5.05504	-3.19392	-1.23087
H	-2.92768	-3.38339	-0.99124
H	-7.72485	-3.85408	-5.8732
C	-6.71485	-2.87714	-4.23308
C	-7.47196	-2.89109	-5.43707
N	-4.96929	-1.81141	-1.48358
C	-6.38305	-1.66138	-3.65972
C	-5.62695	-1.20654	-2.4822
C	-7.90087	-1.7345	-6.0608
Ni	-4.11446	-0.49999	-0.348
H	-8.48785	-1.78836	-6.97436
C	-6.80615	-0.47418	-4.32846
C	-7.5668	-0.4649	-5.50694
C	-5.57051	0.23556	-2.51509
N	-4.87609	0.85269	-1.55828
C	-6.3547	0.70389	-3.66887
H	-5.95501	2.57208	0.15167
C	-7.91863	0.81398	-6.02719
H	-8.51195	0.88132	-6.93589
C	-4.71043	2.25702	-1.57239
C	-5.30994	3.04947	-0.58074
C	-6.71542	1.93052	-4.19694
C	-7.50603	1.96328	-5.37851
H	-6.4072	2.86264	-3.73715
C	-3.88602	2.87743	-2.52716
C	-5.10048	4.42921	-0.55292
H	-5.57919	5.02816	0.21763
H	-3.40983	2.26366	-3.2863
H	-7.78518	2.93174	-5.78529
C	-3.68073	4.2564	-2.49498
C	-4.28627	5.03968	-1.50864
H	-3.03973	4.71977	-3.24077
H	-4.12201	6.11329	-1.48385
C	-4.16038	-0.30489	2.08225
C	-3.43462	0.53471	1.19777
C	-3.67465	-1.55699	2.45479
H	-5.07918	0.07046	2.52475
C	-2.41978	-1.99548	1.96549
C	-1.71158	-1.23355	1.06142
C	-2.21066	0.03777	0.59499
H	-3.68992	1.58621	1.10733
H	-2.02353	-2.95318	2.29128
C	-1.50899	0.79626	-0.36032
H	-0.60163	0.41228	-0.81499
H	-1.85484	1.77671	-0.66638
H	-0.75883	-1.58376	0.67249
H	-4.24954	-2.18795	3.12498

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF= -2812.1720495

A1'

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.451879 (Hartree/Particle)
Thermal correction to Energy= 0.478748
Thermal correction to Enthalpy= 0.479693
Thermal correction to Gibbs Free Energy= 0.392088
Sum of electronic and zero-point Energies= -2812.473317
Sum of electronic and thermal Energies= -2812.446447
Sum of electronic and thermal Enthalpies= -2812.445503
Sum of electronic and thermal Free Energies= -2812.533108

H	-5.5571	-6.52836	0.04481
C	-5.47229	-5.48277	-0.2376
H	-7.48992	-4.98873	0.35245
H	-3.42717	-5.65677	-0.90382
C	-6.55769	-4.61761	-0.06512
C	-4.27704	-4.99275	-0.77043
C	-6.44909	-3.27382	-0.42479
C	-4.16397	-3.64822	-1.12713
H	-7.28445	-2.59227	-0.29086
H	-6.75948	-3.63169	-3.18779
C	-5.25121	-2.78168	-0.9627
H	-3.23492	-3.25333	-1.52688
H	-8.01826	-3.92315	-5.29917
C	-6.94745	-2.76916	-3.81748
C	-7.67045	-2.92858	-5.03353
N	-5.11764	-1.40842	-1.28615
C	-6.50294	-1.50645	-3.46943
C	-5.7321	-0.92064	-2.36657
C	-7.94091	-1.86973	-5.88333
Ni	-4.26973	0.02367	-0.31231
H	-8.49286	-2.03379	-6.80515
C	-6.78791	-0.42088	-4.34928
C	-7.48897	-0.5573	-5.55547
C	-5.5856	0.48589	-2.60631
N	-4.84706	1.16227	-1.71297
C	-6.24792	0.81351	-3.87393
H	-6.81044	2.96526	-1.59284
C	-7.65953	0.6274	-6.33104
H	-8.19678	0.58132	-7.27467
C	-4.70897	2.5665	-1.82044
C	-5.8285	3.40857	-1.73154
C	-6.42265	1.94275	-4.65496
C	-7.13427	1.82694	-5.88264
H	-6.03459	2.90867	-4.35258
C	-3.43759	3.1356	-1.98428
C	-5.67873	4.79267	-1.82793
H	-6.55443	5.43264	-1.75944
H	-2.57478	2.47841	-2.04062
H	-7.26615	2.72114	-6.48579
C	-3.29196	4.51941	-2.07919
C	-4.41096	5.3547	-2.00383
H	-2.30172	4.94623	-2.21455
H	-4.29525	6.43239	-2.07603
C	-3.67917	-2.25359	1.77721
C	-4.03839	-0.89577	1.55137
C	-2.3742	-2.66712	1.64019
H	-4.45425	-2.96751	2.03766
C	-1.36367	-1.7273	1.30723
C	-1.66855	-0.39874	1.11779
C	-3.01211	0.07089	1.2792
H	-5.00611	-0.56365	1.92972
H	-0.33512	-2.06366	1.20558

C	-3.48597	1.3547	0.8433
H	-2.75019	2.05421	0.45147
H	-4.27529	1.83915	1.42347
H	-0.89355	0.32153	0.87013
H	-2.11031	-3.70957	1.7912

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -2812.2104737

UB3LYP/6-31G(d)
Zero-point correction= 0.451698 (Hartree/Particle)
Thermal correction to Energy= 0.478600
Thermal correction to Enthalpy= 0.479544
Thermal correction to Gibbs Free Energy= 0.392040
Sum of electronic and zero-point Energies= -2812.393630
Sum of electronic and thermal Energies= -2812.366728
Sum of electronic and thermal Enthalpies= -2812.365784
Sum of electronic and thermal Free Energies= -2812.453288

H	-5.68233	-6.56659	-0.00705
C	-5.57763	-5.51764	-0.27059
H	-7.56522	-4.98422	0.37967
H	-3.55823	-5.7302	-0.99792
C	-6.63396	-4.62889	-0.05435
C	-4.38579	-5.04668	-0.82551
C	-6.50097	-3.28187	-0.39314
C	-4.24696	-3.69924	-1.16085
H	-7.31841	-2.58561	-0.22704
H	-6.74394	-3.64837	-3.24317
C	-5.30639	-2.80515	-0.95444
H	-3.32103	-3.32454	-1.58662
H	-7.9719	-3.91817	-5.36972
C	-6.92301	-2.77748	-3.86388
C	-7.62846	-2.92552	-5.09022
N	-5.15496	-1.42956	-1.27014
C	-6.48215	-1.5189	-3.49608
C	-5.73094	-0.94084	-2.37387
C	-7.88797	-1.86036	-5.93324
Ni	-4.29648	0.00663	-0.29179
H	-8.42831	-2.01781	-6.86353
C	-6.75452	-0.42683	-4.37193
C	-7.4413	-0.55176	-5.58759
C	-5.57834	0.46624	-2.60583
N	-4.87289	1.14622	-1.69121
C	-6.22388	0.80324	-3.87979
H	-6.77964	2.97336	-1.31556
C	-7.60626	0.64073	-6.35069
H	-8.13235	0.60482	-7.30152
C	-4.72894	2.55361	-1.80909
C	-5.81817	3.40672	-1.57617
C	-6.39452	1.94088	-4.64864
C	-7.09212	1.83663	-5.88387
H	-6.01145	2.90468	-4.3326
C	-3.48355	3.11279	-2.12958
C	-5.66544	4.78999	-1.6765
H	-6.51825	5.4384	-1.49203
H	-2.64202	2.44902	-2.30634
H	-7.22123	2.73695	-6.479
C	-3.33551	4.49605	-2.22943
C	-4.42483	5.34106	-2.00452
H	-2.3656	4.91448	-2.48601
H	-4.30673	6.41853	-2.07964
C	-3.58558	-2.24194	1.82345
C	-3.99782	-0.90447	1.56806
C	-2.26333	-2.60432	1.71232
H	-4.3302	-2.98021	2.10555
C	-1.28875	-1.63101	1.37082
C	-1.64592	-0.32186	1.149
C	-3.00846	0.09631	1.28702
H	-4.97574	-0.60072	1.94325
H	-0.24481	-1.92492	1.2933
C	-3.53191	1.35761	0.84622
H	-2.82745	2.08213	0.44315
H	-4.33247	1.81686	1.42998
H	-0.89566	0.4249	0.90226
H	-1.95761	-3.62978	1.89885

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -2812.2102753

B1

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.606374 (Hartree/Particle)
Thermal correction to Energy= 0.641602
Thermal correction to Enthalpy= 0.642546
Thermal correction to Gibbs Free Energy= 0.538024
Sum of electronic and zero-point Energies= -3273.418836
Sum of electronic and thermal Energies= -3273.383608
Sum of electronic and thermal Enthalpies= -3273.382664
Sum of electronic and thermal Free Energies= -3273.487186

H	5.57889	-4.23138	4.85584
C	5.25371	-3.21707	5.06834
H	3.33515	-3.8162	5.85526
H	7.05585	-2.30217	4.30764
C	3.99548	-2.98331	5.62995
C	6.08508	-2.13383	4.76566
C	3.57243	-1.68232	5.89745
C	5.67315	-0.83054	5.03815
H	2.58854	-1.4893	6.30589
H	6.84971	-0.21366	7.27711
C	4.41912	-0.5962	5.62732
H	6.30973	0.01224	4.78783
H	8.76709	0.59289	8.60508
C	6.91426	0.83925	7.52393
C	8.01262	1.30917	8.29274
N	3.93892	0.7103	5.85324
C	5.94933	1.74035	7.1125
C	4.66453	1.65958	6.40029
C	8.14807	2.63777	8.65754
Ni	2.07134	1.29105	5.61727
H	9.00047	2.95981	9.2497
C	6.08787	3.10351	7.50108
C	7.15991	3.58684	8.27268
C	4.06441	3.00095	6.40472
N	2.86357	3.10484	5.89091
C	4.9951	3.91479	7.0864
H	0.49069	3.7489	6.8359
C	7.12709	4.96838	8.61529
H	7.93421	5.39353	9.20586
C	2.22337	4.35141	5.7204
C	0.94266	4.54687	6.25806
C	4.98256	5.24874	7.44704
C	6.06663	5.76107	8.21073

H	4.16809	5.90607	7.1661
C	2.81156	5.36582	4.94777
C	0.27558	5.75452	6.05286
H	-0.71099	5.90009	6.4841
H	3.79374	5.19976	4.51531
H	6.05232	6.81119	8.488
C	2.13491	6.56736	4.74109
C	0.86715	6.76944	5.29576
H	2.59829	7.34557	4.14099
H	0.34304	7.70673	5.13321
H	2.2875	-0.64072	2.99278
H	0.79666	-0.64796	0.37265
C	1.37217	-0.13021	3.28861
H	1.89209	2.10061	3.05185
C	-0.04383	-0.49883	1.04552
C	1.47509	1.34545	3.70961
C	0.14482	-0.2772	2.39737
O	0.85398	-0.70075	4.53428
H	-1.54381	-0.723	-0.49487
C	-1.36596	-0.53647	0.56082
C	0.38288	1.5376	4.59359
C	-0.94773	-0.08091	3.26434
C	-0.31875	0.17234	4.62931
C	-2.44854	-0.34333	1.41965
H	-0.16879	2.46401	4.70921
C	-2.24777	-0.10572	2.79364
H	-0.90243	-0.07022	5.516
H	-3.46059	-0.38061	1.02556
H	-3.09444	0.04681	3.45797
H	4.65287	-0.76692	10.26676
H	2.82805	-1.03508	8.63708
C	4.10572	0.10919	9.92556
C	3.07354	-0.04235	9.00578
H	5.26356	1.49713	11.11918
C	4.44756	1.37845	10.41162
C	2.33668	1.06626	8.52499
C	1.31133	0.92471	7.48515
C	3.72968	2.48724	9.96234
C	2.69952	2.33375	9.03356
H	3.98725	3.48314	10.31478
H	2.16532	3.2114	8.67795
H	0.48172	1.62553	7.61581
H	0.91573	-0.09591	7.42002

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0550436

UB3LYP/6-31G(d)
Zero-point correction= 0.605229 (Hartree/Particle)
Thermal correction to Energy= 0.640964
Thermal correction to Enthalpy= 0.641908
Thermal correction to Gibbs Free Energy= 0.533988
Sum of electronic and zero-point Energies= -3273.296806
Sum of electronic and thermal Energies= -3273.261072
Sum of electronic and thermal Enthalpies= -3273.260127
Sum of electronic and thermal Free Energies= -3273.368047

H	5.71224	-4.15407	4.74986
C	5.36608	-3.15703	5.00732
H	3.55249	-3.84551	5.95039
H	7.05086	-2.15624	4.10218
C	4.15605	-2.98298	5.68134
C	6.11963	-2.03582	4.64977
C	3.70255	-1.70533	6.00485
C	5.67922	-0.75545	4.97788
H	2.75378	-1.56743	6.50837
H	6.97808	-0.13085	7.21256
C	4.47218	-0.57852	5.67759
H	6.25354	0.11552	4.6779
H	8.99242	0.75178	8.32986
C	7.04433	0.93149	7.41615
C	8.20078	1.44593	8.06122
N	3.96056	0.71095	5.94775
C	6.02897	1.80189	7.06358
C	4.69513	1.68428	6.44613
C	8.34983	2.78841	8.35719
Ni	2.08499	1.26631	5.71494
H	9.25071	3.14351	8.85138
C	6.18151	3.18052	7.3874
C	7.31582	3.70926	8.02879
C	4.08285	3.01444	6.44505
N	2.86031	3.10067	5.97229
C	5.04757	3.96234	7.03127
H	0.56554	3.90465	7.03891
C	7.29985	5.10587	8.30179
H	8.15358	5.56752	8.79181
C	2.22866	4.34701	5.74952
C	0.99411	4.62834	6.35419
C	5.05689	5.31394	7.32256
C	6.19991	5.87024	7.95665
H	4.21671	5.95422	7.07916
C	2.77593	5.27576	4.84799
C	0.33802	5.82922	6.08451
H	-0.61143	6.03902	6.56994
H	3.71782	5.04584	4.35849
H	6.20106	6.93376	8.17943
C	2.10909	6.46963	4.57748
C	0.88994	6.75511	5.19707
H	2.5421	7.1762	3.87418
H	0.37234	7.68613	4.98424
H	2.31121	-0.62445	2.99267
H	0.85747	-0.51491	0.35017
C	1.3959	-0.11997	3.30037
H	1.92658	2.1202	3.16935
C	0.00949	-0.38933	1.0192
C	1.49768	1.33665	3.78463
C	0.18097	-0.21991	2.38065
O	0.85722	-0.74088	4.5062
H	-1.46729	-0.55531	-0.5495
C	-1.30428	-0.40882	0.51504
C	0.39594	1.49582	4.65764
C	-0.92254	-0.05795	3.23851
C	-0.30825	0.12975	4.62392
C	-2.39749	-0.24978	1.36474
H	-0.15459	2.42024	4.79597
C	-2.21523	-0.06599	2.74816
H	-0.90812	-0.15372	5.48825
H	-3.40425	-0.27319	0.95589
H	-3.07355	0.05724	3.40433
H	3.99005	-1.1184	10.71918
H	2.40749	-1.19722	8.83719
C	3.59923	-0.1899	10.3087
C	2.70911	-0.23317	9.24042
H	4.67705	1.06906	11.69978
C	3.98301	1.03533	10.86424
C	2.16245	0.94311	8.67887
C	1.23346	0.89686	7.53623
C	3.45457	2.21217	10.33265

C	2.56751	2.16659	9.25734
H	3.73553	3.17455	10.75434
H	2.16099	3.0947	8.86294
H	0.433	1.63624	7.63238
H	0.78338	-0.09588	7.42011

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0525342

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UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.486583
(Hartree/Particle)
Thermal correction to Energy= 0.515287
Thermal correction to Enthalpy= 0.516231
Thermal correction to Gibbs Free Energy= 0.426257
Sum of electronic and zero-point Energies= -3002.552129
Sum of electronic and thermal Energies= -3002.523426
Sum of electronic and thermal Enthalpies= -3002.522481
Sum of electronic and thermal Free Energies= -3002.612455

H	0.97531	-6.2375	1.75975
C	0.94751	-5.22524	1.36679
H	-1.17629	-5.25223	0.97916
H	3.05826	-4.87345	1.65339
C	-0.25834	-4.67294	0.92384
C	2.11532	-4.45782	1.30802
C	-0.29851	-3.37216	0.42344
C	2.08041	-3.15626	0.81076
H	-1.23882	-2.93273	0.10625
H	-0.13243	-3.65981	-2.17988
C	0.87535	-2.60041	0.35065
H	2.97992	-2.55046	0.77259
H	-1.1654	-4.1014	-4.37826
C	-0.49352	-2.82523	-2.76947
C	-1.08923	-3.07258	-4.03744
N	0.85553	-1.25662	-0.06709
C	-0.39368	-1.52077	-2.31825
C	0.17177	-0.84634	-1.13871
C	-1.56892	-2.05554	-4.84422
Ni	1.40434	0.28964	1.01681
H	-2.01562	-2.28357	-5.80837
C	-0.88317	-0.47963	-3.15927
C	-1.46593	-0.69992	-4.41714
C	0.00317	0.58129	-1.30975
N	0.54599	1.37534	-0.38248
C	-0.66987	0.81303	-2.59811
H	-1.87942	2.52305	-0.55459
C	-1.86741	0.45702	-5.14588
H	-2.3284	0.34416	-6.1236
C	0.24639	2.74685	-0.28717
C	-1.07367	3.22589	-0.36852
C	-1.05578	1.91667	-3.33871
C	-1.65759	1.71663	-4.61222
H	-0.91405	2.92616	-2.97058
C	1.27879	3.65374	0.00413
C	-1.34563	4.58103	-0.18453
H	-2.3724	4.93235	-0.24445
H	2.29318	3.27677	0.08586
H	-1.95981	2.59136	-5.18138
C	1.00155	5.00768	0.18494
C	-0.31125	5.4808	0.09053
H	1.81423	5.69569	0.40255
H	-0.52631	6.53537	0.23708
H	2.01547	-1.34677	4.2856
H	-0.61348	-2.24818	3.11579
C	1.76338	-0.45439	3.71527
H	3.53782	-0.67458	2.26105
C	-0.73567	-1.17625	2.99944
C	2.62874	-0.12171	2.47707
C	0.3139	-0.29895	3.24146
O	1.90328	0.74962	4.52176
H	-2.79462	-1.29902	2.37414
C	-1.95852	-0.63484	2.57453
C	2.46272	1.2878	2.31584
C	0.15004	1.09476	3.08257
C	1.5122	1.67951	3.47174
C	-2.11996	0.74651	2.41439
H	3.22633	1.97246	1.95929
C	-1.06426	1.6333	2.67553
H	1.53806	2.70958	3.82311
H	-3.07948	1.14016	2.09081
H	-1.19157	2.70301	2.54413

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3002.244906

UB3LYP/6-31G(d)
Zero-point correction= 0.486317
(Hartree/Particle)
Thermal correction to Energy= 0.515288
Thermal correction to Enthalpy= 0.516232
Thermal correction to Gibbs Free Energy= 0.424626
Sum of electronic and zero-point Energies= -3002.458645
Sum of electronic and thermal Energies= -3002.429674
Sum of electronic and thermal Enthalpies= -3002.428730
Sum of electronic and thermal Free Energies= -3002.520336

H	1.36347	-6.54361	0.96442
C	1.20486	-5.49027	0.75082
H	-0.94109	-5.60182	0.94617
H	3.30173	-5.05469	0.4935
C	-0.08793	-4.96058	0.73951
C	2.29154	-4.6534	0.48957
C	-0.29456	-3.60782	0.47011
C	2.09122	-3.29933	0.21859
H	-1.29693	-3.18915	0.46754
H	0.05707	-3.73597	-2.33896
C	0.79498	-2.76433	0.20219
H	2.93181	-2.64563	0.00443
H	-0.65926	-4.14112	-4.668
C	-0.25621	-2.89647	-2.94915
C	-0.66908	-3.1219	-4.2908
N	0.59367	-1.37871	-0.02894
C	-0.26623	-1.6034	-2.45586
C	0.08521	-0.95207	-1.18988
C	-1.07426	-2.09743	-5.12682
Ni	1.00289	0.11095	1.13388
H	-1.3764	-2.31178	-6.14894
C	-0.68922	-0.55344	-3.32242
C	-1.08809	-0.75364	-4.65288
C	-0.13998	0.47065	-1.32641
N	0.20901	1.23568	-0.2938
C	-0.62917	0.72432	-2.69463

H	-2.2123	2.35272	-0.62654
C	-1.44424	0.41025	-5.39172
H	-1.76129	0.31568	-6.42743
C	-0.10923	2.60986	-0.23919
C	-1.42607	3.07017	-0.41174
C	-0.97079	1.8354	-3.44493
C	-1.37693	1.65627	-4.79547
H	-0.93921	2.83568	-3.0284
C	0.89486	3.53744	0.08138
C	-1.72233	4.42656	-0.28387
H	-2.74745	4.76455	-0.4136
H	1.9097	3.17863	0.2227
H	-1.64422	2.53662	-5.37391
C	0.5935	4.89319	0.20279
C	-0.71566	5.34635	0.02107
H	1.38587	5.59863	0.43975
H	-0.94977	6.4025	0.12106
H	1.65494	-1.37844	4.55001
H	-1.31398	-1.49476	4.06212
C	1.54794	-0.4907	3.92779
H	2.85368	-1.34471	2.23916
C	-1.14312	-0.4485	3.82164
C	2.20673	-0.52196	2.52802
C	0.13847	0.0716	3.72802
O	2.19536	0.65507	4.53904
H	-3.24119	0.04369	3.69546
C	-2.22601	0.42313	3.61387
C	2.44164	0.85154	2.2309
C	0.35237	1.43298	3.43046
C	1.87797	1.58767	3.47407
C	-2.01487	1.77154	3.32138
H	3.31008	1.2377	1.70439
C	-0.7143	2.29507	3.22497
H	2.27689	2.57776	3.69171
H	-2.86666	2.42977	3.17387
H	-0.55943	3.34597	2.99788

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.2367467

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UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -411.41 cm^{-1}
Zero-point correction= 0.483757
(Hartree/Particle)
Thermal correction to Energy= 0.512771
Thermal correction to Enthalpy= 0.513715
Thermal correction to Gibbs Free Energy= 0.423170
Sum of electronic and zero-point Energies= -3002.507609
Sum of electronic and thermal Energies= -3002.478595
Sum of electronic and thermal Enthalpies= -3002.477651
Sum of electronic and thermal Free Energies= -3002.568196

H	3.04773	-4.64026	-2.13973
C	2.60197	-3.69918	-1.83093
H	3.69177	-3.60379	0.02982
H	1.36932	-3.51306	-3.59389
C	2.96149	-3.11799	-0.61135
C	1.6614	-3.06519	-2.64808
C	2.38619	-1.91298	-0.20749
C	1.08662	-1.85725	-2.2527
H	2.65849	-1.45353	0.7373
H	3.03754	-0.1487	-3.11428
C	1.45265	-1.27181	-1.0314
H	0.3478	-1.3609	-2.87397
H	4.14585	1.21984	-4.85208
C	2.75598	0.89151	-3.23087
C	3.38819	1.68445	-4.22764
N	0.83468	-0.0703	-0.6011
C	1.78737	1.47399	-2.43381
C	0.94757	1.04566	-1.31063
C	3.07437	3.01862	-4.42512
Ni	-0.45822	0.11579	0.79501
H	3.58234	3.59248	-5.19551
C	1.4679	2.84703	-2.64171
C	2.08835	3.64953	-3.61304
C	0.13346	2.17163	-0.88752
N	-0.65059	1.95627	0.16073
C	0.47565	3.32414	-1.73558
H	-1.11767	2.63937	2.64807
C	1.67833	5.01237	-3.66846
H	2.12355	5.67832	-4.40271
C	-1.64127	2.8721	0.57851
C	-1.80262	3.1122	1.95107
C	0.10938	4.65624	-1.807
C	0.72403	5.48623	-2.78429
H	-0.63409	5.07802	-1.14066
C	-2.54051	3.45146	-0.3312
C	-2.82946	3.93888	2.40396
H	-2.93958	4.1218	3.46921
H	-2.44195	3.23042	-1.38905
H	0.42689	6.52984	-2.83356
C	-3.56868	4.27378	0.12813
C	-3.71721	4.52409	1.4956
H	-4.26404	4.70835	-0.58472
H	-4.52189	5.16146	1.85034
H	-0.83769	-3.39826	1.15263
H	-1.64234	-2.84725	-1.45924
C	-1.29662	-2.45235	1.48199
C	-2.15308	-1.99736	-1.01647
C	-0.22974	-1.4524	2.00133
C	-1.95499	-1.68505	0.32897
O	-2.28674	-2.60387	2.43752
H	-3.18053	-1.44428	-2.8273
C	-3.02015	-1.20844	-1.77868
C	-0.91558	-0.42577	2.69442
C	-2.6404	-0.58677	0.9112
C	-2.30813	-0.3863	2.33811
C	-3.71454	-0.13568	-1.19663
C	-3.54087	0.17648	0.15133
H	-3.00627	0.1871	2.94455
H	-4.39586	0.45644	-1.80082
H	-4.06349	1.01607	0.59902
H	0.78011	-1.75007	2.26527
H	-0.54307	0.11716	3.5566

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3002.1991019

UB3LYP/6-31G(d)
Imaginary frequency = -388.25 cm^{-1}
Zero-point correction= 0.482590
(Hartree/Particle)
Thermal correction to Energy= 0.512029
Thermal correction to Enthalpy= 0.512973
Thermal correction to Gibbs Free Energy= 0.420322
Sum of electronic and zero-point Energies= -3002.406376

Sum of electronic and thermal Energies= -3002.376936
Sum of electronic and thermal Enthalpies= -3002.375992
Sum of electronic and thermal Free Energies= -3002.46864

H	2.73068	-4.56544	-2.61909
C	2.29035	-3.63473	-2.27254
H	3.06468	-3.82064	-0.26775
H	1.36811	-3.17061	-4.16769
C	2.47498	-3.2172	-0.95274
C	1.52845	-2.84955	-3.14168
C	1.9055	-2.02601	-0.50239
C	0.95912	-1.65639	-2.69863
H	2.04565	-1.69685	0.52214
H	3.10637	0.02231	-3.05548
C	1.15087	-1.22989	-1.375
H	0.3512	-1.05207	-3.36534
H	4.49328	1.49272	-4.47548
C	2.88679	1.08323	-3.09057
C	3.67855	1.93465	-3.90831
N	0.53232	-0.04539	-0.89869
C	1.84723	1.63425	-2.36363
C	0.82931	1.13891	-1.42206
C	3.44327	3.29381	-4.01143
Ni	-0.86571	0.13465	0.45304
H	4.0672	3.90914	-4.65493
C	1.62477	3.03799	-2.45926
C	2.38426	3.89381	-3.27249
C	0.05325	2.27062	-0.95949
N	-0.91392	2.00575	-0.08146
C	0.54794	3.47748	-1.63454
H	-0.00081	3.92734	1.55195
C	2.01641	5.2699	-3.26672
H	2.56909	5.97838	-3.87861
C	-1.67042	3.05023	0.51301
C	-1.07052	3.98471	1.3715
C	0.21293	4.81981	-1.65625
C	0.96001	5.7008	-2.48492
H	-0.59849	5.21413	-1.05512
C	-3.05468	3.1073	0.29881
C	-1.84418	4.96633	1.9911
H	-1.36891	5.68054	2.65848
H	-3.51183	2.37611	-0.36143
H	0.68863	6.75303	-2.4938
C	-3.82143	4.09554	0.91584
C	-3.22099	5.02877	1.76397
H	-4.89229	4.13469	0.73422
H	-3.82123	5.79335	2.24898
H	-0.50566	-3.13465	1.90924
H	-1.10001	-3.65969	-0.75346
C	-1.19065	-2.2734	1.88115
C	-1.84457	-2.87666	-0.63929
C	-0.46605	-0.93442	2.13707
C	-1.86677	-2.09435	0.51667
O	-2.22903	-2.39433	2.79256
H	-2.80486	-3.2883	-2.52296
C	-2.80961	-2.6711	-1.6285
C	-1.45772	0.02485	2.40481
C	-2.86372	-1.09748	0.67872
C	-2.7663	-0.37379	1.9588
C	-3.80947	-1.70325	-1.45815
C	-3.8457	-0.91494	-0.3085
H	-3.64012	0.17554	2.30328
H	-4.56717	-1.56943	-2.22559
H	-4.62564	-0.16919	-0.17446
H	0.53356	-0.86329	2.55449
H	-1.32716	0.9027	3.03012

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.195824

A2''

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.486511 (Hartree/Particle)
Thermal correction to Energy= 0.515901
Thermal correction to Enthalpy= 0.516845
Thermal correction to Gibbs Free Energy= 0.424685
Sum of electronic and zero-point Energies= -3002.555891
Sum of electronic and thermal Energies= -3002.526501
Sum of electronic and thermal Enthalpies= -3002.525557
Sum of electronic and thermal Free Energies= -3002.617716

H	4.09056	-5.1254	-1.27692
C	3.51507	-4.23871	-1.0281
H	4.50797	-3.92773	0.86333
H	2.34008	-4.29434	-2.83834
C	3.7489	-3.56694	0.17546
C	2.53368	-3.77158	-1.90626
C	3.00609	-2.43297	0.5046
C	1.79262	-2.6322	-1.5901
H	3.17001	-1.90563	1.43917
H	3.68094	-0.78047	-2.37099
C	2.0399	-1.95957	-0.38805
H	1.0245	-2.2603	-2.26108
H	4.83386	0.65517	-4.0275
C	3.3517	0.24205	-2.51338
C	4.00584	1.071	-3.46173
N	1.26756	-0.80854	-0.04936
C	2.29516	0.77	-1.79337
C	1.40709	0.29131	-0.73491
C	3.62448	2.38428	-3.68708
Ni	-0.10429	-0.66883	1.26803
H	4.152	2.98624	-4.42168
C	1.90412	2.12062	-2.02605
C	2.5449	2.95713	-2.95801
C	0.48718	1.3944	-0.37202
N	-0.35259	1.12777	0.58826
C	0.81844	2.54977	-1.20801
H	-0.6416	2.24748	2.96861
C	2.05131	4.28791	-3.05981
H	2.50882	4.97559	-3.76549
C	-1.36103	2.06431	0.95145
C	-1.40693	2.55234	2.26161
C	0.36486	3.85131	-1.32553
C	0.99851	4.70845	-2.26271
H	-0.45792	4.22204	-0.72574
C	-2.34806	2.42683	0.02754
C	-2.42819	3.42416	2.63751
H	-2.45615	3.81003	3.65231
H	-2.31504	2.01596	-0.9765
H	0.63992	5.72912	-2.35381
C	-3.37169	3.29207	0.41407
C	-3.41447	3.79398	1.71742
H	-4.1409	3.56443	-0.30259
H	-4.21427	4.46463	2.01709
H	-0.53963	-3.46518	0.09017
H	-2.96742	-3.65098	-0.84935

C	-1.08311	-3.29788	1.06162
C	-3.17179	-2.75021	-0.2741
C	-0.07739	-2.51584	1.96226
C	-2.27053	-2.38097	0.73038
O	-1.47617	-4.41247	1.68947
H	-4.97068	-2.26623	-1.35997
C	-4.29794	-1.97854	-0.55588
C	-0.54048	-1.63821	2.9651
C	-2.54512	-1.22383	1.50126
C	-1.61198	-0.80993	2.55911
C	-4.55906	-0.82406	0.19819
C	-3.69092	-0.45147	1.21782
H	-1.90479	0.03191	3.17931
H	-5.43682	-0.21922	-0.0138
H	-3.88599	0.44353	1.80324
H	0.86687	-3.03011	2.12492
H	0.02025	-1.41192	3.86944

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3002.2609834

UB3LYP/6-31G(d)
Zero-point correction= 0.485122 (Hartree/Particle)
Thermal correction to Energy= 0.514817
Thermal correction to Enthalpy= 0.515761
Thermal correction to Gibbs Free Energy= 0.421884
Sum of electronic and zero-point Energies= -3002.443314
Sum of electronic and thermal Energies= -3002.413619
Sum of electronic and thermal Enthalpies= -3002.412675
Sum of electronic and thermal Free Energies= -3002.506552

H	4.08803	-5.09501	-1.38427
C	3.51011	-4.21122	-1.12995
H	4.51484	-3.89637	0.753
H	2.31466	-4.27533	-2.92465
C	3.74796	-3.53954	0.07119
C	2.51642	-3.74995	-1.99529
C	2.99794	-2.41362	0.40951
C	1.76868	-2.61804	-1.66945
H	3.17178	-1.88816	1.3437
H	3.75336	-0.70721	-2.3574
C	2.01407	-1.94199	-0.46731
H	0.98636	-2.25974	-2.33195
H	4.99916	0.77682	-3.89538
C	3.44442	0.32617	-2.46601
C	4.15299	1.18394	-3.34912
N	1.23745	-0.79651	-0.11694
C	2.36525	0.83731	-1.76791
C	1.41282	0.32995	-0.77357
C	3.80297	2.50958	-3.53727
Ni	-0.21581	-0.67321	1.12789
H	4.3719	3.13117	-4.22399
C	2.01189	2.2052	-1.96181
C	2.69938	3.0677	-2.83177
C	0.50267	1.41737	-0.41804
N	-0.42895	1.11711	0.4603
C	0.89724	2.61151	-1.17096
H	-0.21772	2.67001	2.61184
C	2.22211	4.40735	-2.90535
H	2.7155	5.11827	-3.56322
C	-1.35275	2.12822	0.86603
C	-1.11688	2.86404	2.03408
C	0.45863	3.9201	-1.26343
C	1.13839	4.80529	-2.14223
H	-0.38454	4.27976	-0.68458
C	-2.51219	2.36083	0.11688
C	-2.0303	3.83746	2.43941
H	-1.83923	4.40699	3.34487
H	-2.69748	1.7687	-0.77363
H	0.79026	5.83203	-2.21162
C	-3.41947	3.3386	0.52867
C	-3.18254	4.08016	1.68794
H	-4.31719	3.51473	-0.05771
H	-3.8933	4.83704	2.00716
H	-0.63226	-3.62512	0.1217
H	-3.1448	-4.12947	-0.55597
C	-1.14265	-3.38507	1.08889
C	-3.36935	-3.17174	-0.09257
C	-0.15425	-2.47763	1.91211
C	-2.42176	-2.60772	0.76665
O	-1.36259	-4.42246	1.88588
H	-5.29056	-2.96713	-1.04681
C	-4.57418	-2.52512	-0.35876
C	-0.6607	-1.55275	2.85153
C	-2.72059	-1.38654	1.4131
C	-1.76107	-0.8041	2.36731
C	-4.86247	-1.30489	0.26601
C	-3.94423	-0.74193	1.14512
H	-2.09168	0.07215	2.92018
H	-5.80753	-0.80275	0.07432
H	-4.17388	0.19387	1.64916
H	0.79457	-2.96598	2.11165
H	-0.12874	-1.25764	3.75339

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.2562502

$TS_{A2''-C}$

UB3LYP/6-31G(d)
Imaginary frequency = -131.47 cm^{-1}
Zero-point correction= 0.602103 (Hartree/Particle)
Thermal correction to Energy= 0.638287
Thermal correction to Enthalpy= 0.639231
Thermal correction to Gibbs Free Energy= 0.531665
Sum of electronic and zero-point Energies= -3273.274002
Sum of electronic and thermal Energies= -3273.237818
Sum of electronic and thermal Enthalpies= -3273.236874
Sum of electronic and thermal Free Energies= -3273.344440

H	3.44647	-5.42096	-1.80463
C	2.92892	-4.51555	-1.50181
H	3.80213	-4.47829	0.47157
H	1.88141	-4.28825	-3.37555
C	3.12704	-3.98755	-0.22354
C	2.05343	-3.87816	-2.38456
C	2.45689	-2.83044	0.17385
C	1.38831	-2.71404	-1.99906
H	2.60161	-2.42372	1.16793
H	3.37827	-0.93675	-2.57239
C	1.59868	-2.17864	-0.71984
H	0.70085	-2.22056	-2.67932
H	4.57628	0.51294	-4.17059
C	3.05548	0.08949	-2.6994
C	3.73922	0.92762	-3.61725

N	0.89137	-1.0061	-0.31648
C	1.98463	0.60924	-1.99261
C	1.06776	0.11675	-0.95855
C	3.37484	2.24708	-3.82831
Ni	-0.46506	-0.83273	1.06486
H	3.92397	2.85676	-4.54049
C	1.61594	1.96845	-2.20704
C	2.2862	2.81555	-3.11049
C	0.15699	1.22821	-0.59072
N	-0.73314	0.95769	0.32481
C	0.52272	2.3964	-1.40027
H	-1.12687	2.12657	2.69807
C	1.8132	4.15448	-3.19802
H	2.2929	4.84915	-3.88189
C	-1.74561	1.91157	0.64493
C	-1.84493	2.42798	1.94315
C	0.0922	3.70785	-1.50316
C	0.75268	4.57398	-2.41245
H	-0.73294	4.08573	-0.91159
C	-2.68779	2.28271	-0.32467
C	-2.85851	3.33394	2.25666
H	-2.91891	3.73931	3.26254
H	-2.62454	1.85941	-1.32239
H	0.40887	5.60095	-2.48963
C	-3.70431	3.18183	-0.00025
C	-3.79146	3.71424	1.28834
H	-4.43178	3.46049	-0.75725
H	-4.58326	4.4142	1.53808
H	-0.95931	-3.62522	-0.28509
H	-3.44626	-4.01453	-1.15685
C	-1.52485	-3.50642	0.67602
C	-3.67258	-3.10235	-0.60845
C	-0.58386	-2.73295	1.65062
C	-2.76306	-2.65658	0.35605
O	-1.8516	-4.66656	1.27176
H	-5.52871	-2.74853	-1.64852
C	-4.84542	-2.39737	-0.87929
C	-1.12303	-1.87706	2.63276
C	-3.0666	-1.48841	1.09227
C	-2.14713	-1.03025	2.15032
C	-5.14036	-1.23497	-0.1551
C	-4.25734	-0.78599	0.82297
H	-2.48533	-0.20388	2.76978
H	-6.05708	-0.6852	-0.35189
H	-4.48904	0.10845	1.39619
H	0.33045	-3.27277	1.88312
H	-0.64333	-1.68382	3.58877
C	3.66166	0.46356	1.72585
C	4.61947	1.27844	1.13819
C	4.36549	2.64303	0.93822
C	3.13615	3.18017	1.34107
C	2.17213	2.37034	1.92912
C	2.40399	0.98295	2.14552
H	3.87648	-0.58923	1.88752
H	5.57352	0.85475	0.83558
H	5.11693	3.27833	0.47835
H	2.93175	4.23724	1.19299
H	1.22463	2.80127	2.24102
C	1.42798	0.15199	2.7619
H	1.69963	-0.85437	3.06308
H	0.59876	0.60505	3.29408

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0376084

C

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.605970
(Hartree/Particle)
Thermal correction to Energy= 0.641617
Thermal correction to Enthalpy= 0.642561
Thermal correction to Gibbs Free Energy= 0.537564
Sum of electronic and zero-point Energies= -3273.435899
Sum of electronic and thermal Energies= -3273.400253
Sum of electronic and thermal Enthalpies= -3273.399309
Sum of electronic and thermal Free Energies= -3273.504305

H	1.69476	-5.33939	-2.51734
C	1.42064	-4.3586	-2.13982
H	1.71567	-4.8859	-0.0679
H	0.99943	-3.54011	-4.09331
C	1.43479	-4.10299	-0.76657
C	1.03571	-3.34589	-3.02493
C	1.07522	-2.84828	-0.27932
C	0.68092	-2.08678	-2.54607
H	1.07255	-2.64947	0.78635
H	2.73731	-0.5157	-2.94191
C	0.7141	-1.82025	-1.16587
H	0.35563	-1.30951	-3.23003
H	4.14503	0.98292	-4.3092
C	2.5558	0.55218	-2.91194
C	3.36546	1.42078	-3.69237
N	0.27378	-0.59273	-0.6395
C	1.55605	1.09466	-2.1257
C	0.58764	0.58088	-1.14636
C	3.19726	2.79493	-3.68855
Ni	-0.68203	-0.38582	1.06227
H	3.83866	3.42758	-4.29626
C	1.3951	2.50996	-2.11747
C	2.19209	3.38775	-2.8731
C	-0.11421	1.72829	-0.56349
N	-0.94552	1.46839	0.41964
C	0.38947	2.94929	-1.21145
H	-1.01318	2.13085	2.97108
C	1.93188	4.779	-2.71655
H	2.51611	5.50077	-3.28115
C	-1.76905	2.46476	0.98828
C	-1.72116	2.69224	2.37149
C	0.16844	4.3061	-1.07009
C	0.95035	5.2098	-1.84021
H	-0.57933	4.69247	-0.38731
C	-2.69353	3.17089	0.20211
C	-2.5667	3.63627	2.95395
H	-2.51322	3.81344	4.02451
H	-2.73936	2.97455	-0.86497
H	0.76985	6.2749	-1.72713
C	-3.53967	4.10862	0.79298
C	-3.47806	4.3484	2.16932
H	-4.25218	4.64943	0.17633
H	-4.13869	5.07936	2.62627
H	-1.026	-4.03925	3.16538
H	-1.56763	-5.63609	1.34481
C	-1.70868	-3.31302	2.72273
C	-1.95701	-4.82238	0.73699
C	-1.75147	-1.94237	3.2683
C	-2.07607	-3.54997	1.3
O	-2.78162	-2.90757	3.61522
H	-2.24206	-6.05223	-1.01158
C	-2.33671	-5.05781	-0.58517

C	-2.1501	-0.82332	2.37433
C	-2.56506	-2.47199	0.52082
C	-2.61217	-1.11487	1.07449
C	-2.84272	-4.00338	-1.35381
C	-2.94882	-2.72673	-0.80744
H	-3.24164	-0.3971	0.55369
H	-3.14424	-4.17604	-2.38347
H	-3.3217	-1.90432	-1.41375
H	-1.09262	-1.69084	4.09884
H	-2.48977	0.08592	2.8649
C	3.07586	-0.28525	1.16648
C	4.12011	0.33361	0.48684
C	4.15069	1.72703	0.34408
C	3.12077	2.48472	0.90254
C	2.07103	1.86108	1.57815
C	2.01413	0.45842	1.73157
H	3.06649	-1.3684	1.25963
H	4.91651	-0.27241	0.06063
H	4.95901	2.20819	-0.19961
H	3.11767	3.56646	0.79246
H	1.26586	2.46568	1.9881
C	0.86196	-0.19638	2.36898
H	1.09647	-1.21285	2.70849
H	0.47228	0.37686	3.21592

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0741057

UB3LYP/6-31G(d)
Zero-point correction= 0.604420 (Hartree/Particle)
Thermal correction to Energy= 0.640700
Thermal correction to Enthalpy= 0.641644
Thermal correction to Gibbs Free Energy= 0.532821
Sum of electronic and zero-point Energies= -3273.305775
Sum of electronic and thermal Energies= -3273.269494
Sum of electronic and thermal Enthalpies= -3273.268550
Sum of electronic and thermal Free Energies= -3273.377373

H	1.72971	-5.23007	-2.73568
C	1.46651	-4.26027	-2.32308
H	1.90512	-4.81737	-0.28644
H	0.90863	-3.41378	-4.22814
C	1.5643	-4.02768	-0.95053
C	1.01263	-3.23768	-3.16055
C	1.2206	-2.78688	-0.41785
C	0.67476	-1.99212	-2.63753
H	1.29718	-2.6041	0.64805
H	2.72851	-0.37934	-3.1114
C	0.79265	-1.74588	-1.25747
H	0.2946	-1.2104	-3.2873
H	3.95403	1.14757	-4.61178
C	2.49905	0.6797	-3.08639
C	3.20282	1.56489	-3.94673
N	0.37326	-0.53075	-0.68212
C	1.53681	1.193	-2.23564
C	0.64179	0.65705	-1.1948
C	2.96651	2.92712	-3.96415
Ni	-0.57538	-0.3668	1.03059
H	3.5256	3.57159	-4.6379
C	1.31159	2.59978	-2.24683
C	1.99864	3.4929	-3.08698
C	-0.07063	1.78006	-0.59413
N	-0.87124	1.50299	0.4156
C	0.34692	3.01207	-1.28557
H	-0.88075	2.36097	2.9326
C	1.6709	4.87162	-2.95422
H	2.1692	5.6055	-3.58285
C	-1.73999	2.47757	0.96377
C	-1.6581	2.81156	2.32417
C	0.06024	4.35998	-1.17157
C	0.73247	5.27766	-2.02266
H	-0.66158	4.73002	-0.45238
C	-2.75306	3.05298	0.17829
C	-2.55667	3.72291	2.8788
H	-2.47444	3.98014	3.93141
H	-2.83067	2.77707	-0.8694
H	0.49942	6.33486	-1.92944
C	-3.65132	3.95788	0.74207
C	-3.55626	4.29995	2.09313
H	-4.43253	4.39164	0.12333
H	-4.25853	5.0039	2.53034
H	-1.22722	-4.06821	3.27281
H	-1.8673	-5.68732	1.4974
C	-1.83724	-3.30677	2.78396
C	-2.17014	-4.86719	0.84976
C	-1.7846	-1.91455	3.27744
C	-2.18795	-3.56834	1.36138
O	-2.88654	-2.78103	3.62577
H	-2.5454	-6.13949	-0.84972
C	-2.55529	-5.12301	-0.46642
C	-2.08711	-0.80502	2.33292
C	-2.57662	-2.48771	0.53243
C	-2.54089	-1.11246	1.04015
C	-2.96495	-4.06471	-1.28235
C	-2.96877	-2.76352	-0.78856
H	-3.12035	-0.37768	0.48745
H	-3.27385	-4.25452	-2.30683
H	-3.27288	-1.93943	-1.42995
H	-1.13208	-1.68195	4.11899
H	-2.39028	0.13657	2.78499
C	3.26808	-0.46467	1.5416
C	4.44788	0.09505	1.06011
C	4.57177	1.48127	0.92488
C	3.49531	2.29366	1.28342
C	2.31197	1.72963	1.75937
C	2.16253	0.33389	1.90778
H	3.20037	-1.54407	1.65758
H	5.28087	-0.55323	0.79741
H	5.49355	1.91888	0.55113
H	3.5737	3.37437	1.19053
H	1.48731	2.38075	2.03888
C	0.90638	-0.2619	2.40759
H	1.06702	-1.28814	2.76178
H	0.486	0.32044	3.23392

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0703756

C-TS

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -349.19 cm^{-1}
Zero-point correction= 0.604480 (Hartree/Particle)
Thermal correction to Energy= 0.640382
Thermal correction to Enthalpy= 0.641326
Thermal correction to Gibbs Free Energy= 0.533835
Sum of electronic and zero-point Energies= -3273.371845

Sum of electronic and thermal Energies= -3273.335943
Sum of electronic and thermal Enthalpies= -3273.334998
Sum of electronic and thermal Free Energies= -3273.442490

H	2.45799	-3.352	-3.28343
H	1.11472	-5.29039	-2.48609
H	1.3051	-0.11047	3.72077
C	1.58782	-3.19164	-2.65367
C	0.83435	-4.28016	-2.20289
C	0.53179	-0.39175	3.01513
H	0.93338	-2.52337	2.95817
H	1.83029	-1.04463	-2.60973
C	1.23625	-1.89345	-2.28539
C	0.10322	-1.85759	3.29139
O	-0.18213	-1.89325	4.6074
H	-0.42228	1.6053	3.17283
C	-0.27362	-4.0633	-1.37894
C	-0.55593	0.5706	2.86823
H	-0.86132	-4.90147	-1.01631
C	0.12189	-1.6829	-1.45971
H	-0.73561	-4.34061	2.5883
C	-0.62674	-2.76973	-0.99739
C	-1.13342	-2.23689	2.4689
C	-1.45164	-3.58486	2.2711
C	-1.74504	0.16693	2.25934
N	-0.18917	-0.38241	-0.97849
H	-0.3086	-1.10212	-4.2546
Ni	-0.13557	0.18904	0.94428
H	-1.47673	-2.59445	-0.35065
C	-2.06528	-1.25129	2.06302
H	-2.54046	0.89309	2.11553
C	-0.48154	-0.03674	-4.34763
C	-2.65435	-3.96887	1.67838
C	-0.35758	0.62183	-1.79105
H	-2.87633	-5.02159	1.52339
H	-0.67885	-0.12926	-6.49485
C	-0.49407	0.79646	-3.24294
C	-0.69152	0.52967	-5.63209
C	-3.27981	-1.6432	1.46562
C	-3.57582	-2.98998	1.27639
N	-0.41663	1.99687	0.13382
C	-0.52847	1.9552	-1.15941
H	1.38715	3.25471	1.5876
H	-3.98704	-0.87858	1.15068
C	-0.733	2.18742	-3.43721
C	-0.90038	1.88631	-5.81939
C	0.41476	3.73742	1.61134
C	-0.63552	3.19902	0.85876
H	-4.51561	-3.28008	0.81443
C	-0.76057	2.93433	-2.22618
C	-0.92735	2.76895	-4.70416
H	-1.04597	2.28322	-6.82019
C	0.20026	4.88731	2.37104
H	1.01992	5.31135	2.94368
C	-1.90645	3.78609	0.89773
H	-2.71635	3.34082	0.32788
C	-0.95911	4.30187	-2.28451
C	-1.06305	5.48549	2.40359
C	-2.11474	4.92922	1.67036
C	-1.13193	4.17666	-4.73219
H	-0.98727	4.91096	-1.38885
C	-1.13885	4.90792	-3.55537
H	-1.22862	6.37519	3.0038
H	-1.28352	4.676	-5.68512
H	-3.10148	5.38209	1.70051
H	-1.29456	5.98151	-3.59884
C	1.97173	-0.08763	1.54443
C	2.84773	-1.25691	1.80002
C	3.7262	-1.27148	2.89639
C	4.53846	-2.3774	3.15415
C	4.49182	-3.49548	2.31788
C	3.62505	-3.49276	1.21944
C	2.81428	-2.38875	0.96623
H	2.34187	0.82986	1.99938
H	1.90863	0.08085	0.46332
H	3.77398	-0.40476	3.55218
H	5.21139	-2.36303	4.0078
H	5.12399	-4.3566	2.51675
H	3.57779	-4.35382	0.55734
H	2.13803	-2.40387	0.1186

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0244287

UB3LYP/6-31G(d)
Imaginary frequency = -360.10 cm^{-1}
Zero-point correction= 0.602464 (Hartree/Particle)
Thermal correction to Energy= 0.638693
Thermal correction to Enthalpy= 0.639637
Thermal correction to Gibbs Free Energy= 0.531248
Sum of electronic and zero-point Energies= -3273.233873
Sum of electronic and thermal Energies= -3273.197644
Sum of electronic and thermal Enthalpies= -3273.196700
Sum of electronic and thermal Free Energies= -3273.305089

H	2.47475	-3.28559	-3.37727
H	1.04681	-5.23501	-2.77344
H	1.28685	-0.22239	3.71543
C	1.59218	-3.14624	-2.75834
C	0.79307	-4.24052	-2.41718
C	0.51233	-0.47191	2.99979
H	0.90216	-2.60997	2.88559
H	1.89531	-1.01893	-2.5548
C	1.26922	-1.86928	-2.29976
C	0.08149	-1.94733	3.22238
O	-0.10597	-1.94526	4.56468
H	-0.42708	1.52255	3.21849
C	-0.32796	-4.04684	-1.60736
C	-0.56038	0.50321	2.8671
H	-0.95396	-4.89029	-1.32968
C	0.13578	-1.67167	-1.49193
H	-0.86992	-4.41474	2.66891
C	-0.65455	-2.77451	-1.13884
C	-1.20125	-2.30546	2.47794
C	-1.56226	-3.6461	2.33314
C	-1.73982	0.11381	2.22922
N	-0.17265	-0.38909	-0.96736
H	-0.39842	-1.10953	-4.238
Ni	-0.10737	0.20303	0.94886
H	-1.52648	-2.62626	-0.51162
C	-2.10478	-1.29955	2.06941
H	-2.52931	0.84866	2.09598
C	-0.55096	-0.04101	-4.33403
C	-2.79188	-4.0061	1.77845
C	-0.3471	0.64315	-1.78067
H	-3.05744	-5.05496	1.67425

H	-0.79875	-0.15478	-6.47605
C	-0.52125	0.79984	-3.23497
C	-0.77886	0.51606	-5.62147
C	-3.34111	-1.6687	1.51044
C	-3.68521	-3.01058	1.36799
N	-0.36029	2.02586	0.14514
C	-0.49383	1.95675	-1.1673
H	1.4013	3.37998	1.58234
H	-4.0349	-0.89199	1.19525
C	-0.74144	2.1917	-3.44816
C	-0.96525	1.87147	-5.82239
C	0.40977	3.82356	1.59988
C	-0.61466	3.23003	0.84728
H	-4.64825	-3.28079	0.94256
C	-0.73014	2.9397	-2.23676
C	-0.9509	2.76437	-4.71343
H	-1.12582	2.25949	-6.8251
C	0.15958	4.97676	2.34349
H	0.96532	5.43179	2.91331
C	-1.89908	3.79745	0.87471
H	-2.69718	3.32656	0.3079
C	-0.90128	4.31087	-2.30795
C	-1.11705	5.54302	2.36107
C	-2.1444	4.94629	1.62666
C	-1.12921	4.17652	-4.75118
H	-0.89683	4.93264	-1.4201
C	-1.09545	4.91239	-3.58051
H	-1.31133	6.43621	2.94786
H	-1.29135	4.67326	-5.70451
H	-3.14423	5.37209	1.64275
H	-1.22906	5.98974	-3.62678
C	2.00214	-0.16142	1.55524
C	2.91094	-1.28903	1.8777
C	3.74181	-1.23772	3.01088
C	4.6187	-2.27837	3.31156
C	4.68477	-3.40128	2.4848
C	3.86657	-3.46895	1.35478
C	2.99116	-2.42717	1.05507
H	2.3351	0.77647	1.99866
H	1.95912	-0.038	0.46936
H	3.70708	-0.36476	3.65941
H	5.25231	-2.21042	4.19199
H	5.36745	-4.214	2.71759
H	3.9097	-4.33623	0.70093
H	2.36385	-2.49255	0.17071

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0179661

P3

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.606996
(Hartree/Particle)
Thermal correction to Energy= 0.643019
Thermal correction to Enthalpy= 0.643963
Thermal correction to Gibbs Free Energy= 0.535850
Sum of electronic and zero-point Energies= -3273.411141
Sum of electronic and thermal Energies= -3273.375118
Sum of electronic and thermal Enthalpies= -3273.374174
Sum of electronic and thermal Free Energies= -3273.482288

H	2.81034	-3.20731	-3.21044
H	1.5452	-5.16869	-2.34804
H	1.82011	-0.67195	3.87446
C	1.92211	-3.05908	-2.60328
C	1.21335	-4.16136	-2.11487
C	1.15561	-0.84021	3.01522
H	0.89113	-2.98443	3.10016
H	2.06007	-0.90333	-2.6658
C	1.50356	-1.76276	-2.30515
C	0.29651	-2.08701	3.41458
O	-0.06588	-2.07421	4.7165
H	0.75207	1.36308	3.09483
C	0.08948	-3.96053	-1.30797
C	0.30093	0.40189	2.85894
H	-0.45735	-4.8093	-0.90773
C	0.36303	-1.56497	-1.51387
H	-1.09248	-4.27106	2.46711
C	-0.32809	-2.6683	-0.9924
C	-1.02577	-2.13204	2.64606
C	-1.64393	-3.34499	2.31712
C	-1.06738	0.34772	2.6866
N	-0.05061	-0.26853	-1.11476
H	0.09982	-1.01446	-4.3903
Ni	-0.32823	0.27834	0.75389
H	-1.18534	-2.50543	-0.3467
C	-1.7483	-0.92677	2.4356
H	-1.67129	1.24954	2.77949
C	-0.14692	0.03404	-4.50609
C	-2.93839	-3.37879	1.80025
C	-0.27823	0.70792	-1.95584
H	-3.39136	-4.33034	1.53321
H	-0.15166	-0.07649	-6.66161
C	-0.31995	0.86463	-3.41244
C	-0.29074	0.58043	-5.80837
C	-3.06951	-0.97009	1.93869
C	-3.6609	-2.18723	1.61993
N	-0.64509	2.06763	-0.04595
C	-0.62996	2.01848	-1.34943
H	0.81578	3.37025	1.7103
H	-3.60907	-0.03673	1.79149
C	-0.65253	2.23236	-3.63909
C	-0.58972	1.91578	-6.02415
C	-0.18252	3.7833	1.60579
C	-1.05813	3.21955	0.66921
H	-4.67274	-2.21545	1.22566
C	-0.84596	2.97392	-2.43929
C	-0.78298	2.79463	-4.92185
H	-0.68026	2.2988	-7.03678
C	-0.59566	4.87157	2.3741
H	0.09149	5.31342	3.08988
C	-2.35828	3.72557	0.53017
H	-3.03631	3.26194	-0.18001
C	-1.15098	4.3204	-2.52648
C	-1.88737	5.38607	2.23023
C	-2.76668	4.80752	1.31014
C	-1.09812	4.18125	-4.97917
H	-1.30814	4.92557	-1.6414
C	-1.26728	4.90958	-3.81283
H	-2.20956	6.22744	2.83655
H	-1.20721	4.6656	-5.94557
H	-3.77561	5.19488	1.20121
H	-1.50587	5.96687	-3.87736
C	2.04572	-1.05604	1.75974
C	3.10913	-2.11921	1.90532
C	4.16298	-1.96054	2.81696
C	5.14936	-2.93958	2.94888
C	5.10031	-4.09645	2.16508
C	4.0579	-4.26309	1.25019

C	3.07145	-3.28213	1.12447
H	2.51829	-0.09935	1.49903
H	1.40773	-1.32077	0.90827
H	4.21255	-1.05995	3.42508
H	5.95877	-2.79803	3.66061
H	5.86879	-4.85829	2.2658
H	4.00981	-5.15665	0.63278
H	2.26173	-3.4198	0.413

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0758107

UB3LYP/6-31G(d)
Zero-point correction= 0.605244 (Hartree/Particle)
Thermal correction to Energy= 0.641675
Thermal correction to Enthalpy= 0.642619
Thermal correction to Gibbs Free Energy= 0.531640
Sum of electronic and zero-point Energies= -3273.287150
Sum of electronic and thermal Energies= -3273.250720
Sum of electronic and thermal Enthalpies= -3273.249775
Sum of electronic and thermal Free Energies= -3273.360755

H	2.5686	-3.1276	-3.59829
H	1.32895	-5.11975	-2.76413
H	1.70886	-0.4071	3.70785
C	1.70506	-3.00063	-2.9503
C	1.01496	-4.12016	-2.47722
C	1.05687	-0.79045	2.91211
H	0.99308	-2.8943	3.49034
H	1.86372	-0.85073	-2.93338
C	1.30786	-1.71579	-2.58497
C	0.33469	-2.0105	3.53189
O	-0.11449	-1.76336	4.81187
H	0.37854	1.33492	2.8043
C	-0.07609	-3.93945	-1.62346
C	0.07875	0.3223	2.5439
H	-0.62135	-4.79965	-1.24393
C	0.19922	-1.52581	-1.73893
H	-0.86906	-4.45191	3.31228
C	-0.47757	-2.65754	-1.24991
C	-1.00606	-2.35155	2.87935
C	-1.49467	-3.66246	2.90404
C	-1.28347	0.06897	2.35084
N	-0.18835	-0.25102	-1.28014
H	-0.14452	-0.83629	-4.60711
Ni	-0.38836	0.26179	0.59003
H	-1.32939	-2.51928	-0.58958
C	-1.81548	-1.30076	2.39179
H	-2.00547	0.88092	2.42619
C	-0.29902	0.23479	-4.66914
C	-2.76546	-3.95249	2.4144
C	-0.33519	0.80999	-2.08167
H	-3.13272	-4.97488	2.42262
H	-0.34862	0.21287	-6.82761
C	-0.38046	1.025	-3.53451
C	-0.41632	0.84617	-5.94699
C	-3.10304	-1.60736	1.91624
C	-3.57411	-2.91679	1.92801
N	-0.62454	2.09759	-0.10484
C	-0.5833	2.08437	-1.43167
H	0.99315	3.48707	1.47139
H	-3.73155	-0.80449	1.53761
C	-0.60196	2.42392	-3.71157
C	-0.60348	2.20693	-6.10742
C	-0.01919	3.88015	1.44913
C	-0.96713	3.26539	0.6166
H	-4.57369	-3.13418	1.56109
C	-0.72061	3.11407	-2.47251
C	-0.70562	3.04945	-4.96339
H	-0.67764	2.63663	-7.10327
C	-0.36887	4.99142	2.21693
H	0.37892	5.46095	2.8507
C	-2.27549	3.77704	0.58218
H	-3.01376	3.29238	-0.05055
C	-0.91658	4.48308	-2.49689
C	-1.6683	5.50028	2.17317
C	-2.61891	4.88698	1.35329
C	-0.90913	4.45935	-4.95475
H	-1.0112	5.06133	-1.5847
C	-1.00198	5.14031	-3.75453
H	-1.93943	6.36268	2.77554
H	-0.99227	4.99694	-5.89611
H	-3.63557	5.27	1.31731
H	-1.15456	6.21621	-3.76524
C	1.96301	-1.17377	1.70837
C	3.07182	-2.15948	2.01617
C	4.11733	-1.81562	2.88593
C	5.1436	-2.71687	3.16685
C	5.14525	-3.98359	2.5782
C	4.11482	-4.33683	1.70675
C	3.08801	-3.43175	1.42966
H	2.4046	-0.24564	1.32068
H	1.33737	-1.57132	0.8993
H	4.13196	-0.82832	3.34312
H	5.94463	-2.42884	3.84289
H	5.94516	-4.68655	2.79522
H	4.10873	-5.31788	1.23847
H	2.29328	-3.71129	0.74166

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0596035

$TS_{A2'-A3'}$

UB3LYP/6-31G(d)
Imaginary frequency = -105.93 cm^{-1}
Zero-point correction= 0.602644 (Hartree/Particle)
Thermal correction to Energy= 0.638335
Thermal correction to Enthalpy= 0.639279
Thermal correction to Gibbs Free Energy= 0.531287
Sum of electronic and zero-point Energies= -3273.255455
Sum of electronic and thermal Energies= -3273.219764
Sum of electronic and thermal Enthalpies= -3273.218820
Sum of electronic and thermal Free Energies= -3273.326812

H	0.01916	-6.43743	2.26383
C	-0.05502	-5.42045	1.8892
H	-2.19983	-5.48059	1.66024
H	2.0634	-5.03496	2.02222
C	-1.29848	-4.88358	1.54602
C	1.0899	-4.63225	1.75506
C	-1.39776	-3.57842	1.06613
C	0.99622	-3.32436	1.28119
H	-2.367	-3.15544	0.82162
H	-1.1475	-3.95535	-1.55651

C	-0.24682	-2.78465	0.91534
H	1.88684	-2.71294	1.18349
H	-2.24388	-4.53381	-3.68929
C	-1.57301	-3.16293	-2.16096
C	-2.21005	-3.49022	-3.38812
N	-0.33314	-1.43614	0.4932
C	-1.5218	-1.83804	-1.76448
C	-0.97317	-1.09441	-0.61598
C	-2.79616	-2.5335	-4.19644
Ni	0.12789	0.18315	1.55284
H	-3.28915	-2.82518	-5.12056
C	-2.09528	-0.8555	-2.61995
C	-2.755	-1.16071	-3.82236
C	-1.18069	0.32899	-0.85865
N	-0.73443	1.16491	0.07111
C	-1.92936	0.46861	-2.12102
H	-1.59998	2.88611	1.84534
C	-3.31427	-0.06549	-4.53954
H	-3.83916	-0.24449	-5.47462
C	-0.75492	2.56919	-0.09944
C	-1.22234	3.37206	0.95298
C	-2.49686	1.50788	-2.83743
C	-3.19118	1.21867	-4.04321
H	-2.41884	2.53652	-2.5064
C	-0.25354	3.19127	-1.25523
C	-1.22155	4.76015	0.84048
H	-1.60174	5.3644	1.66023
H	0.14876	2.58298	-2.05697
H	-3.62972	2.04579	-4.59504
C	-0.24365	4.58275	-1.3556
C	-0.73171	5.37502	-0.31468
H	0.15669	5.04833	-2.25276
H	-0.72305	6.45822	-0.39836
H	0.99562	-1.35551	4.94194
H	-1.58404	-2.63928	4.09182
C	0.56347	-0.51858	4.39443
H	2.28006	-0.45888	2.88614
C	-1.86891	-1.59608	3.98899
C	1.28616	-0.0755	3.10006
C	-0.93468	-0.5781	4.08995
O	0.60947	0.69802	5.18794
H	-3.96431	-2.02214	3.68989
C	-3.2099	-1.24273	3.75827
C	0.90518	1.29522	2.95454
C	-1.31289	0.77317	3.96102
C	-0.00929	1.54488	4.1831
C	-3.58824	0.09481	3.64023
H	1.56576	2.08599	2.61
C	-2.63618	1.12419	3.74325
H	-0.08831	2.57191	4.53853
H	-4.63361	0.3467	3.48288
H	-2.94592	2.16417	3.67535
H	1.7971	-1.66444	-1.71571
H	1.63033	-1.44181	-4.16764
C	2.02521	-0.71386	-2.18943
C	1.93942	-0.58802	-3.56995
H	2.56794	-0.73282	0.48227
C	2.5342	0.2519	0.03507
C	2.42604	0.38101	-1.36921
C	2.24623	0.62662	-4.19431
H	2.18176	0.72058	-5.27467
H	2.91759	1.07466	0.63035
C	2.72344	1.60889	-2.03089
C	2.64255	1.72105	-3.41085
H	3.03364	2.46199	-1.43256
H	2.89198	2.6657	-3.8886

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0197685

A3'

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.606944
(Hartree/Particle)
Thermal correction to Energy= 0.641817
Thermal correction to Enthalpy= 0.642761
Thermal correction to Gibbs Free Energy= 0.539446
Sum of electronic and zero-point Energies= -3273.410894
Sum of electronic and thermal Energies= -3273.376020
Sum of electronic and thermal Enthalpies= -3273.375076
Sum of electronic and thermal Free Energies= -3273.478391

H	0.59798	-6.31367	2.07848
C	0.51759	-5.28735	1.73231
H	-1.59311	-5.42014	1.29728
H	2.59585	-4.82314	2.08883
C	-0.71038	-4.78634	1.28878
C	1.63733	-4.44978	1.73847
C	-0.81861	-3.46884	0.84633
C	1.53402	-3.12963	1.30438
H	-1.77714	-3.07134	0.52877
H	-0.66913	-3.6491	-1.72002
C	0.30925	-2.62816	0.83361
H	2.39202	-2.46822	1.32714
H	-1.53558	-4.04521	-3.9962
C	-1.00176	-2.8043	-2.31103
C	-1.49622	-3.02491	-3.62516
N	0.21417	-1.2746	0.47016
C	-0.94785	-1.51107	-1.82305
C	-0.43248	-0.8615	-0.6071
C	-1.91875	-1.99093	-4.44251
Ni	1.06445	0.26285	1.39687
H	-2.28314	-2.19743	-5.44534
C	-1.38331	-0.45166	-2.6695
C	-1.86027	-0.64637	-3.97743
C	-0.59382	0.58204	-0.763
N	-0.07987	1.34409	0.18823
C	-1.20795	0.83149	-2.07696
H	-2.4188	2.62447	-0.09352
C	-2.199	0.52352	-4.71491
H	-2.5764	0.42879	-5.72965
C	-0.29609	2.73007	0.25874
C	-1.58176	3.28278	0.11541
C	-1.53103	1.94871	-2.82601
C	-2.03085	1.77353	-4.14487
H	-1.40511	2.95111	-2.43482
C	0.77335	3.57884	0.58938
C	-1.78061	4.65429	0.26615
H	-2.78164	5.063	0.15726
H	1.75609	3.14586	0.73445
H	-2.28274	2.65878	-4.72205
C	0.5693	4.95	0.73193
C	-0.70707	5.4976	0.56916
H	1.41104	5.59217	0.97687
H	-0.86539	6.56553	0.6879
H	1.17226	-1.44315	4.78882
H	-1.36265	-2.33749	3.45502
C	0.95365	-0.54379	4.21469
H	2.89406	-0.70054	3.01978

C	-1.48506	-1.26427	3.34914
C	1.9412	-0.1818	3.07733
C	-0.4626	-0.38523	3.66744
O	1.03326	0.64969	5.05321
H	-3.50781	-1.39019	2.60896
C	-2.68764	-0.72427	2.86369
C	1.77781	1.23248	2.92614
C	-0.6234	1.00567	3.5171
C	0.70629	1.59151	3.98551
C	-2.84745	0.65673	2.71451
H	2.58996	1.92958	2.73964
C	-1.80991	1.54402	3.04582
H	0.70141	2.61667	4.35325
H	-3.79032	1.0513	2.34528
H	-1.93529	2.61484	2.92052
C	2.75838	0.34226	0.30919
C	2.55357	0.19172	-1.14174
H	3.37538	-0.45951	0.72296
H	3.19345	1.31195	0.56451
C	2.53027	-1.07952	-1.74896
C	2.28727	-1.22791	-3.11244
C	2.05244	-0.10568	-3.91241
C	2.07635	1.166	-3.33082
C	2.32106	1.30977	-1.96759
H	2.31082	2.30058	-1.52075
H	1.8867	2.04627	-3.93959
H	2.68241	-1.95993	-1.12965
H	2.2611	-2.22278	-3.5493
H	1.84649	-0.22079	-4.973

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0466436

UB3LYP/6-31G(d)
Zero-point correction= 0.605837 (Hartree/Particle)
Thermal correction to Energy= 0.641176
Thermal correction to Enthalpy= 0.642120
Thermal correction to Gibbs Free Energy= 0.536693
Sum of electronic and zero-point Energies= -3273.278149
Sum of electronic and thermal Energies= -3273.242809
Sum of electronic and thermal Enthalpies= -3273.241865
Sum of electronic and thermal Free Energies= -3273.347293

H	0.42711	-6.40979	2.05894
C	0.38785	-5.38244	1.70826
H	-1.76142	-5.3487	1.51734
H	2.52163	-5.08379	1.81105
C	-0.83796	-4.78711	1.39976
C	1.56043	-4.63686	1.57077
C	-0.89219	-3.4688	0.95081
C	1.51328	-3.31586	1.1282
H	-1.84769	-3.00158	0.73502
H	-0.78747	-3.79049	-1.6557
C	0.2873	-2.71609	0.79544
H	2.42729	-2.7418	1.02953
H	-1.86224	-4.26028	-3.82483
C	-1.15218	-2.96227	-2.25159
C	-1.77039	-3.22627	-3.50333
N	0.23842	-1.36005	0.4047
C	-1.03285	-1.6512	-1.82414
C	-0.43409	-0.96386	-0.66606
C	-2.25098	-2.21907	-4.31956
Ni	1.06894	0.21073	1.32551
H	-2.71431	-2.46063	-5.27297
C	-1.52505	-0.61926	-2.67299
C	-2.12677	-0.85832	-3.92047
C	-0.59963	0.47344	-0.85809
N	-0.07298	1.26776	0.06063
C	-1.29097	0.682	-2.14487
H	-2.46501	2.47172	-0.13703
C	-2.52233	0.28637	-4.668
H	-2.99717	0.15904	-5.63773
C	-0.33041	2.65317	0.10355
C	-1.63948	3.16123	0.00713
C	-1.66783	1.77292	-2.90834
C	-2.28739	1.55372	-4.16779
H	-1.50236	2.78863	-2.56936
C	0.72004	3.55171	0.35397
C	-1.87922	4.52959	0.12289
H	-2.89877	4.90013	0.05109
H	1.72599	3.16331	0.45789
H	-2.58207	2.41971	-4.75441
C	0.47441	4.91906	0.46055
C	-0.82459	5.41888	0.34304
H	1.30438	5.59737	0.64114
H	-1.01411	6.48467	0.43364
H	1.21006	-1.333	4.84872
H	-1.40456	-2.30423	3.75427
C	0.95696	-0.46809	4.23625
H	2.86775	-0.65819	3.00415
C	-1.53392	-1.2389	3.58613
C	1.90568	-0.15538	3.0506
C	-0.48773	-0.34706	3.75701
O	1.0644	0.76079	5.00841
H	-3.62489	-1.39934	3.07331
C	-2.78175	-0.7242	3.19623
C	1.72466	1.24802	2.83911
C	-0.66686	1.03289	3.54831
C	0.68264	1.64457	3.91688
C	-2.95909	0.64464	2.98738
H	2.53285	1.94175	2.62553
C	-1.89514	1.54523	3.16302
H	0.68806	2.6847	4.24107
H	-3.93823	1.02174	2.70315
H	-2.04217	2.6102	3.00773
C	2.83402	0.16292	0.36721
C	2.81278	0.3453	-1.09758
H	3.22164	-0.81991	0.64286
H	3.42901	0.93598	0.85911
C	2.53279	-0.72551	-1.97017
C	2.54333	-0.55605	-3.35356
C	2.82998	0.69246	-3.90835
C	3.11671	1.76774	-3.06217
C	3.10633	1.59501	-1.68136
H	3.35103	2.43525	-1.03613
H	3.35556	2.74193	-3.48169
H	2.31886	-1.70536	-1.55231
H	2.32602	-1.40262	-3.9999
H	2.83605	0.826	-4.98679

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0430011

$TS_{A3'-A4'}$

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -246.22 cm^{-1}
Zero-point correction= 0.607076 (Hartree/Particle)

Thermal correction to Energy= 0.641708
Thermal correction to Enthalpy= 0.642652
Thermal correction to Gibbs Free Energy= 0.538574
Sum of electronic and zero-point Energies= -3273.368174
Sum of electronic and thermal Energies= -3273.333542
Sum of electronic and thermal Enthalpies= -3273.332597
Sum of electronic and thermal Free Energies= -3273.436676

H	3.87678	-4.50966	-2.13015
C	3.29703	-3.64983	-1.80648
H	4.79364	-2.95704	-0.41377
H	1.62345	-4.08395	-3.09879
C	3.81107	-2.77872	-0.84227
C	2.0311	-3.41044	-2.34955
C	3.06579	-1.67431	-0.42544
C	1.28216	-2.30875	-1.9331
H	3.45735	-0.98686	0.31941
H	2.93849	-0.43213	-3.26663
C	1.79914	-1.42874	-0.97325
H	0.29781	-2.11385	-2.34375
H	3.88262	0.91557	-5.11652
C	2.69815	0.62316	-3.33151
C	3.23867	1.40516	-4.3911
N	1.039	-0.31525	-0.52555
C	1.87562	1.23885	-2.40578
C	1.14373	0.82658	-1.20052
C	2.97832	2.75827	-4.5237
Ni	-0.22797	-0.08935	1.00444
H	3.41566	3.3226	-5.34326
C	1.60659	2.62983	-2.55283
C	2.13918	3.42111	-3.5802
C	0.45739	1.96334	-0.66723
N	-0.18298	1.77154	0.4978
C	0.75634	3.12566	-1.51587
H	0.21732	2.78124	2.90122
C	1.79715	4.80539	-3.56248
H	2.17988	5.46619	-4.33576
C	-0.90924	2.84341	1.07476
C	-0.59567	3.27157	2.3729
C	0.45593	4.47747	-1.52172
C	0.9864	5.29969	-2.55609
H	-0.17474	4.92392	-0.76221
C	-1.97142	3.45741	0.39364
C	-1.32131	4.30085	2.9723
H	-1.06333	4.62428	3.97716
H	-2.21299	3.12646	-0.61105
H	0.73742	6.35743	-2.54774
C	-2.69563	4.48733	0.99549
C	-2.37475	4.91422	2.28709
H	-3.51539	4.95238	0.45445
H	-2.94129	5.71366	2.75594
H	-2.96159	-2.87415	1.90006
H	-2.09948	-3.5828	-0.87614
C	-2.72928	-1.87728	1.53096
H	-1.29058	-1.47104	3.24091
C	-2.31347	-2.52883	-1.03064
C	-1.55985	-1.1392	2.24921
C	-2.60045	-1.68634	0.02804
O	-3.80703	-0.94384	1.81988
H	-2.11496	-2.62316	-3.17946
C	-2.31606	-1.98065	-2.32651
C	-1.82709	0.23646	2.01653
C	-2.87721	-0.32193	-0.17642
C	-3.15191	0.22254	1.21749
C	-2.58108	-0.62487	-2.53034
H	-1.7162	0.95904	2.81892
C	-2.86475	0.22609	-1.44744
H	-3.77526	1.11056	1.29874
H	-2.58246	-0.22393	-3.54013
C	0.2776	-2.06971	1.55916
C	0.2671	-3.02774	2.69834
H	1.27455	-1.62575	1.52145
H	0.05454	-2.57457	0.6193
C	0.92483	-2.72031	3.90243
C	0.92415	-3.61529	4.97179
C	0.26453	-4.84356	4.86049
C	-0.39064	-5.16511	3.6693
C	-0.3894	-4.26508	2.60197
H	-0.89519	-4.52851	1.67594
H	-0.90162	-6.11912	3.56865
H	1.43914	-1.76558	3.99419
H	1.44166	-3.35653	5.8919
H	0.26452	-5.54255	5.69227
H	-3.0795	1.27706	-1.61315

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0165052

UB3LYP/6-31G(d)
Imaginary frequency = -251.33 cm^{-1}
Zero-point correction= 0.605786 (Hartree/Particle)
Thermal correction to Energy= 0.640815
Thermal correction to Enthalpy= 0.641759
Thermal correction to Gibbs Free Energy= 0.535250
Sum of electronic and zero-point Energies= -3273.248282
Sum of electronic and thermal Energies= -3273.213254
Sum of electronic and thermal Enthalpies= -3273.212310
Sum of electronic and thermal Free Energies= -3273.318819

H	3.86679	-4.85193	-1.81484
C	3.31293	-3.9827	-1.47086
H	4.8988	-3.27081	-0.19284
H	1.55792	-4.43248	-2.64093
C	3.89129	-3.09537	-0.56104
C	2.01568	-3.74705	-1.93198
C	3.17977	-1.97965	-0.11863
C	1.29875	-2.63427	-1.48958
H	3.62733	-1.28092	0.58305
H	3.22997	-0.63054	-2.74482
C	1.87863	-1.73477	-0.58381
H	0.29006	-2.44501	-1.84251
H	4.33566	0.78761	-4.43932
C	3.04702	0.43814	-2.74014
C	3.68157	1.26079	-3.71159
N	1.14854	-0.6085	-0.11331
C	2.2124	1.02968	-1.80942
C	1.38793	0.5742	-0.6792
C	3.50073	2.63107	-3.75738
Ni	-0.15284	-0.40024	1.4042
H	4.00969	3.22514	-4.51258
C	2.02322	2.44017	-1.87099
C	2.64774	3.2709	-2.81207
C	0.72637	1.70924	-0.11195
N	-0.02302	1.47963	0.97701
C	1.1348	2.90873	-0.85622

H	0.45472	2.59145	3.33468
C	2.36732	4.66494	-2.71693
H	2.82363	5.35734	-3.42008
C	-0.73772	2.56789	1.54879
C	-0.38281	3.05005	2.81638
C	0.89266	4.26988	-0.78642
C	1.52096	5.13129	-1.72817
H	0.23621	4.69496	-0.03603
C	-1.82138	3.15591	0.87817
C	-1.08975	4.10429	3.39601
H	-0.79845	4.46997	4.37725
H	-2.09816	2.77998	-0.10284
H	1.31989	6.19745	-1.66218
C	-2.52671	4.20921	1.46112
C	-2.16403	4.68897	2.72204
H	-3.36396	4.65399	0.92912
H	-2.71562	5.50758	3.17584
H	-2.76064	-3.2303	2.65557
H	-2.11807	-4.19563	-0.10727
C	-2.59037	-2.2681	2.17595
H	-1.08431	-1.65147	3.75633
C	-2.36945	-3.16387	-0.34063
C	-1.41458	-1.41942	2.75343
C	-2.57477	-2.22452	0.65421
O	-3.68465	-1.35643	2.44576
H	-2.39516	-3.47962	-2.47766
C	-2.52232	-2.75474	-1.67773
C	-1.75913	-0.08279	2.40968
C	-2.92215	-0.89781	0.34258
C	-3.12461	-0.23271	1.69655
C	-2.85442	-1.43567	-1.98791
H	-1.65558	0.70988	3.14384
C	-3.05552	-0.48511	-0.97214
H	-3.78839	0.62906	1.7401
H	-2.97775	-1.14278	-3.02714
C	0.44495	-2.32914	2.05817
C	0.49802	-3.24339	3.235
H	1.41826	-1.83838	1.98342
H	0.24417	-2.88586	1.14345
C	1.13218	-2.85414	4.42844
C	1.20731	-3.71551	5.52147
C	0.64931	-4.99431	5.44925
C	0.02048	-5.40008	4.27133
C	-0.05392	-4.53334	3.1804
H	-0.53238	-4.8668	2.26196
H	-0.40957	-6.39584	4.1983
H	1.57624	-1.86228	4.49273
H	1.7071	-3.39009	6.43035
H	0.70916	-5.66772	6.29986
H	-3.32883	0.53694	-1.22139

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.014331

A4'

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.608710
(Hartree/Particle)
Thermal correction to Energy= 0.643817
Thermal correction to Enthalpy= 0.644761
Thermal correction to Gibbs Free Energy= 0.538805
Sum of electronic and zero-point Energies= -3273.424436
Sum of electronic and thermal Energies= -3273.389329
Sum of electronic and thermal Enthalpies= -3273.388385
Sum of electronic and thermal Free Energies= -3273.494341

H	3.21655	-4.44117	-1.82233
C	2.69901	-3.49705	-1.67938
H	4.4581	-2.44589	-1.00191
H	0.77551	-4.26728	-2.28563
C	3.39607	-2.37529	-1.22072
C	1.32884	-3.39883	-1.93869
C	2.73366	-1.16294	-1.02567
C	0.66098	-2.19035	-1.74297
H	3.26634	-0.29505	-0.64882
H	3.2046	0.21391	-3.19577
C	1.36075	-1.05892	-1.29611
H	-0.40931	-2.10965	-1.91268
H	4.55714	1.6944	-4.63336
C	2.98353	1.27469	-3.21394
C	3.7604	2.13455	-4.04012
N	0.62556	0.11573	-1.01885
C	1.96617	1.81854	-2.44919
C	0.95408	1.31501	-1.5109
C	3.54353	3.49972	-4.10682
Ni	-0.74778	0.29486	0.35675
H	4.16592	4.12479	-4.74157
C	1.73518	3.22349	-2.54345
C	2.49699	4.09108	-3.34053
C	0.12262	2.42513	-1.10341
N	-0.86913	2.15923	-0.25649
C	0.63907	3.64672	-1.73861
H	-1.48597	2.86811	2.20027
C	2.14348	5.47095	-3.29699
H	2.70337	6.18822	-3.8913
C	-1.84827	3.10834	0.09755
C	-2.10341	3.35868	1.45505
C	0.32121	4.99245	-1.71462
C	1.09282	5.8932	-2.50047
H	-0.50247	5.37165	-1.12041
C	-2.63929	3.74145	-0.87686
C	-3.11944	4.23829	1.83012
H	-3.30014	4.42838	2.88466
H	-2.45213	3.53285	-1.92602
H	0.83672	6.94868	-2.47538
C	-3.65206	4.62028	-0.49466
C	-3.89772	4.87377	0.85894
H	-4.25751	5.10213	-1.25765
H	-4.69026	5.55607	1.15229
H	-1.7545	-2.96394	3.52405
H	-2.31433	-4.0357	0.75237
C	-1.73395	-2.03873	2.94818
H	0.08363	-1.32217	3.8106
C	-2.61387	-3.00199	0.60476
C	-0.33352	-1.36386	2.79617
C	-2.41874	-2.05061	1.58985
O	-2.46123	-0.98989	3.63067
H	-3.40049	-3.33479	-1.38057
C	-3.21649	-2.5978	-0.60399
C	-0.73869	0.07051	2.33111
C	-2.79102	-0.70401	1.3762
C	-2.26893	0.02577	2.6082
C	-3.58062	-1.26792	-0.81747
H	-0.23323	0.83738	2.92793
C	-3.35391	-0.28861	0.17142
H	-2.7642	0.95535	2.88396

H	-4.047	-0.98052	-1.75537
C	0.6596	-2.09128	1.88211
C	1.02066	-3.48739	2.33912
H	1.56293	-1.47352	1.80006
H	0.24664	-2.14575	0.87194
C	1.70469	-3.70046	3.54562
C	2.01909	-4.99109	3.97432
C	1.65431	-6.09724	3.20026
C	0.97752	-5.89928	1.99492
C	0.66523	-4.60483	1.57115
H	0.15233	-4.45471	0.62489
H	0.69415	-6.75095	1.38164
H	1.99714	-2.84559	4.15137
H	2.55171	-5.13437	4.91109
H	1.8993	-7.10237	3.53299
H	-3.63756	0.74744	0.00713

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0676034

UB3LYP/6-31G(d)
Zero-point correction= 0.607493 (Hartree/Particle)
Thermal correction to Energy= 0.643116
Thermal correction to Enthalpy= 0.644060
Thermal correction to Gibbs Free Energy= 0.534436
Sum of electronic and zero-point Energies= -3273.304282
Sum of electronic and thermal Energies= -3273.268659
Sum of electronic and thermal Enthalpies= -3273.267715
Sum of electronic and thermal Free Energies= -3273.377339

H	3.86679	-4.85193	-1.81484
C	3.31293	-3.9827	-1.47086
H	4.8988	-3.27081	-0.19284
H	1.55792	-4.43248	-2.64093
C	3.89129	-3.09537	-0.56104
C	2.01568	-3.74705	-1.93198
C	3.17977	-1.97965	-0.11863
C	1.29875	-2.63427	-1.48958
H	3.62733	-1.28092	0.58305
H	3.22997	-0.63054	-2.74482
C	1.87863	-1.73477	-0.58381
H	0.29006	-2.44501	-1.84251
H	4.33566	0.78761	-4.43932
C	3.04702	0.43814	-2.74014
C	3.68157	1.26079	-3.71159
N	1.14854	-0.6085	-0.11331
C	2.2124	1.02968	-1.80942
C	1.38793	0.5742	-0.6792
C	3.50073	2.63107	-3.75738
Ni	-0.15284	-0.40024	1.4042
H	4.00969	3.22514	-4.51258
C	2.02322	2.44017	-1.87099
C	2.64774	3.2709	-2.81207
C	0.72637	1.70924	-0.11195
N	-0.02302	1.47963	0.97701
C	1.1348	2.90873	-0.85622
H	0.45472	2.59145	3.33468
C	2.36732	4.66494	-2.71693
H	2.82363	5.35734	-3.42008
C	-0.73772	2.56789	1.54879
C	-0.38281	3.05005	2.81638
C	0.89266	4.26988	-0.78642
C	1.52096	5.13129	-1.72817
H	0.23621	4.69496	-0.03603
C	-1.82138	3.15591	0.87817
C	-1.08975	4.10429	3.39601
H	-0.79845	4.46997	4.37725
H	-2.09816	2.77998	-0.10284
H	1.31989	6.19745	-1.66218
C	-2.52671	4.20921	1.46112
C	-2.16403	4.68897	2.72204
H	-3.36396	4.65399	0.92912
H	-2.71562	5.50758	3.17584
H	-2.76064	-3.2303	2.65557
H	-2.11807	-4.19563	-0.10727
C	-2.59037	-2.2681	2.17595
H	-1.08431	-1.65147	3.75633
C	-2.36945	-3.16387	-0.34063
C	-1.41458	-1.41942	2.75343
C	-2.57477	-2.22452	0.65421
O	-3.68465	-1.35643	2.44576
H	-2.39516	-3.47962	-2.47766
C	-2.52232	-2.75474	-1.67773
C	-1.75913	-0.08279	2.40968
C	-2.92215	-0.89781	0.34258
C	-3.12461	-0.23271	1.69655
C	-2.85442	-1.43567	-1.98791
H	-1.65558	0.70988	3.14384
C	-3.05552	-0.48511	-0.97214
H	-3.78839	0.62906	1.7401
H	-2.97775	-1.14278	-3.02714
C	0.44495	-2.32914	2.05817
C	0.49802	-3.24339	3.235
H	1.41826	-1.83838	1.98342
H	0.24417	-2.88586	1.14345
C	1.13218	-2.85414	4.42844
C	1.20731	-3.71551	5.52147
C	0.64931	-4.99431	5.44925
C	0.02048	-5.40008	4.27133
C	-0.05392	-4.53334	3.1804
H	-0.53238	-4.8668	2.26196
H	-0.40957	-6.39584	4.1983
H	1.57624	-1.86228	4.49273
H	1.7071	-3.39009	6.43035
H	0.70916	-5.66772	6.29986
H	-3.32883	0.53694	-1.22139

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.014331

P2

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.609308 (Hartree/Particle)
Thermal correction to Energy= 0.644522
Thermal correction to Enthalpy= 0.645466
Thermal correction to Gibbs Free Energy= 0.539010
Sum of electronic and zero-point Energies= -3273.469460
Sum of electronic and thermal Energies= -3273.434246
Sum of electronic and thermal Enthalpies= -3273.433302
Sum of electronic and thermal Free Energies= -3273.539758

H	6.13291	1.17661	1.8021
C	5.12222	0.79964	1.67384
H	5.57288	-1.1562	2.46996

H	4.36598	2.63595	0.8275
C	4.80686	-0.50941	2.05071
C	4.13016	1.61785	1.12543
C	3.51023	-0.99583	1.88385
C	2.83243	1.13558	0.95783
H	3.25885	-2.01391	2.16707
H	2.44628	-0.26322	4.26597
C	2.50887	-0.17129	1.34729
H	2.05688	1.76708	0.53903
H	1.99068	-0.64078	6.66769
C	1.53089	-0.76449	4.55973
C	1.26358	-0.98905	5.93945
N	1.1951	-0.6559	1.15298
C	0.61307	-1.20453	3.62342
C	0.48365	-1.16767	2.16161
C	0.1226	-1.63718	6.38106
Ni	0.3755	-1.04943	-0.54214
H	-0.04061	-1.79684	7.44357
C	-0.56739	-1.85727	4.08831
C	-0.84465	-2.09925	5.44123
C	-0.75779	-1.78517	1.79832
N	-1.00472	-1.88015	0.4861
C	-1.43361	-2.23595	3.01911
H	-1.32977	-4.09232	-0.92526
C	-2.06303	-2.78172	5.72904
H	-2.32855	-2.99709	6.76062
C	-2.24336	-2.39838	0.02933
C	-2.26355	-3.57075	-0.73722
C	-2.60566	-2.90157	3.33008
C	-2.90105	-3.16745	4.69688
H	-3.30259	-3.2172	2.5619
C	-3.44415	-1.71772	0.28381
C	-3.47269	-4.06534	-1.22998
H	-3.47886	-4.97897	-1.81783
H	-3.41534	-0.80006	0.86409
H	-3.82474	-3.68925	4.93112
C	-4.64967	-2.21724	-0.20837
C	-4.66838	-3.39262	-0.96641
H	-5.5745	-1.68431	-0.00556
H	-5.6079	-3.77771	-1.3521
H	2.04625	-1.81159	-3.18534
C	1.4065	-1.00833	-2.79465
C	0.00396	-1.50961	-2.47498
O	1.84282	-0.58351	-1.50397
C	-0.90131	-0.52312	-2.14486
C	-0.71415	0.93527	-2.53939
H	-1.67861	1.25482	-2.95625
C	-0.45711	1.8327	-1.28569
C	-0.50051	3.31378	-1.5662
C	0.6819	4.05739	-1.67276
C	0.6459	5.42218	-1.96843
C	-0.5789	6.06344	-2.16711
C	-1.76622	5.33205	-2.06259
C	-1.7243	3.96964	-1.76218
H	1.63827	3.55958	-1.53049
H	-0.60967	7.1246	-2.39906
H	1.57395	5.9825	-2.04632
H	-2.65077	3.40492	-1.67987
H	-2.724	5.82394	-2.21113
H	0.51684	1.54883	-0.88417
H	-1.20988	1.56769	-0.53214
C	0.34558	1.10782	-3.61401
C	1.36815	0.15334	-3.75914
C	2.335	0.31326	-4.7552
C	2.29835	1.41435	-5.61312
C	1.27832	2.35887	-5.47828
C	0.30633	2.20064	-4.48754
H	3.11863	-0.43412	-4.85983
H	3.05435	1.5301	-6.38513
H	1.23319	3.21463	-6.14661
H	-0.4911	2.93217	-4.39195
H	-1.91663	-0.79839	-1.87529
H	-0.26819	-2.55928	-2.54153

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.1052974

UB3LYP/6-31G(d)
Zero-point correction= 0.608195 (Hartree/Particle)
Thermal correction to Energy= 0.643588
Thermal correction to Enthalpy= 0.644532
Thermal correction to Gibbs Free Energy= 0.537257
Sum of electronic and zero-point Energies= -3273.353618
Sum of electronic and thermal Energies= -3273.318225
Sum of electronic and thermal Enthalpies= -3273.317281
Sum of electronic and thermal Free Energies= -3273.424556

H	6.28013	0.8745	1.91234
C	5.25124	0.55425	1.77256
H	5.61024	-1.46105	2.45676
H	4.58478	2.46342	1.02275
C	4.87416	-0.75494	2.08089
C	4.29914	1.44497	1.27255
C	3.55514	-1.16746	1.89851
C	2.97986	1.03637	1.08556
H	3.26009	-2.18855	2.12274
H	2.51492	-0.40709	4.33131
C	2.59213	-0.26957	1.41193
H	2.23686	1.72403	0.69627
H	2.0558	-0.83955	6.72076
C	1.58677	-0.89185	4.61251
C	1.31735	-1.14762	5.98535
N	1.25194	-0.68168	1.20959
C	0.6555	-1.27898	3.6664
C	0.52272	-1.19439	2.20438
C	0.16143	-1.77573	6.412
Ni	0.402	-0.96067	-0.49549
H	-0.00224	-1.96012	7.4709
C	-0.54061	-1.91065	4.11695
C	-0.82057	-2.18336	5.46357
C	-0.74059	-1.75875	1.83035
N	-1.00871	-1.78866	0.51657
C	-1.42134	-2.23161	3.04085
H	-1.39297	-4.07663	-0.76742
C	-2.05645	-2.8382	5.73674
H	-2.32559	-3.07659	6.76277
C	-2.25658	-2.29265	0.06271
C	-2.30972	-3.51018	-0.63077
C	-2.61069	-2.87234	3.34007
C	-2.90812	-3.16942	4.69872
H	-3.32034	-3.14861	2.56822
C	-3.44295	-1.56617	0.25599
C	-3.52637	-3.99571	-1.11324
H	-3.55313	-4.94419	-1.64312
H	-3.39836	-0.6183	0.78512
H	-3.84553	-3.67197	4.92208
C	-4.65641	-2.05595	-0.22675
C	-4.70322	-3.2722	-0.91347

H	-5.5669	-1.48342	-0.06976
H	-5.64888	-3.65043	-1.29144
H	2.18087	-1.73214	-3.05264
C	1.50671	-0.932	-2.71408
C	0.10345	-1.44797	-2.42507
O	1.8721	-0.46593	-1.42053
C	-0.81799	-0.46086	-2.13605
C	-0.65046	0.98534	-2.59386
H	-1.60936	1.24857	-3.06376
C	-0.47755	1.95949	-1.38083
C	-0.64623	3.42661	-1.70724
C	0.46436	4.26805	-1.85342
C	0.30436	5.62143	-2.1566
C	-0.97357	6.15737	-2.32077
C	-2.09035	5.33101	-2.17619
C	-1.92476	3.98029	-1.86972
H	1.46282	3.85556	-1.73245
H	-1.09977	7.21109	-2.55516
H	1.17985	6.25666	-2.26424
H	-2.80086	3.34567	-1.74773
H	-3.09054	5.74019	-2.29467
H	0.50955	1.77284	-0.9506
H	-1.21962	1.67373	-0.6232
C	0.43443	1.12938	-3.65142
C	1.47741	0.18918	-3.72597
C	2.45687	0.31172	-4.71377
C	2.41323	1.35891	-5.63449
C	1.37291	2.28642	-5.57185
C	0.38823	2.16706	-4.58917
H	3.25749	-0.42351	-4.75986
H	3.18012	1.44527	-6.39988
H	1.32066	3.09972	-6.29105
H	-0.42602	2.88556	-4.55519
H	-1.83708	-0.74522	-1.8897
H	-0.1572	-2.50177	-2.47418

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.1046374

$TS_{4\text{-}P2}$

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -256.89 cm^{-1}
Zero-point correction= 0.604955
(Hartree/Particle)
Thermal correction to Energy= 0.640221
Thermal correction to Enthalpy= 0.641165
Thermal correction to Gibbs Free Energy= 0.536878
Sum of electronic and zero-point Energies= -3273.388615
Sum of electronic and thermal Energies= -3273.353349
Sum of electronic and thermal Enthalpies= -3273.352404
Sum of electronic and thermal Free Energies= -3273.456692

H	6.70404	-0.06993	2.40843
C	5.64161	-0.15094	2.19652
H	5.65171	-2.30895	2.12572
H	5.31312	1.98248	2.18872
C	5.05031	-1.40794	2.03929
C	4.85936	1.0019	2.07231
C	3.68573	-1.51235	1.76744
C	3.49644	0.9013	1.79616
H	3.21586	-2.48373	1.64153
H	2.82847	-1.42968	4.31893
C	2.89834	-0.35702	1.65477
H	2.88001	1.78837	1.68979
H	2.29481	-2.45153	6.50575
C	1.81972	-1.77907	4.5074
C	1.50578	-2.37247	5.76306
N	1.51391	-0.44637	1.376
C	0.82503	-1.67488	3.55262
C	0.70532	-1.13047	2.19114
C	0.24405	-2.85531	6.06417
Ni	0.69532	-0.1743	-0.35861
H	0.04726	-3.31028	7.03135
C	-0.47648	-2.15664	3.87918
C	-0.80484	-2.75642	5.10345
C	-0.64089	-1.30686	1.74548
N	-0.9265	-0.9251	0.4898
C	-1.40724	-1.95495	2.81766
H	-2.28098	-2.05063	-1.54384
C	-2.15148	-3.19963	5.25373
H	-2.46223	-3.67286	6.1814
C	-2.28988	-0.72251	0.15258
C	-2.86937	-1.35629	-0.95566
C	-2.70513	-2.401	2.9914
C	-3.05677	-3.02624	4.22047
H	-3.45742	-2.27576	2.22068
C	-3.07844	0.15469	0.92008
C	-4.2057	-1.12115	-1.28586
H	-4.63869	-1.62323	-2.14642
H	-2.62722	0.65488	1.77199
H	-4.07906	-3.37126	4.34818
C	-4.41419	0.3801	0.59341
C	-4.98464	-0.25524	-0.5144
H	-5.00636	1.06277	1.19638
H	-6.02319	-0.07408	-0.77508
H	3.66483	-0.47683	-2.32268
C	2.59313	-0.25707	-2.21918
C	1.75692	-1.52754	-2.14709
O	2.33878	0.44311	-1.01492
C	0.41255	-1.32078	-2.15003
C	-0.11168	0.04631	-2.41517
H	-1.18631	0.07285	-2.54805
C	-0.32826	1.78555	-0.9802
C	-1.20614	2.5849	-1.84403
C	-0.68761	3.69382	-2.53955
C	-1.50752	4.48612	-3.3428
C	-2.86052	4.17198	-3.48852
C	-3.3896	3.06663	-2.81122
C	-2.57522	2.28798	-1.9935
H	0.36825	3.9314	-2.44472
H	-3.49883	4.78179	-4.12198
H	-1.08592	5.34034	-3.86563
H	-2.99533	1.4372	-1.47087
H	-4.44158	2.81443	-2.9161
H	0.66838	2.20816	-0.87989
H	-0.80688	1.55632	-0.02987
C	0.69446	0.75133	-3.43988
C	2.09252	0.56621	-3.39149
C	2.90869	1.16142	-4.34765
C	2.34331	1.93308	-5.372
C	0.95945	2.10041	-5.43501
C	0.13425	1.51179	-4.46974
H	3.98593	1.01754	-4.30032
H	2.98279	2.39153	-6.12176
H	0.51604	2.68833	-6.23405
H	-0.94268	1.63526	-4.52515
H	-0.28506	-2.13545	-1.99613
H	2.19936	-2.50955	-2.01787

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0151507

UB3LYP/6-31G(d)
Imaginary frequency = -253.14 cm^{-1}
Zero-point correction= 0.603745 (Hartree/Particle)
Thermal correction to Energy= 0.639305
Thermal correction to Enthalpy= 0.640249
Thermal correction to Gibbs Free Energy= 0.534502
Sum of electronic and zero-point Energies= -3273.265741
Sum of electronic and thermal Energies= -3273.230181
Sum of electronic and thermal Enthalpies= -3273.229237
Sum of electronic and thermal Free Energies= -3273.334984

H	6.66949	0.02487	2.3755
C	5.60865	-0.07797	2.16364
H	5.64117	-2.23562	2.19859
H	5.25858	2.04711	2.03962
C	5.03086	-1.34569	2.06658
C	4.81545	1.05675	1.97541
C	3.66927	-1.47799	1.79437
C	3.45663	0.92909	1.69636
H	3.21606	-2.46186	1.7108
H	2.7821	-1.3069	4.33094
C	2.86778	-0.33972	1.61941
H	2.83718	1.80506	1.53557
H	2.26256	-2.30399	6.52916
C	1.78335	-1.68548	4.51529
C	1.4781	-2.26521	5.778
N	1.48304	-0.45742	1.34045
C	0.79565	-1.63042	3.54919
C	0.67359	-1.11689	2.17251
C	0.23226	-2.78558	6.07531
Ni	0.65794	-0.19991	-0.40498
H	0.04296	-3.2316	7.04866
C	-0.49218	-2.14441	3.87429
C	-0.80987	-2.73763	5.10505
C	-0.67065	-1.32091	1.72843
N	-0.97098	-0.94749	0.46928
C	-1.42086	-1.98633	2.80353
H	-2.30272	-2.14351	-1.54195
C	-2.13948	-3.22797	5.25146
H	-2.44146	-3.70005	6.1831
C	-2.34257	-0.79548	0.13846
C	-2.91152	-1.46251	-0.95811
C	-2.70174	-2.48191	2.97598
C	-3.0397	-3.10423	4.20892
H	-3.45418	-2.40101	2.19972
C	-3.16763	0.05152	0.90394
C	-4.2597	-1.29085	-1.2766
H	-4.67905	-1.82403	-2.12578
H	-2.7363	0.57876	1.74995
H	-4.0493	-3.48754	4.33179
C	-4.51514	0.21454	0.58829
C	-5.06953	-0.45433	-0.50661
H	-5.13116	0.8737	1.1945
H	-6.11908	-0.32527	-0.75546
H	3.65844	-0.55373	-2.30258
C	2.58788	-0.31641	-2.23445
H	-0.4793	5.10769	4.7923
C	-0.44775	3.4493	3.40603
C	1.7224	-1.56798	-2.19556
O	2.30994	0.37996	-1.03825
C	0.38362	-1.32632	-2.21787
C	-0.09817	0.05583	-2.47788
H	-1.17056	0.12432	-2.62441
C	-0.25529	1.80504	-1.00361
C	-1.15166	2.64434	-1.8115
C	-0.62458	3.7347	-2.53205
C	-1.45583	4.59616	-3.24638
C	-2.83344	4.37484	-3.27945
C	-3.37301	3.29009	-2.58071
C	-2.54586	2.44058	-1.8513
H	0.44715	3.91002	-2.51465
H	-3.48254	5.04229	-3.84012
H	-1.02481	5.43742	-3.7829
H	-2.97967	1.6127	-1.3006
H	-4.4451	3.11111	-2.59611
H	0.7659	2.17429	-0.96557
H	-0.68208	1.59738	-0.02266
C	0.74404	0.74627	-3.48515
C	2.13511	0.51945	-3.41683
C	2.98165	1.08023	-4.36669
C	2.45535	1.85667	-5.40608
C	1.07948	2.06619	-5.48983
C	0.22335	1.51552	-4.52985
H	4.05355	0.90611	-4.30143
H	3.11893	2.28611	-6.15237
H	0.6654	2.6554	-6.3038
H	-0.84865	1.66802	-4.60866
H	-0.33699	-2.12587	-2.09132
H	2.13819	-2.56442	-2.08194

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0145397

TS_{B1}

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -354.17 cm^{-1}
Zero-point correction= 0.605670 (Hartree/Particle)
Thermal correction to Energy= 0.640624
Thermal correction to Enthalpy= 0.641568
Thermal correction to Gibbs Free Energy= 0.536032
Sum of electronic and zero-point Energies= -3273.374681
Sum of electronic and thermal Energies= -3273.339727
Sum of electronic and thermal Enthalpies= -3273.338783
Sum of electronic and thermal Free Energies= -3273.444319

H	4.97953	1.32262	3.36065
C	3.97971	1.24854	2.94307
H	3.0447	0.77797	4.83136
H	4.60808	1.67693	0.92329
C	2.89169	0.94559	3.76866
C	3.77015	1.44652	1.57552
C	1.60706	0.84253	3.23575
C	2.48819	1.34085	1.03558
H	0.7623	0.59205	3.87055
H	0.62251	3.30765	3.505
C	1.39115	1.04607	1.8615
H	2.32132	1.48324	-0.02703

C	-1.0894	4.48087	4.14782
N	0.1238	0.85173	1.2793
C	-1.21376	2.64437	2.58266
C	-0.96623	1.51231	1.67474
C	-2.45413	4.70234	4.08396
Ni	-0.35055	-0.46658	-0.1108
H	-2.90965	5.49292	4.67458
C	-2.61361	2.89554	2.50459
C	-3.26982	3.89243	3.24084
C	-2.21316	1.14307	1.05897
N	-2.17314	0.10031	0.21352
C	-3.26946	2.01227	1.59548
H	-2.94464	-2.33734	-0.28944
C	-4.68189	3.9899	3.06751
H	-5.24137	4.74512	3.61313
C	-3.2291	-0.24059	-0.65495
C	-3.51301	-1.60211	-0.85278
C	-4.64198	2.1264	1.45856
C	-5.3311	3.12201	2.20743
H	-5.20269	1.48137	0.79157
C	-3.9357	0.71864	-1.40174
C	-4.50284	-1.99498	-1.7519
H	-4.7157	-3.05194	-1.88734
H	-3.69436	1.76982	-1.27886
H	-6.40811	3.20099	2.08717
C	-4.9243	0.31951	-2.30086
C	-5.21698	-1.03649	-2.47762
H	-5.4613	1.0715	-2.87292
H	-5.98656	-1.34282	-3.18028
H	1.18038	-3.26146	-2.09888
H	3.45109	-2.95042	-4.00557
C	1.02985	-2.22289	-2.37905
H	2.33019	-0.9668	-0.99928
C	2.82059	-2.13886	-4.35932

C	1.30829	-1.13671	-1.31924
C	1.68253	-1.75722	-3.67196
O	-0.36888	-1.96114	-2.66472
H	4.01447	-1.73329	-6.11462
C	3.13663	-1.44526	-5.5427
C	0.50393	-0.00816	-1.7976
C	0.87235	-0.69914	-4.12216
C	-0.19909	-0.56383	-3.04777
C	2.33333	-0.3948	-5.99175
H	0.95795	0.97837	-1.85518
C	1.18804	-0.00048	-5.27492
H	-1.15915	-0.12894	-3.3251
H	2.594	0.12444	-6.91019
C	0.85008	-2.27246	0.4006
C	2.19387	-2.85475	0.60762
H	0.12005	-3.0027	0.04382
H	0.50824	-1.8197	1.33823
C	2.55421	-4.09492	0.04924
C	3.8371	-4.61834	0.21951
C	4.79318	-3.91372	0.95506
C	4.44617	-2.68644	1.52976
C	3.16479	-2.16624	1.36101
H	2.90629	-1.21784	1.81834
H	5.17463	-2.13092	2.11504
H	1.81433	-4.66724	-0.50497
H	4.08681	-5.58094	-0.21921
H	5.79256	-4.31921	1.08694
H	0.5726	0.82387	-5.62548

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0126516

UB3LYP/6-31G(d)
Imaginary frequency = -341.62 cm^{-1}
Zero-point correction= 0.604598 (Hartree/Particle)
Thermal correction to Energy= 0.639962
Thermal correction to Enthalpy= 0.640906
Thermal correction to Gibbs Free Energy= 0.533187
Sum of electronic and zero-point Energies= -3273.261867
Sum of electronic and thermal Energies= -3273.226503
Sum of electronic and thermal Enthalpies= -3273.225559
Sum of electronic and thermal Free Energies= -3273.333278

H	1.03275	1.39179	7.04568
C	0.06739	1.2716	6.56214
H	-0.93017	0.58412	8.34783
H	0.76848	1.90995	4.62418
C	-1.03613	0.82265	7.29261
C	-0.08168	1.55889	5.20339
C	-2.27628	0.66565	6.67549
C	-1.31921	1.40119	4.57891
H	-3.13088	0.30468	7.24046
H	-3.34958	3.155	6.95624
C	-2.43553	0.96168	5.30944
H	-1.44018	1.63119	3.5247
H	-4.57872	4.83252	8.28696
C	-4.4253	3.2308	6.84472
C	-5.13959	4.19241	7.61105

N	-3.66273	0.73738	4.64911
C	-5.12669	2.40895	5.98112
C	-4.79582	1.32681	5.03757
C	-6.51307	4.33167	7.53277
Ni	-4.03777	-0.55503	3.18558
H	-7.02369	5.07183	8.14403
C	-6.53776	2.57755	5.88837
C	-7.26467	3.50572	6.64852
C	-6.00938	0.90928	4.38482
N	-5.90318	-0.08957	3.49665
C	-7.12546	1.69185	4.938
H	-6.81539	-2.53672	3.15259
C	-8.67621	3.5233	6.45449
H	-9.29029	4.22191	7.01737
C	-6.97544	-0.4543	2.64717
C	-7.33567	-1.80582	2.5405
C	-8.49994	1.72843	4.78161
C	-9.25856	2.65121	5.55383
H	-9.01107	1.07614	4.08271
C	-7.6368	0.49062	1.84325
C	-8.35134	-2.20059	1.67151
H	-8.62207	-3.25105	1.60655
H	-7.34355	1.53463	1.90325
H	-10.33691	2.66928	5.41918
C	-8.64921	0.08907	0.97264
C	-9.01477	-1.25652	0.88513
H	-9.14915	0.83076	0.35475
H	-9.80233	-1.56669	0.20408
H	-2.8175	-3.46116	1.29909
H	-0.68733	-3.50171	-0.79606
C	-2.87335	-2.4247	0.9748
H	-1.36364	-1.27167	2.2327
C	-1.24858	-2.636	-1.13891
C	-2.41236	-1.33583	1.9642
C	-2.2733	-2.09274	-0.38457
O	-4.25174	-2.01769	0.78005
H	-0.16678	-2.45406	-2.99968
C	-0.95475	-2.03849	-2.37727
C	-3.13017	-0.15036	1.50059
C	-2.99179	-0.96867	-0.82685
C	-3.95884	-0.66783	0.31071
C	-1.66653	-0.92252	-2.81799
H	-2.60536	0.79812	1.42333
C	-2.69505	-0.3662	-2.03759
H	-4.8862	-0.14783	0.07163
H	-1.42633	-0.4793	-3.78096
C	-2.87056	-2.37567	3.775
C	-1.58863	-3.10484	3.90442
H	-3.69981	-3.04708	3.53776
H	-3.07369	-1.83082	4.7018
C	-1.45969	-4.43726	3.47123
C	-0.25115	-5.12401	3.58855
C	0.86422	-4.49342	4.14147
C	0.75403	-3.17123	4.58105
C	-0.45318	-2.48624	4.46461
H	-0.52496	-1.45988	4.81571
H	1.61299	-2.67089	5.0212
H	-2.32796	-4.95008	3.06269
H	-0.18446	-6.1561	3.25343
H	1.80634	-5.0267	4.23533
H	-3.24135	0.50615	-2.3879

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0115119

B2

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.609139
(Hartree/Particle)
Thermal correction to Energy= 0.643758
Thermal correction to Enthalpy= 0.644702
Thermal correction to Gibbs Free Energy= 0.540348
Sum of electronic and zero-point Energies= -3273.423163
Sum of electronic and thermal Energies= -3273.388544
Sum of electronic and thermal Enthalpies= -3273.387600
Sum of electronic and thermal Free Energies= -3273.491954

H	3.13997	3.33733	-4.38220
C	2.58118	2.96499	-3.52819
H	0.67415	3.67750	-4.25072
H	4.30624	2.10179	-2.55818
C	1.19684	3.15469	-3.45408
C	3.23535	2.27893	-2.50147
C	0.47939	2.67096	-2.36181
C	2.52089	1.79501	-1.40497
H	-0.59830	2.79461	-2.30057
H	3.00236	3.51096	0.42140
C	1.13741	2.00172	-1.31774
H	3.02045	1.23116	-0.62714
H	4.28770	4.58385	2.23248
C	2.72441	3.31408	1.45004
C	3.46040	3.93213	2.49995
N	0.36661	1.48788	-0.25257
C	1.66978	2.47733	1.77109
C	0.66636	1.68855	1.03867
C	3.15925	3.73524	3.83583
Ni	-1.06321	0.32039	-0.45140
H	3.74310	4.22724	4.60938
C	1.36491	2.28527	3.15219
C	2.06969	2.89190	4.20191
C	-0.21276	1.07067	1.99110
N	-1.26969	0.41810	1.47714
C	0.23098	1.43923	3.34056
H	-3.84635	0.07077	1.18961
C	1.60877	2.61990	5.52388
H	2.12298	3.05953	6.37450
C	-2.03735	-0.50342	2.19741
C	-3.41349	-0.60729	1.91754
C	-0.20146	1.20906	4.63510
C	0.50496	1.80779	5.71588
H	-1.06116	0.58171	4.84265
C	-1.46659	-1.40819	3.11618
C	-4.19664	-1.56525	2.55725
H	-5.25844	-1.62439	2.33226
H	-0.39935	-1.36243	3.30938
H	0.15777	1.61459	6.72730
C	-2.25749	-2.36233	3.75396
C	-3.62698	-2.44664	3.48293
H	-1.79787	-3.05228	4.45706
H	-4.23974	-3.19394	3.97885
H	-2.42633	-2.73316	-0.50510
H	-3.62657	-4.43330	-2.63806
C	-2.23317	-2.10926	-1.37643
H	-0.51116	-2.55589	-2.64978
C	-3.61243	-3.48875	-3.17463
C	-0.73149	-1.91536	-1.78640
C	-3.01986	-2.35915	-2.63217
O	-2.63676	-0.70725	-1.06162
H	-4.67974	-4.23985	-4.89262

C	-4.19639	-3.37516	-4.44651
C	-0.77553	-0.41229	-2.17936
C	-2.99583	-1.14175	-3.32757
C	-2.26615	-0.16880	-2.44048
C	-4.16744	-2.16356	-5.14482
H	-0.05364	-0.05628	-2.91135
C	-3.55949	-1.02647	-4.58983
H	-2.57474	0.87330	-2.53116
H	-4.63055	-2.09883	-6.12551
H	-3.54161	-0.08492	-5.13205
H	4.28318	-1.73680	-2.87579
C	3.73336	-1.65185	-1.94199
H	1.88836	-2.33706	-2.80928
H	5.43869	-0.95632	-0.81423
C	2.37821	-1.98747	-1.90404
C	4.38319	-1.21323	-0.78541
C	1.64520	-1.88394	-0.71382
C	3.66077	-1.09465	0.40484
C	2.30307	-1.41932	0.43376
C	0.20016	-2.32466	-0.62341
H	4.14908	-0.73729	1.30789
H	1.74156	-1.30698	1.35827
H	-0.21820	-1.95985	0.32177
H	0.16739	-3.42261	-0.55549

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0688815

UB3LYP/6-31G(d)
Zero-point correction= 0.608399 (Hartree/Particle)
Thermal correction to Energy= 0.643348
Thermal correction to Enthalpy= 0.644293
Thermal correction to Gibbs Free Energy= 0.536780
Sum of electronic and zero-point Energies= -3273.308662
Sum of electronic and thermal Energies= -3273.273713
Sum of electronic and thermal Enthalpies= -3273.272769
Sum of electronic and thermal Free Energies= -3273.380282

H	4.16493	3.33631	-3.23035
C	3.43184	2.95196	-2.52667
H	1.73171	3.64982	-3.657
H	4.90418	2.1294	-1.18033
C	2.06607	3.12423	-2.76625
C	3.8451	2.27821	-1.37506
C	1.12365	2.63143	-1.86517
C	2.90479	1.77991	-0.47225
H	0.06179	2.77448	-2.04075
H	2.69377	3.943	1.03264
C	1.5302	1.95846	-0.70245
H	3.22564	1.24386	0.4161
H	3.41316	5.43175	2.85843
C	2.24691	3.82292	2.01261
C	2.65629	4.68092	3.07022
N	0.56547	1.44864	0.19813
C	1.28631	2.85764	2.2626
C	0.57575	1.82864	1.48981
C	2.12718	4.59656	4.34438
Ni	-0.7801	0.18316	-0.12946
H	2.46419	5.27452	5.1247
C	0.7421	2.78363	3.58043
C	1.12479	3.62632	4.63431
C	-0.37618	1.18826	2.35028
N	-1.19808	0.31163	1.76286
C	-0.27077	1.78666	3.69008
H	-3.77684	-0.07916	1.32509
C	0.45235	3.44023	5.87658
H	0.71237	4.06318	6.72894
C	-2.03965	-0.54142	2.50387
C	-3.39238	-0.67289	2.14691
C	-0.91494	1.64214	4.90597
C	-0.53469	2.47908	5.99092
H	-1.69912	0.90766	5.05107
C	-1.5426	-1.32474	3.56283
C	-4.22687	-1.5431	2.84592
H	-5.27299	-1.62282	2.56126
H	-0.49151	-1.24898	3.82604
H	-1.04592	2.35344	6.94183
C	-2.38306	-2.19302	4.25732
C	-3.73063	-2.30585	3.90578
H	-1.97976	-2.79084	5.07099
H	-4.38396	-2.98448	4.44719
H	-1.75825	-2.96575	-0.51388
H	-3.17554	-4.47466	-2.67525
C	-1.76966	-2.20958	-1.29834
H	-0.34041	-2.24829	-2.93033
C	-3.32032	-3.46742	-3.05724
C	-0.38866	-1.79933	-1.92928
C	-2.73408	-2.37025	-2.44644
O	-2.26108	-0.92681	-0.7187
H	-4.59666	-4.08239	-4.68362
C	-4.11417	-3.24203	-4.19203
C	-0.61205	-0.266	-1.99737
C	-2.92099	-1.07232	-2.94509
C	-2.14619	-0.15879	-2.02749
C	-4.29491	-1.95166	-4.69537
H	-0.04519	0.28721	-2.74488
C	-3.6941	-0.84672	-4.07414
H	-2.56099	0.84245	-1.9029
H	-4.91766	-1.80033	-5.57286
H	-3.84328	0.15602	-4.4668
H	3.73317	-4.91176	-3.78683
C	3.49168	-3.91826	-3.41716
H	1.80628	-4.60366	-2.26747
H	5.1178	-2.95506	-4.45923
C	2.40434	-3.74258	-2.55976
C	4.2687	-2.82182	-3.79383
C	2.07198	-2.47507	-2.06214
C	3.94895	-1.55374	-3.3048
C	2.86171	-1.38299	-2.4471
C	0.86562	-2.29644	-1.16136
H	4.54839	-0.69168	-3.58648
H	2.62918	-0.39255	-2.06791
H	1.09955	-1.59583	-0.35174
H	0.63644	-3.26267	-0.69255

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = - 3273.0639423

TS_{B2}

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Imaginary frequency = -439.95 cm^{-1}
Zero-point correction= 0.606993 (Hartree/Particle)
Thermal correction to Energy= 0.641736
Thermal correction to Enthalpy= 0.642680
Thermal correction to Gibbs Free Energy= 0.535817
Sum of electronic and zero-point Energies= -3273.412504

Sum of electronic and thermal Energies= -3273.377762
Sum of electronic and thermal Enthalpies= -3273.376817
Sum of electronic and thermal Free Energies= -3273.483681

H	3.39336	4.50976	-3.36554
C	2.75908	3.98781	-2.65479
H	0.92279	4.81079	-3.43576
H	4.40092	2.99524	-1.66469
C	1.37163	4.15467	-2.69487
C	3.32427	3.13902	-1.69811
C	0.55466	3.48278	-1.78466
C	2.51081	2.46399	-0.78766
H	-0.52479	3.60292	-1.80869
H	2.26597	4.46371	1.03787
C	1.11856	2.63852	-0.81817
H	2.93984	1.79453	-0.04792
H	3.04459	5.77701	2.98267
C	1.93536	4.1842	2.03174
C	2.37906	4.93579	3.15619
N	0.2842	1.93009	0.07926
C	1.09025	3.1086	2.23971
C	0.39569	2.12523	1.40125
C	1.99288	4.6361	4.45103
Ni	-0.82914	0.47029	-0.31081
H	2.35069	5.2368	5.28316
C	0.69732	2.80674	3.57757
C	1.11354	3.54063	4.69743
C	-0.38037	1.26413	2.24409
N	-1.13921	0.3625	1.6055
C	-0.19995	1.69777	3.63779
H	-3.58983	-0.41823	1.11162
C	0.5967	3.12592	5.96015
H	0.88869	3.65626	6.86278
C	-1.80236	-0.68072	2.26983
C	-3.11586	-1.00667	1.88999
C	-0.69411	1.33025	4.87714
C	-0.281	2.05829	6.02868
H	-1.38371	0.50156	4.99083
C	-1.16775	-1.46284	3.25308
C	-3.78892	-2.06084	2.5044
H	-4.80832	-2.29167	2.20601
H	-0.1415	-1.23701	3.52683
H	-0.67462	1.7566	6.99554
C	-1.84636	-2.51638	3.86467
C	-3.16135	-2.81954	3.49802
H	-1.34182	-3.10833	4.62398
H	-3.68737	-3.64197	3.97454
H	-0.75895	-2.80863	-1.13959
H	-2.06075	-4.2926	-3.22284
C	-1.09452	-1.93276	-1.69801
H	0.20145	-1.38878	-3.3707
C	-2.49583	-3.32597	-3.46154
C	0.05335	-1.07363	-2.32776
C	-2.10045	-2.18115	-2.79099
O	-1.82203	-1.02631	-0.80877
H	-3.81792	-4.0946	-4.98541
C	-3.48366	-3.20785	-4.45404
C	-0.58738	0.30949	-2.22104
C	-2.66516	-0.9323	-3.09494
C	-2.04263	0.14577	-2.28443
C	-4.0505	-1.9667	-4.75592
H	-0.14847	1.15659	-2.74399
C	-3.64557	-0.80968	-4.07314
H	-2.66433	1.02238	-2.09939
H	-4.82012	-1.89728	-5.51944
H	-4.08422	0.15646	-4.30804
H	2.4516	-5.53949	-0.1841
C	2.51567	-4.80199	-0.97993
H	1.49642	-3.27875	0.15471
H	3.56137	-6.11539	-2.33693
C	1.97557	-3.52708	-0.79006
C	3.13875	-5.12554	-2.18717
C	2.04674	-2.55673	-1.79915
C	3.21854	-4.16586	-3.20111
C	2.67645	-2.89466	-3.00637
C	1.41732	-1.19597	-1.61228
H	3.7057	-4.4074	-4.14229
H	2.74287	-2.1511	-3.79788
H	2.07402	-0.40955	-2.00497
H	1.29423	-0.9873	-0.5441

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3273.0511328

UB3LYP/6-31G(d)
Imaginary frequency = -437.63 cm^{-1}
Zero-point correction= 0.606545 (Hartree/Particle)
Thermal correction to Energy= 0.641264
Thermal correction to Enthalpy= 0.642208
Thermal correction to Gibbs Free Energy= 0.536483
Sum of electronic and zero-point Energies= -3273.300744
Sum of electronic and thermal Energies= -3273.266026
Sum of electronic and thermal Enthalpies= -3273.265082
Sum of electronic and thermal Free Energies= -3273.370807

H	3.97568	3.34572	-3.70163
C	3.27011	2.96135	-2.97054
H	1.52696	3.47303	-4.13349
H	4.7945	2.33372	-1.57826
C	1.89649	3.02802	-3.21323
C	3.72763	2.39376	-1.77888
C	0.98973	2.53451	-2.27583
C	2.82379	1.89487	-0.84061
H	-0.07965	2.605	-2.45317
H	2.48651	4.1062	0.5521
C	1.43954	1.96419	-1.07485
H	3.17995	1.44809	0.08317
H	3.11065	5.73191	2.29317
C	2.04359	4.01359	1.53676
C	2.39801	4.95099	2.54571
N	0.508	1.44535	-0.14517
C	1.13978	3.00864	1.83819
C	0.49485	1.89752	1.12372
C	1.87019	4.90621	3.82239
Ni	-0.75517	0.05372	-0.39206
H	2.16463	5.6442	4.56452
C	0.59512	2.977	3.15801
C	0.92458	3.89662	4.16436
C	-0.42387	1.25473	2.01714
N	-1.19196	0.30183	1.48189
C	-0.35891	1.93146	3.32214
H	-3.76387	-0.18703	1.0972
C	0.2598	3.73936	5.41473
H	0.4807	4.42165	6.23197
C	-1.9999	-0.54103	2.272
C	-3.3529	-0.7255	1.94314

C	-0.99805	1.81524	4.54333
C	-0.67027	2.73024	5.58146
H	-1.73872	1.04507	4.72687
C	-1.46265	-1.25741	3.35764
C	-4.151	-1.58252	2.69921
H	-5.19883	-1.70543	2.43708
H	-0.41	-1.13889	3.59836
H	-1.17616	2.62694	6.53786
C	-2.26672	-2.11339	4.10821
C	-3.61625	-2.27849	3.7858
H	-1.83426	-2.65974	4.94282
H	-4.24169	-2.94716	4.37097
H	-1.92634	-3.14019	-0.81356
H	-3.6545	-4.2822	-2.83396
C	-1.85699	-2.30016	-1.50911
H	-0.40982	-2.53298	-3.12452
C	-3.64349	-3.26659	-3.22145
C	-0.43643	-2.06468	-2.12932
C	-2.8402	-2.29181	-2.65371
O	-2.18755	-1.06428	-0.81336
H	-5.10748	-3.65522	-4.7586
C	-4.45978	-2.90907	-4.30627
C	-0.46092	-0.53114	-2.22619
C	-2.83742	-0.9795	-3.14951
C	-1.86713	-0.13531	-2.39826
C	-4.45952	-1.60374	-4.80123
H	0.29493	-0.01168	-2.81109
C	-3.64445	-0.6207	-4.22253
H	-2.09997	0.9308	-2.37173
H	-5.10546	-1.34342	-5.63519
H	-3.64659	0.39585	-4.60847
H	3.82987	-4.60749	-4.24352
C	3.5786	-3.76087	-3.60944
H	1.71061	-4.6161	-2.96891
H	5.38393	-2.67074	-4.06919
C	2.38337	-3.76414	-2.88974
C	4.45153	-2.67565	-3.51062
C	2.03648	-2.68894	-2.05918
C	4.11874	-1.59947	-2.68649
C	2.9234	-1.60916	-1.96635
C	0.71807	-2.69191	-1.31418
H	4.78737	-0.74665	-2.60263
H	2.67352	-0.76671	-1.32834
H	0.81874	-2.16775	-0.35643
H	0.44412	-3.72979	-1.08241

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0 499421

$TS_{A4'-P3}$

UB3LYP/6-31G(d)
Imaginary frequency = -486.45 cm^{-1}
Zero-point correction= 0.604361
(Hartree/Particle)
Thermal correction to Energy= 0.640072
Thermal correction to Enthalpy= 0.641016
Thermal correction to Gibbs Free Energy= 0.531834
Sum of electronic and zero-point Energies= -
3273.258719
Sum of electronic and thermal Energies= -
3273.223009
Sum of electronic and thermal Enthalpies= -
3273.222065
Sum of electronic and thermal Free Energies= -
3273.331246

H	2.95777	-4.42117	-2.55138
C	2.44196	-3.49899	-2.29893
H	4.19151	-2.55379	-1.46063
H	0.52598	-4.17006	-3.03006
C	3.13483	-2.44812	-1.69205
C	1.07813	-3.35745	-2.56523
C	2.4763	-1.26418	-1.3645
C	0.4112	-2.17822	-2.23545
H	3.00994	-0.45583	-0.87369
H	2.9002	0.24011	-3.52526
C	1.10718	-1.1121	-1.64632
H	-0.65048	-2.07035	-2.43234
H	4.29844	1.79158	-4.83604
C	2.76662	1.30763	-3.39303
C	3.56943	2.20742	-4.14571
N	0.39597	0.05088	-1.26314
C	1.83499	1.81941	-2.50641
C	0.81391	1.271	-1.59941
C	3.4561	3.58073	-4.02996
Ni	-1.06371	0.16921	0.04749
H	4.09077	4.23485	-4.62252
C	1.71754	3.237	-2.40304
C	2.49816	4.14272	-3.13849
C	0.10524	2.38309	-0.99821
N	-0.91568	2.08846	-0.20145
C	0.69451	3.63398	-1.49513
H	0.04767	3.54567	1.824
C	2.23751	5.52664	-2.92564
H	2.8161	6.27253	-3.46495
C	-1.60049	3.10679	0.51202
C	-0.98224	3.78439	1.57435
C	0.45825	4.98545	-1.31856
C	1.24757	5.91927	-2.04312
H	-0.30987	5.34639	-0.64409
C	-2.93676	3.39649	0.20147
C	-1.6859	4.747	2.29831
H	-1.19655	5.26346	3.11989
H	-3.41217	2.87065	-0.62179
H	1.05752	6.97902	-1.8961
C	-3.63425	4.36287	0.92673
C	-3.01284	5.04164	1.97704
H	-4.66662	4.58437	0.66971
H	-3.55995	5.78879	2.54485
H	-1.9708	-3.20218	2.91978
H	-2.04319	-4.59968	0.52063
C	-2.12305	-2.27142	2.35602
H	-0.91329	-1.09751	3.65823
C	-2.371	-3.65243	0.09975
C	-0.94813	-1.27411	2.57556
C	-2.34973	-2.49998	0.86694
O	-3.28188	-1.60855	2.77183
H	-2.94067	-4.5085	-1.80085
C	-2.88883	-3.59949	-1.20696
C	-1.49457	0.02554	1.94927
C	-2.80437	-1.27039	0.32437
C	-2.76779	-0.17259	1.33108
C	-3.36997	-2.40147	-1.7351
H	-1.3685	0.93616	2.53152
C	-3.33215	-1.22442	-0.97343
H	-3.50209	0.62614	1.27218
H	-3.79294	-2.37955	-2.73574
C	0.45369	-1.70689	2.09857
C	0.98945	-2.94846	2.78315
H	1.14249	-0.86755	2.27013
H	0.44196	-1.86868	1.01503
C	1.29478	-2.94141	4.15248
C	1.78107	-4.08422	4.78665

C	1.97445	-5.26153	4.06015
C	1.68008	-5.28204	2.69672
C	1.19244	-4.13507	2.06626
H	0.97485	-4.15567	1.00076
H	1.83202	-6.19099	2.11978
H	1.15445	-2.0283	4.72736
H	2.0124	-4.05513	5.84852
H	2.35436	-6.15264	4.55296
H	-3.72937	-0.29618	-1.37696

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3273.0275985

A5

UB3LYP-D3/6-31G(d)-CPCM(acetone)
Zero-point correction= 0.486923
(Hartree/Particle)
Thermal correction to Energy= 0.516056
Thermal correction to Enthalpy= 0.517000
Thermal correction to Gibbs Free Energy= 0.425202
Sum of electronic and zero-point Energies= -3002.594413
Sum of electronic and thermal Energies= -3002.565280
Sum of electronic and thermal Enthalpies= -3002.564336
Sum of electronic and thermal Free Energies= -3002.656134

H	5.62802	-3.33699	0.37135
C	4.67818	-2.8131	0.42445
H	5.57914	-0.85383	0.5341
H	3.49335	-4.61413	0.32073
C	4.65139	-1.41842	0.51698
C	3.47935	-3.53054	0.39414
C	3.43271	-0.74228	0.58443
C	2.25653	-2.86062	0.45447
H	3.39656	0.34076	0.65306
H	3.04844	-1.13116	3.2333
C	2.23517	-1.46709	0.56137
H	1.31673	-3.40304	0.42896
H	3.30606	-0.64577	5.64412
C	2.28011	-0.56476	3.74615
C	2.4208	-0.28169	5.13116
N	0.98358	-0.78263	0.60429
C	1.15649	-0.10128	3.08426
C	0.62196	-0.18993	1.72665
C	1.47351	0.43445	5.84375
Ni	-0.25537	-0.62414	-0.77557
H	1.61646	0.62715	6.90341
C	0.18255	0.63631	3.82121
C	0.30162	0.91653	5.19404
C	-0.66824	0.50451	1.68751
N	-1.29656	0.43435	0.54361
C	-0.9371	1.03241	3.03421
H	-1.82149	3.04245	0.90384
C	-0.77075	1.63761	5.78982
H	-0.72833	1.88407	6.84727
C	-2.52113	1.09567	0.29905
C	-2.6624	2.47463	0.51704
C	-1.96805	1.72313	3.64482
C	-1.86505	2.01784	5.03028
H	-2.84295	2.04446	3.09213
C	-3.58461	0.36102	-0.24341
C	-3.87343	3.103	0.22877
H	-3.97675	4.17086	0.39945
H	-3.43613	-0.6922	-0.44897
H	-2.67623	2.56269	5.50388
C	-4.79502	0.99551	-0.51875
C	-4.94566	2.36522	-0.28227
H	-5.62101	0.41924	-0.92615
H	-5.88849	2.85684	-0.50402
O	-1.45265	-0.62918	-2.08494
H	-1.1675	-2.39072	-3.15195
C	-0.67411	-1.41625	-3.01248
C	1.686	0.11732	-3.73492
C	-0.57898	-0.70618	-4.34599
C	0.5424	0.10429	-4.64186
C	0.55417	0.83389	-5.84383
C	-1.6318	-0.78312	-5.25858
H	1.41644	1.45548	-6.07668
H	-2.48603	-1.41658	-5.02662
C	-0.51308	0.76226	-6.73905
C	-1.61106	-0.05364	-6.45159
H	-0.48473	1.33509	-7.66249
H	-2.44325	-0.11987	-7.14738
C	0.62259	-1.53852	-2.22104
C	1.73748	-0.68642	-2.64723
H	0.91326	-2.54899	-1.92228
H	2.63951	-0.70433	-2.04017
H	2.52739	0.75842	-3.98983

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP-D3/6-31G(d)-CPCM(acetone)
HF = -3002.2794691

UB3LYP/6-31G(d)
Zero-point correction= 0.487153
(Hartree/Particle)
Thermal correction to Energy= 0.516331
Thermal correction to Enthalpy= 0.517275
Thermal correction to Gibbs Free Energy= 0.425020
Sum of electronic and zero-point Energies= -3002.499776
Sum of electronic and thermal Energies= -3002.470599
Sum of electronic and thermal Enthalpies= -3002.469655
Sum of electronic and thermal Free Energies= -3002.561910

H	5.6278	-3.33755	0.3714
C	4.67803	-2.81354	0.42448
H	5.57924	-0.85439	0.53417
H	3.49297	-4.61442	0.32071
C	4.65141	-1.41886	0.51703
C	3.47911	-3.53082	0.39413
C	3.43282	-0.74256	0.58446
C	2.25638	-2.86075	0.45443
H	3.39681	0.34048	0.6531
H	3.04837	-1.13148	3.23334
C	2.2352	-1.46722	0.56137
H	1.3165	-3.40304	0.42888
H	3.3059	-0.64625	5.64422
C	2.28007	-0.56505	3.74619
C	2.4207	-0.28207	5.13122
N	0.98369	-0.78261	0.60427
C	1.15653	-0.10144	3.08427
C	0.62206	-0.18998	1.72663
C	1.47343	0.43411	5.84379
Ni	-0.25532	-0.62403	-0.77561
H	1.61633	0.62674	6.90347
C	0.1826	0.63619	3.82119
C	0.30162	0.91634	5.19405
C	-0.66812	0.5046	1.68745

N	-1.29638	0.43454	0.54354
C	-0.93698	1.03245	3.03416
H	-1.82087	3.04271	0.90363
C	-0.77071	1.6375	5.7898
H	-0.72832	1.8839	6.84727
C	-2.52088	1.09602	0.29902
C	-2.66189	2.47502	0.51694
C	-1.96788	1.72326	3.64475
C	-1.86493	2.01789	5.03023
H	-2.84271	2.04471	3.09202
C	-3.58452	0.3615	-0.24328
C	-3.87285	3.10356	0.22873
H	-3.97598	4.17145	0.39935
H	-3.43624	-0.69176	-0.44875
H	-2.67607	2.56279	5.50381
C	-4.79486	0.99617	-0.51854
C	-4.94525	2.36592	-0.28216
H	-5.62098	0.42	-0.92581
H	-5.88802	2.85768	-0.50385
O	-1.45273	-0.62918	-2.08492
H	-1.16754	-2.39078	-3.15183
C	-0.6742	-1.41627	-3.01243
C	1.68568	0.11762	-3.73493
C	-0.57915	-0.70629	-4.346
C	0.5421	0.10437	-4.64188
C	0.55377	0.83392	-5.84389
C	-1.63192	-0.78347	-5.25863
H	1.41593	1.45565	-6.07675
H	-2.48603	-1.41708	-5.02667
C	-0.51344	0.76205	-6.73914
C	-1.61128	-0.05405	-6.45168
H	-0.48517	1.33484	-7.66261
H	-2.44343	-0.12048	-7.1475
C	0.62255	-1.53845	-2.22107
C	1.7373	-0.68614	-2.64725
H	0.91339	-2.54889	-1.92237
H	2.63934	-0.70393	-2.0402
H	2.52695	0.75888	-3.98982

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)
HF = -3002.2791073

$TS_{A5\text{-}A6}$

UB3LYP/6-31G(d)
Imaginary frequency = -227.25 cm^{-1}
Zero-point correction= 0.602920
(Hartree/Particle)
Thermal correction to Energy= 0.638916
Thermal correction to Enthalpy= 0.639860
Thermal correction to Gibbs Free Energy= 0.530984
Sum of electronic and zero-point Energies= -3273.302735
Sum of electronic and thermal Energies= -3273.266740
Sum of electronic and thermal Enthalpies= -3273.265796
Sum of electronic and thermal Free Energies= -3273.374672

H	6.10294	0.11051	2.25053
C	5.03013	0.09162	2.07962
H	5.08765	-1.69009	0.86496
H	4.65303	1.89469	3.20515
C	4.45932	-0.91986	1.30364
C	4.21604	1.08993	2.61972
C	3.0861	-0.94391	1.06961
C	2.83901	1.06724	2.40308
H	2.6386	-1.70326	0.44001
H	1.88676	-0.12744	4.58183
C	2.26248	0.03684	1.64182
H	2.20602	1.85188	2.80686
H	1.09726	-0.06844	6.92392
C	0.82763	-0.013	4.78174
C	0.3675	0.02608	6.12464
N	0.87792	0.01459	1.36105
C	-0.09423	0.10572	3.75799
C	-0.04906	0.09948	2.28222
C	-0.9684	0.19188	6.44432
Ni	0.05068	0.06619	-0.4854
H	-1.27908	0.23138	7.48543
C	-1.46985	0.24636	4.09246
C	-1.94316	0.31079	5.41486
C	-1.42107	0.18358	1.79149
N	-1.57379	0.1537	0.47195
C	-2.31695	0.31609	2.94596
H	-2.66632	1.95086	-1.16564
C	-3.34557	0.48961	5.58287
H	-3.76496	0.55097	6.58384
C	-2.89088	0.11038	-0.07459
C	-3.32653	1.1211	-0.93876
C	-3.67494	0.49764	3.14639
C	-4.1683	0.58751	4.47545
H	-4.36807	0.56521	2.31639
C	-3.73281	-0.97792	0.20001
C	-4.60318	1.05578	-1.49838
H	-4.93394	1.84908	-2.16317
H	-3.37772	-1.77347	0.84817
H	-5.23586	0.73007	4.61911
C	-5.0045	-1.03871	-0.36848
C	-5.44692	-0.02	-1.21632
H	-5.64678	-1.88877	-0.15422
H	-6.43693	-0.07037	-1.66071
H	1.23464	0.60833	-3.28905
H	3.30944	-0.59857	-4.01964
C	0.95577	-0.28692	-2.7144
H	-1.09254	0.5882	-2.65846
C	2.72388	-1.51562	-4.02874
C	-0.51655	-0.27604	-2.32068
C	1.46502	-1.5206	-3.43042
O	1.54149	-0.1884	-1.39992
H	4.23249	-2.64994	-5.07679
C	3.24575	-2.66937	-4.62136
C	-1.22671	-1.55654	-2.41475
C	0.69361	-2.70327	-3.44309
C	-0.65739	-2.68621	-2.89168
C	2.49175	-3.84411	-4.62335
H	-2.26447	-1.58594	-2.09406
C	1.2241	-3.85626	-4.04322
H	-1.22682	-3.61291	-2.92799
H	2.88664	-4.74703	-5.08243
H	0.62798	-4.76657	-4.05861
H	1.79486	2.8794	-2.56053
H	1.14084	4.22919	-4.52537
C	0.86298	3.43885	-2.55064
C	0.49338	4.19857	-3.6525
H	1.45632	2.28326	-0.16194
C	0.42111	2.58819	-0.26117
C	0.04331	3.37444	-1.39101
C	-0.70287	4.92763	-3.64602
H	-0.98794	5.5221	-4.50948
H	-0.14173	2.69894	0.66121
C	-1.16138	4.12871	-1.40675
C	-1.52345	4.88885	-2.51221

H	-1.79538	4.12226	-0.52253	HF =-3273.0483866
H	-2.44654	5.46327	-2.49125	

UM06/6-311+G(d,p)-CPCM(acetone)//UB3LYP/6-31G(d)

Appendix 5: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 5 (Mechanistic Insights into the Nickel-Catalyzed Diarylation of Unactivated Alkenes in Ketimines)

A5.1 Methods

All optimizations of intermediates and transition states were calculated without constraints using unrestricted B3LYP-D3/def2SVP-LANL2DZ(I) level of the theory in implicit solvent (acetonitrile) using CPCM as solvation model with the "guess=mix" keywords as implemented in Gaussian 16.[241] Frequency calculations, at the same level of theory, were used to obtain thermal corrections (at 298K) and to characterize optimized structures as transition states (only a single imaginary frequency) or intermediate (if no imaginary frequencies were found). Intrinsic reaction coordinate (IRCs) calculations were undertaken to ensure transition states connected illustrated ground states. Single point energy calculations with implicit solvent (acetonitrile) corrections using CPCM as the solvation model with unrestricted B3LYP-D3/def2TZVPP were also performed on all structures.[242] For comparison, single point energy calculations with implicit solvent corrections (acetonitrile) using CPCM as solvation model with unrestricted PBEPBE/def2TZVPP and M06L/def2TZVPP were also performed on all structures.[243] All 3-D structures were generated using CYLview.[244]

A5.2 Supplementary Figures

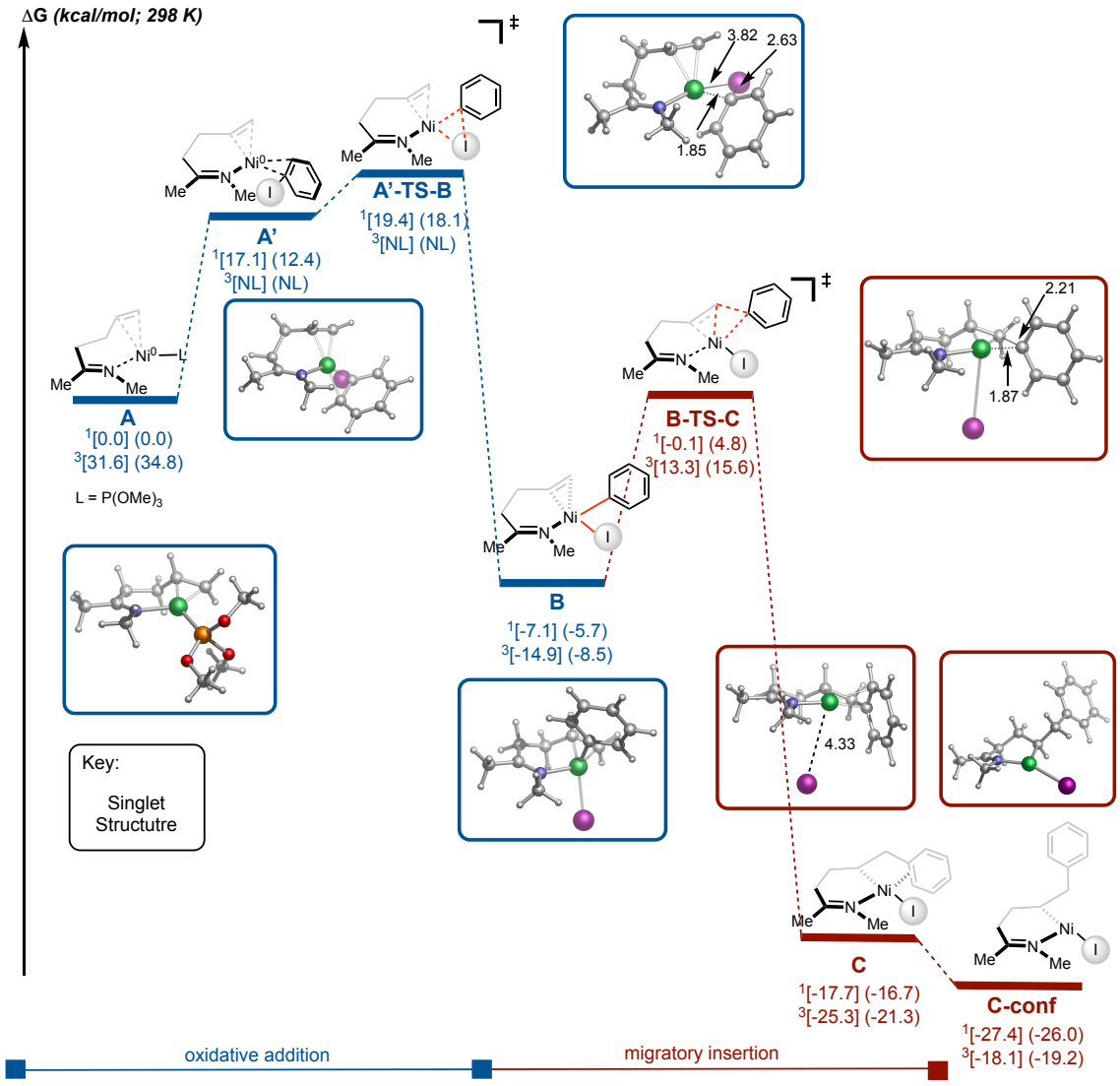


Figure A5.1 Reaction coordinate diagram showing oxidative addition, and migratory insertion leading to intermediate **C-conf**. Free energies are given at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory (parenthesis) and UM06/6-311+G(d,p)-SDD(I)-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) (brackets). NL indicates that these intermediates could not be located at the spin indicated in the superscript.

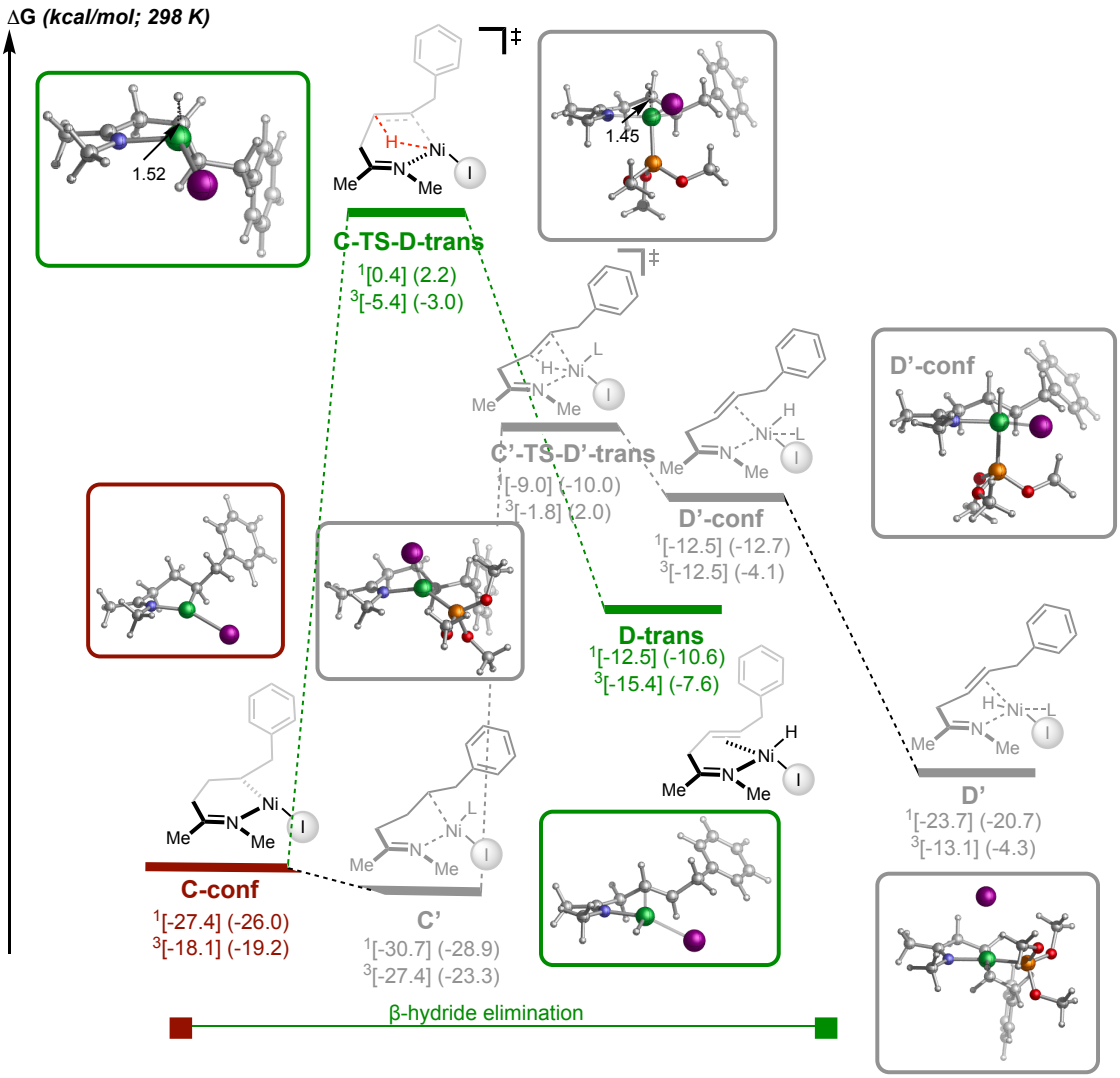


Figure A5.2 Reaction coordinate diagram showing β-hydride elimination leading to intermediate **D-trans** and **D'**. Free energies are given at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory (parenthesis) and UM06/6-311+G(d,p)-SDD(I)-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) (brackets).

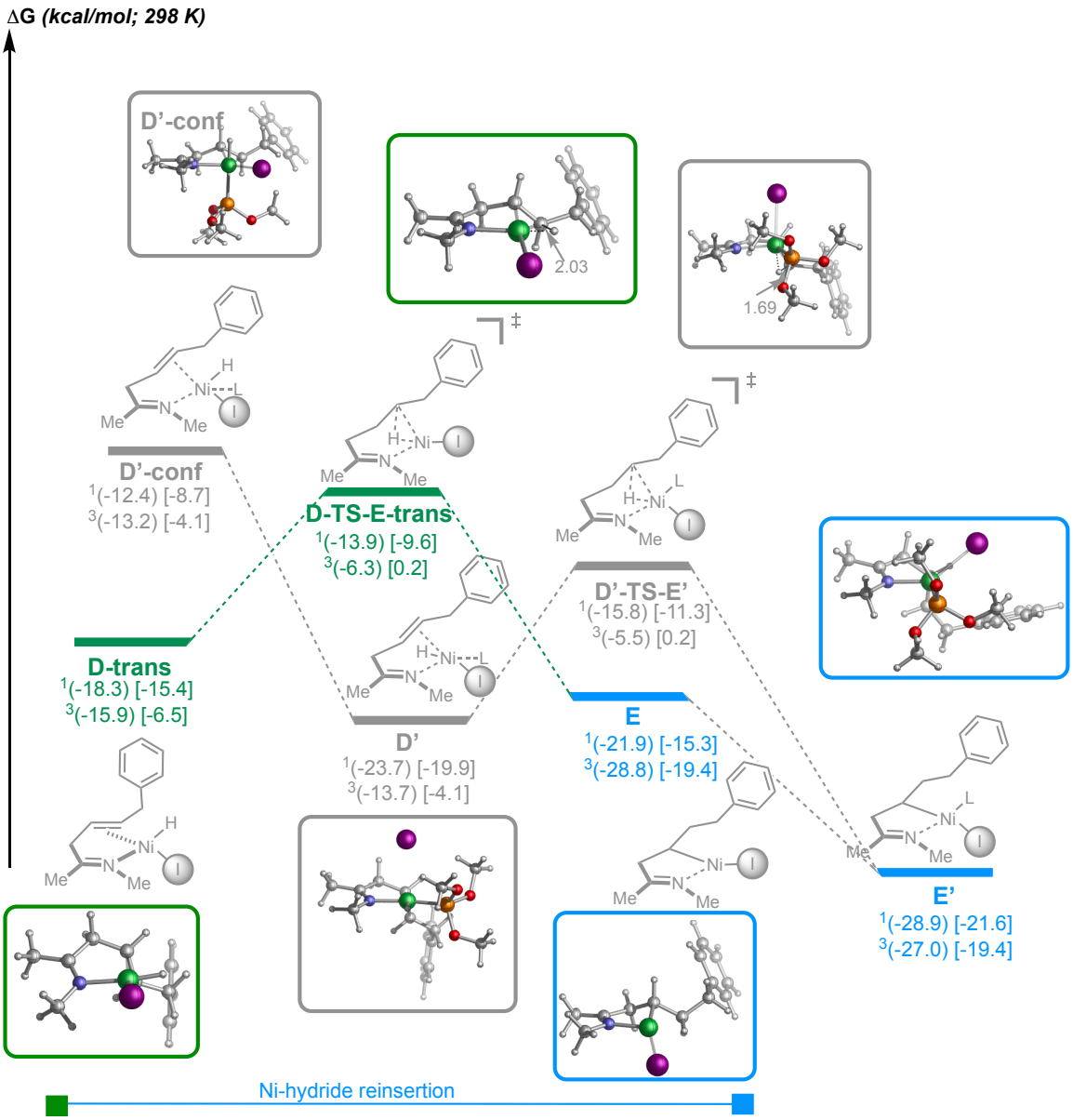


Figure A5.3 Reaction coordinate diagram showing Ni-hydride reinsertion leading to intermediate **E'**. Free energies are given at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory (parenthesis) and UM06/6-311+G(d,p)-SDD(I)-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I) CPCM(acetonitrile) (brackets).

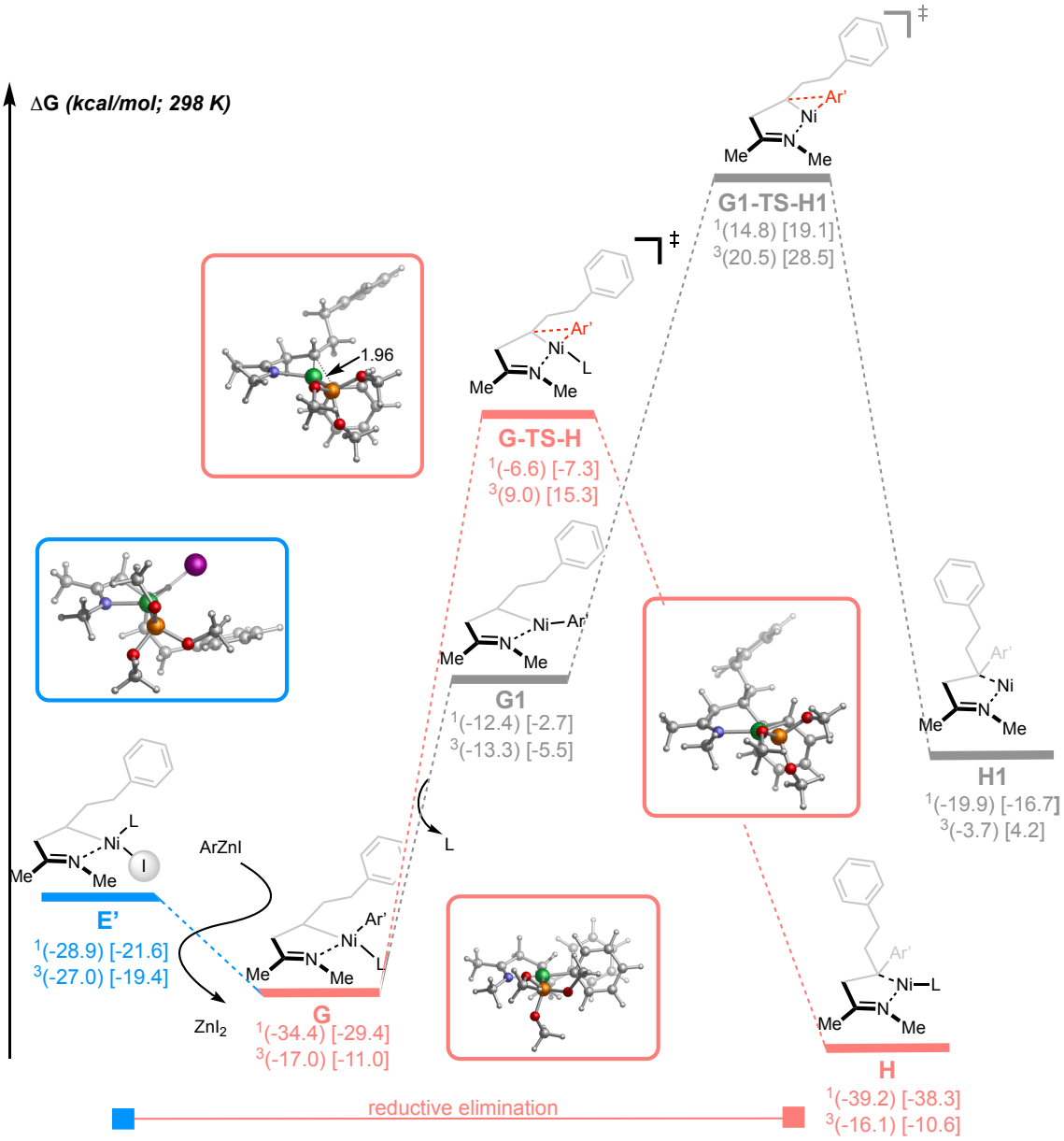


Figure A5.4 Reaction coordinate diagram showing reductive elimination leading to intermediate **H**. Free energies are given at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory (parenthesis) and UM06/6-311+G(d,p)-SDD(I)-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) (brackets).

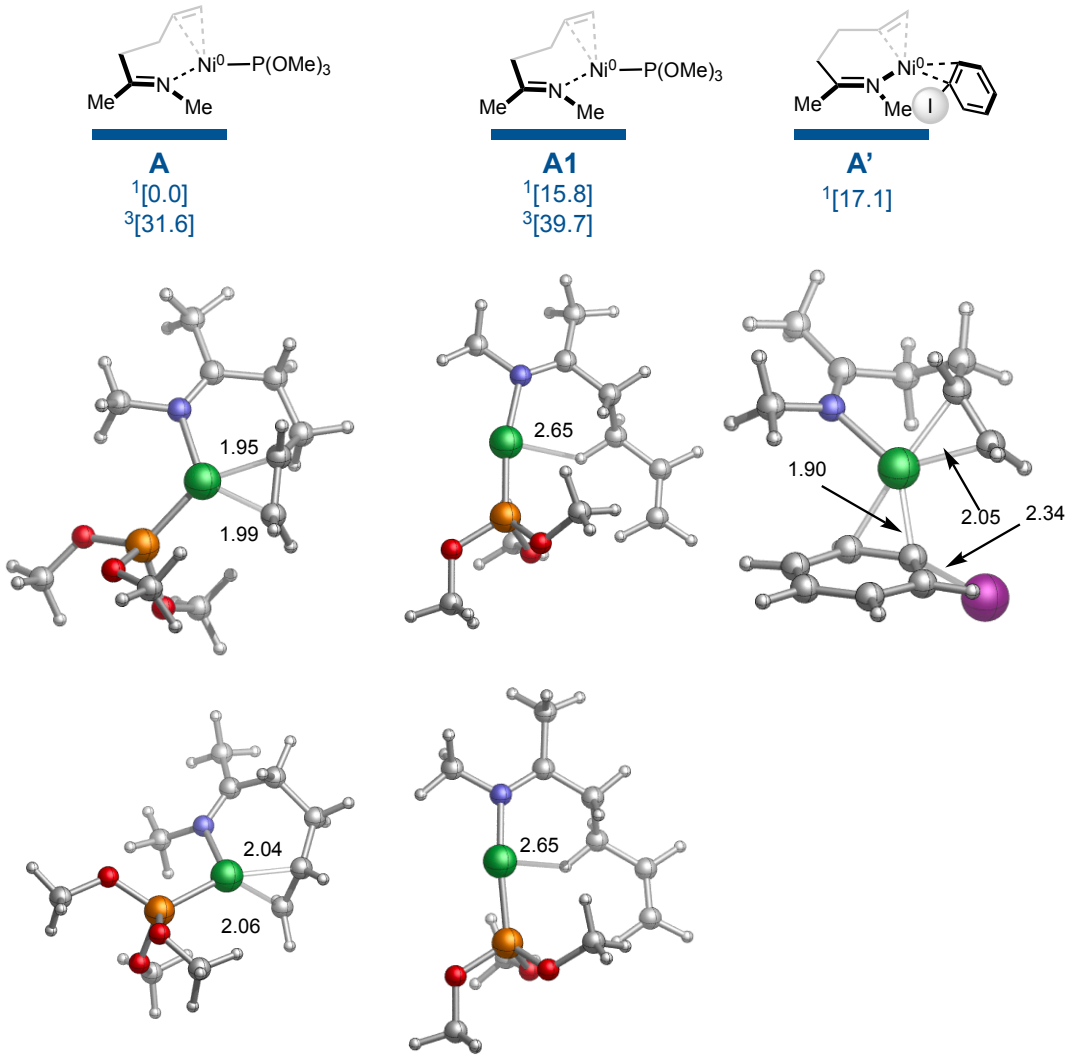


Figure A5.5 Conformers of **A**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

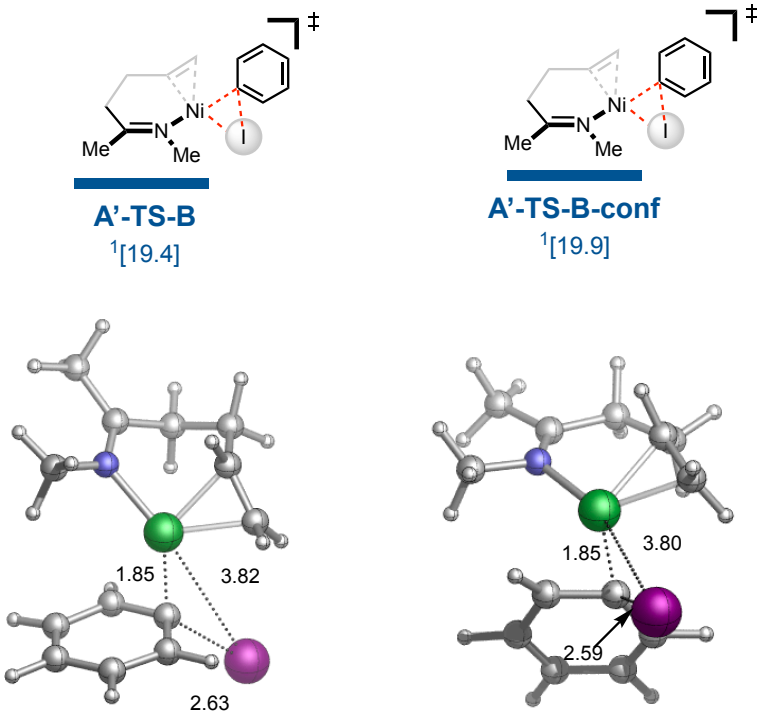


Figure A5.6 Conformers of **A'-TS-B**. Singlet structures are given. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

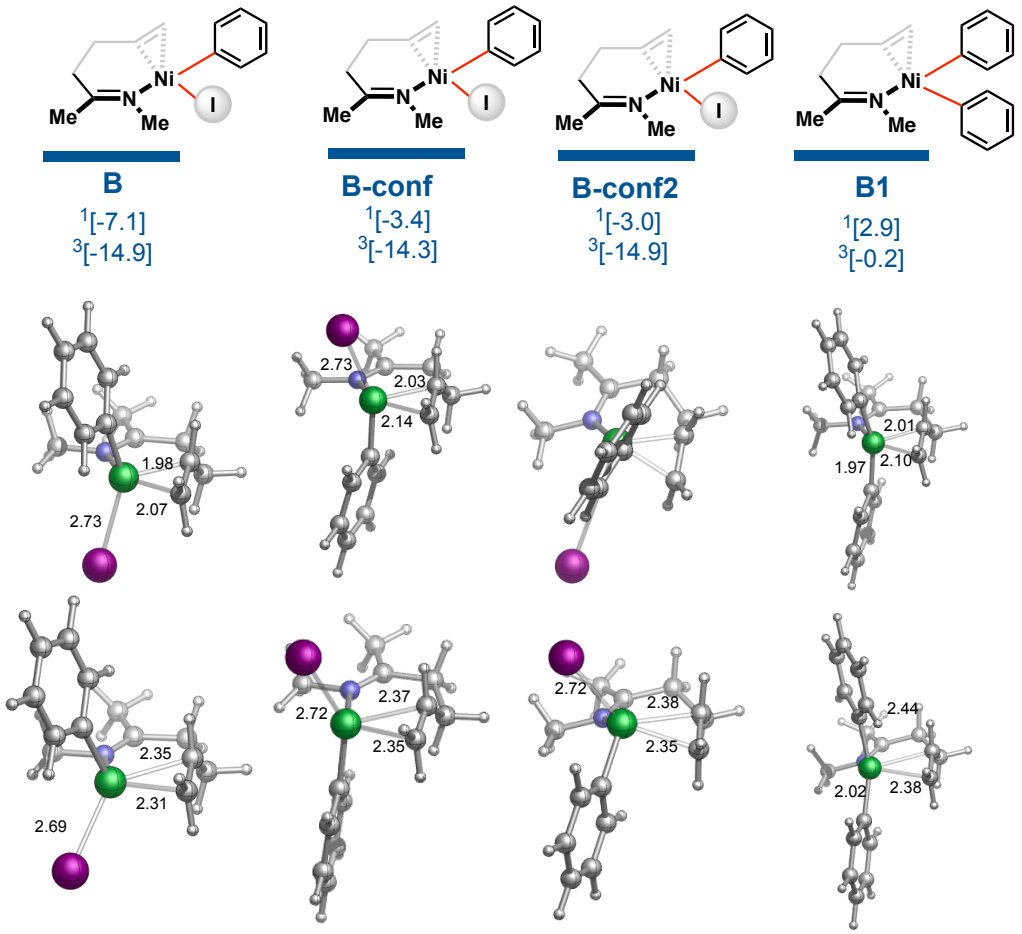


Figure A5.7 Conformers of **B**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

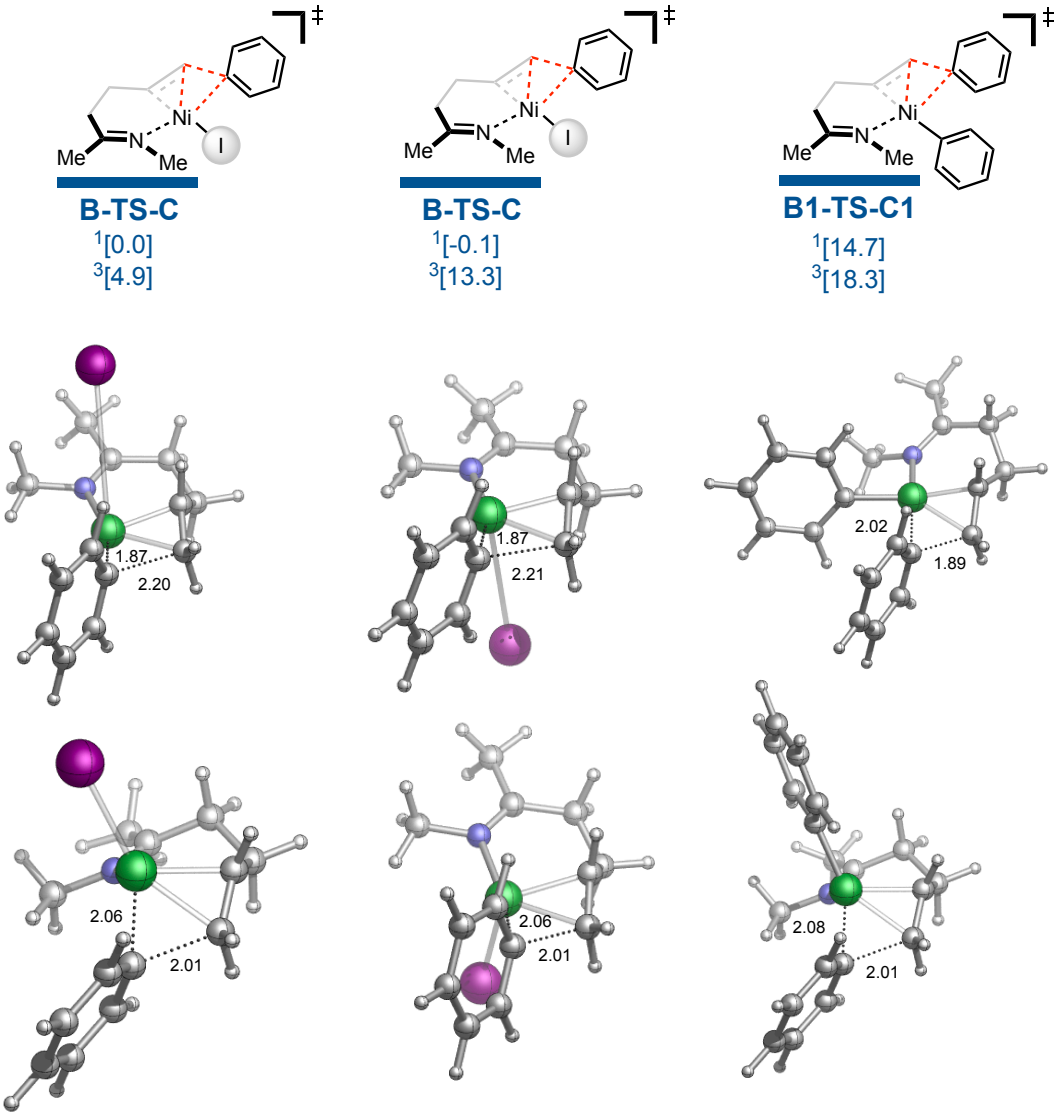


Figure A5.8 Conformers of **B-TS-C**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

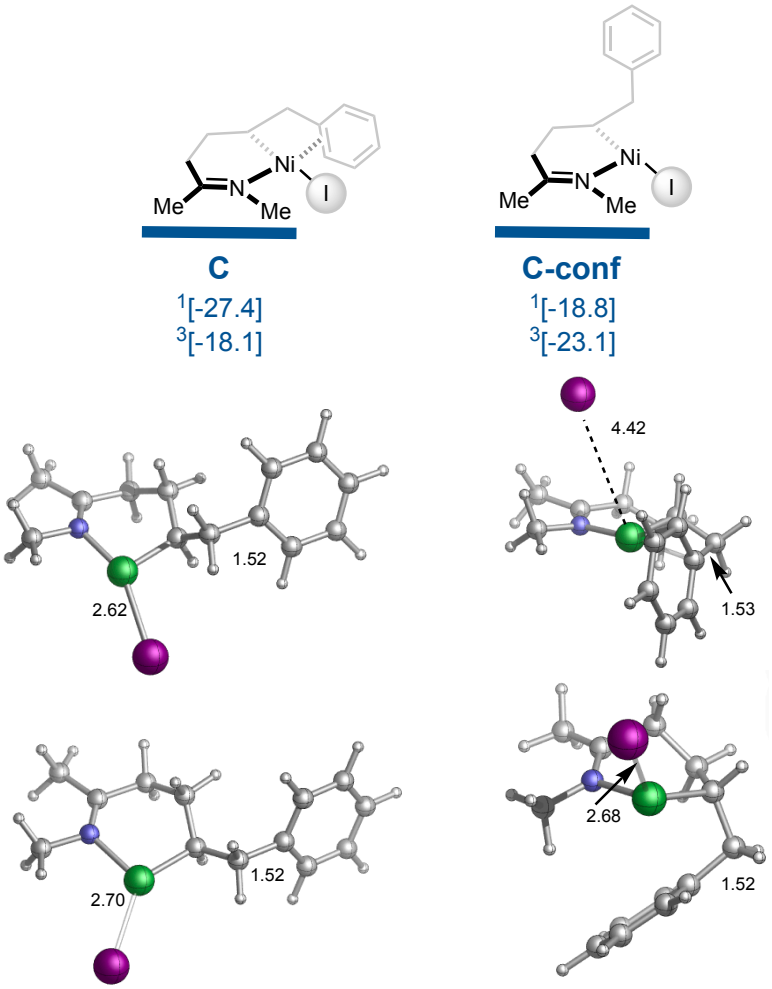


Figure A5.9 Conformers of **C**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

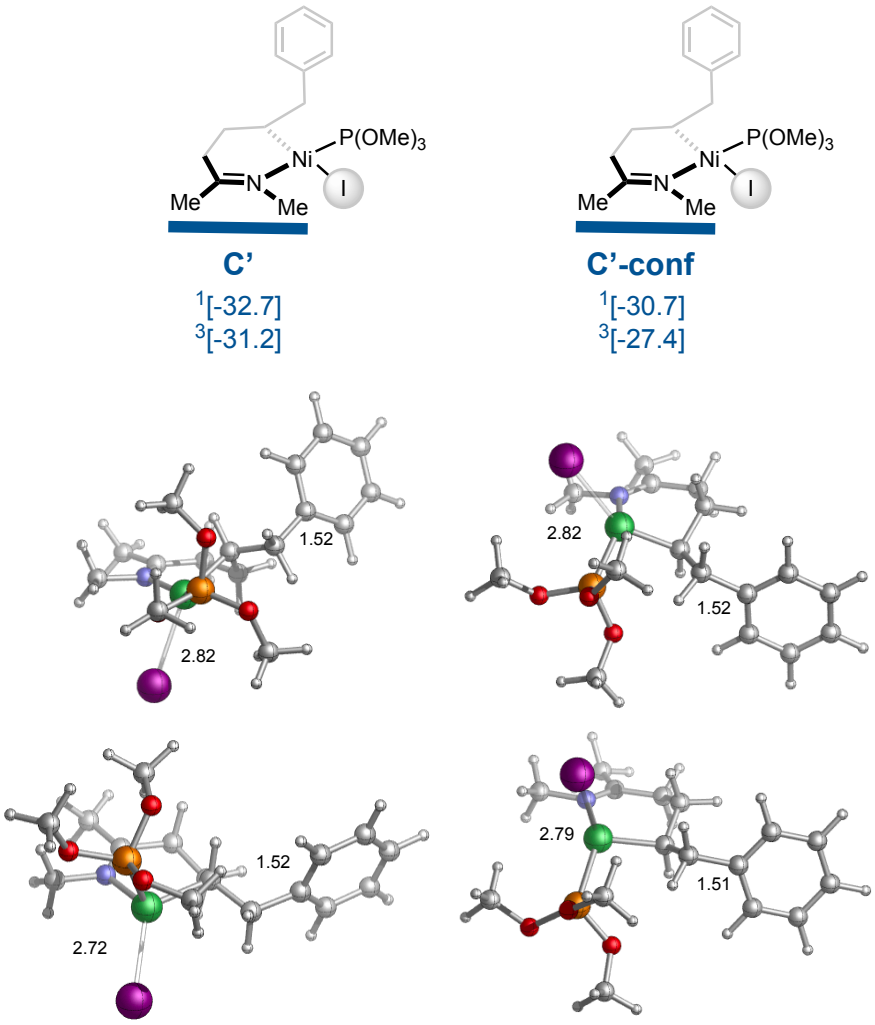


Figure A5.10 Conformers of **C'**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

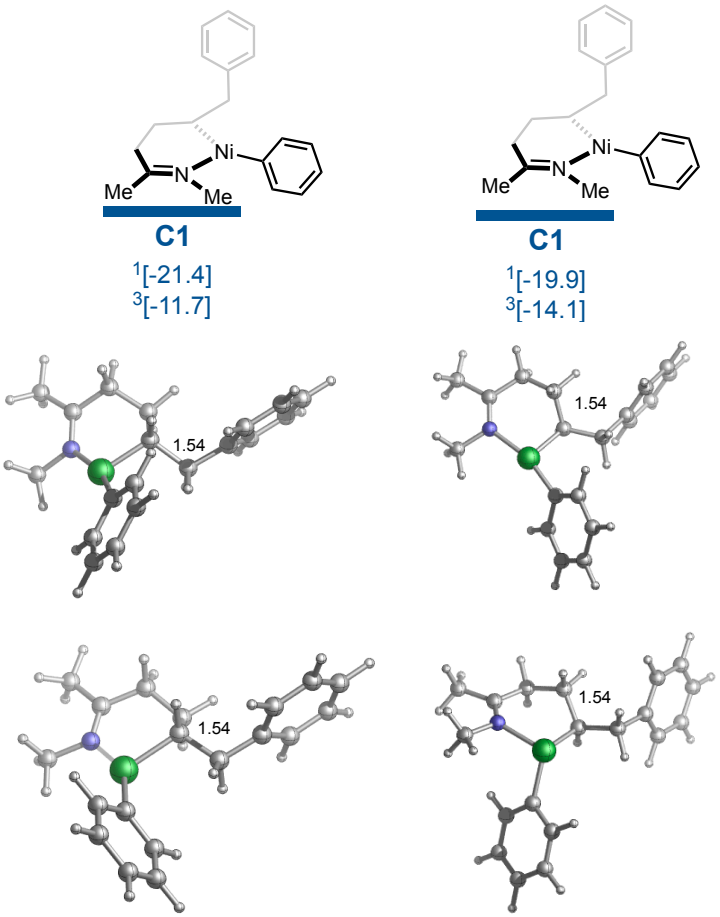


Figure A5.11 Conformers of **C1**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

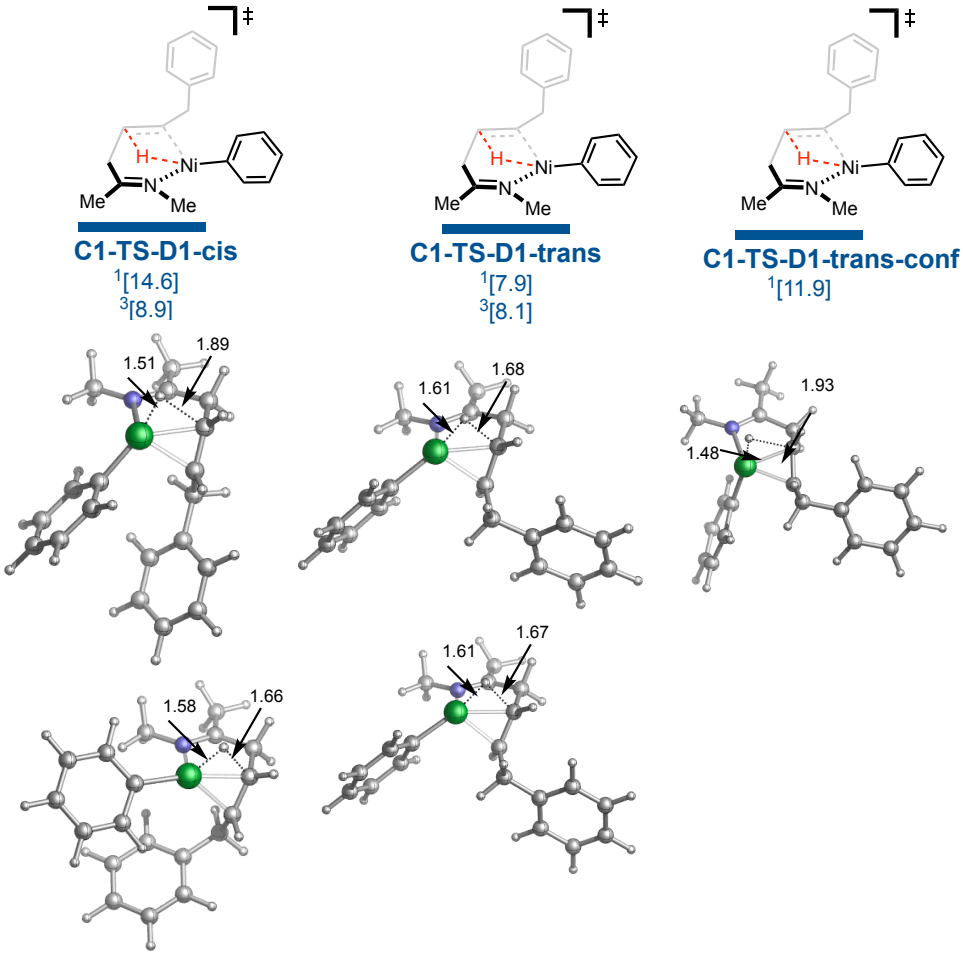


Figure A5.12 Conformers of **C1-TS-D1**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

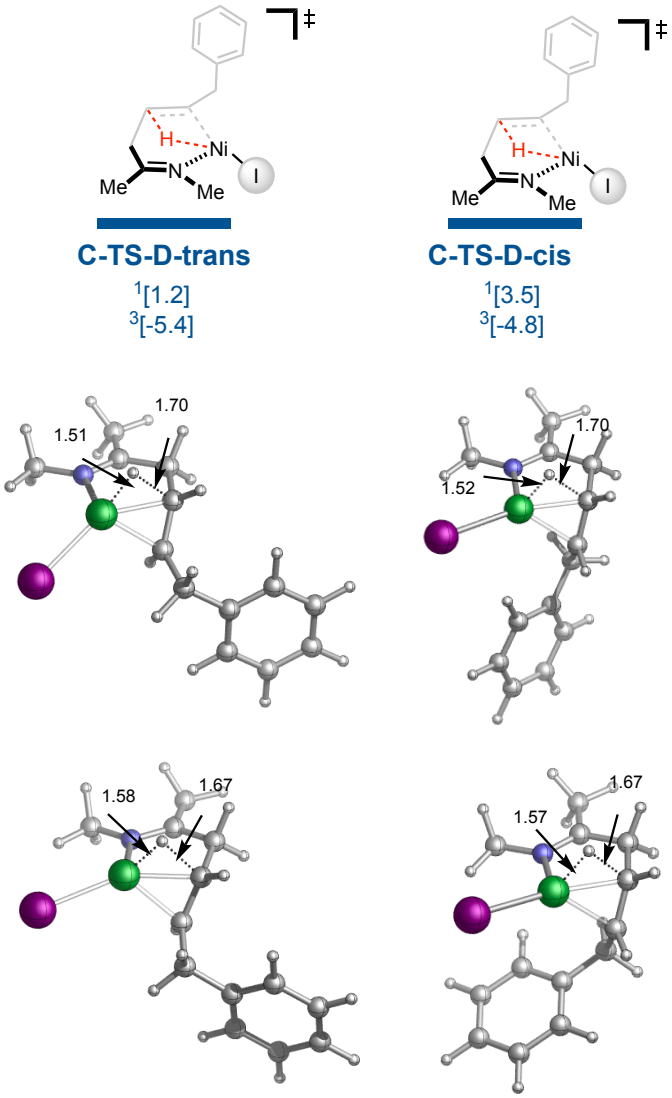


Figure A5.13 Conformers of **C-TS-D**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

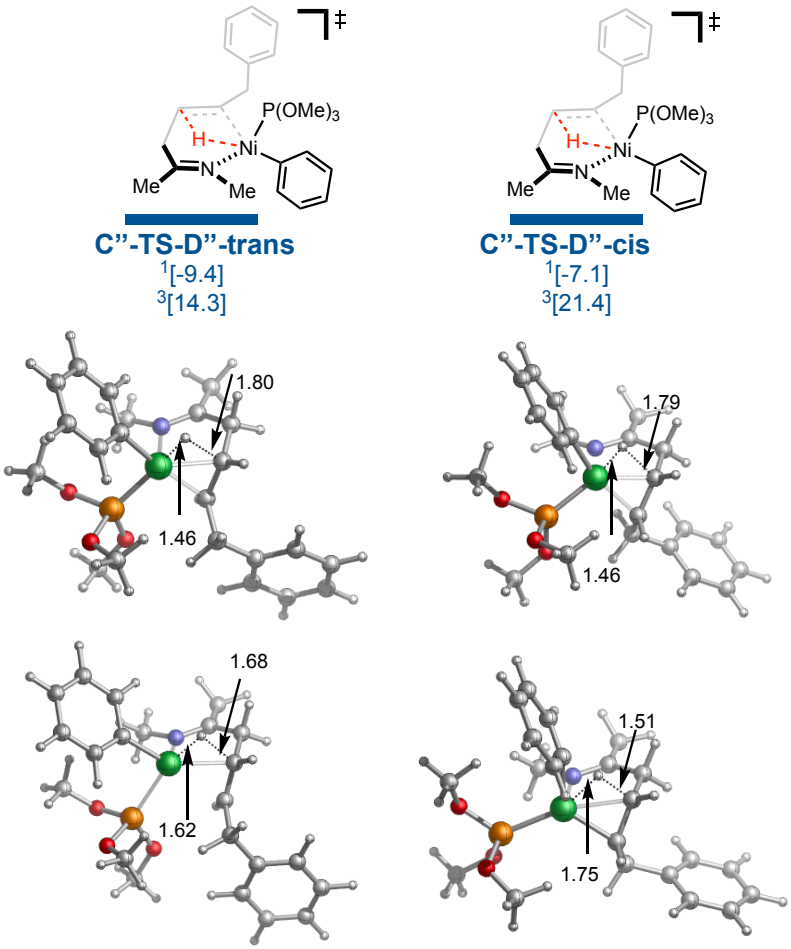


Figure A5.14 Conformers of **C’’-TS-D’’**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

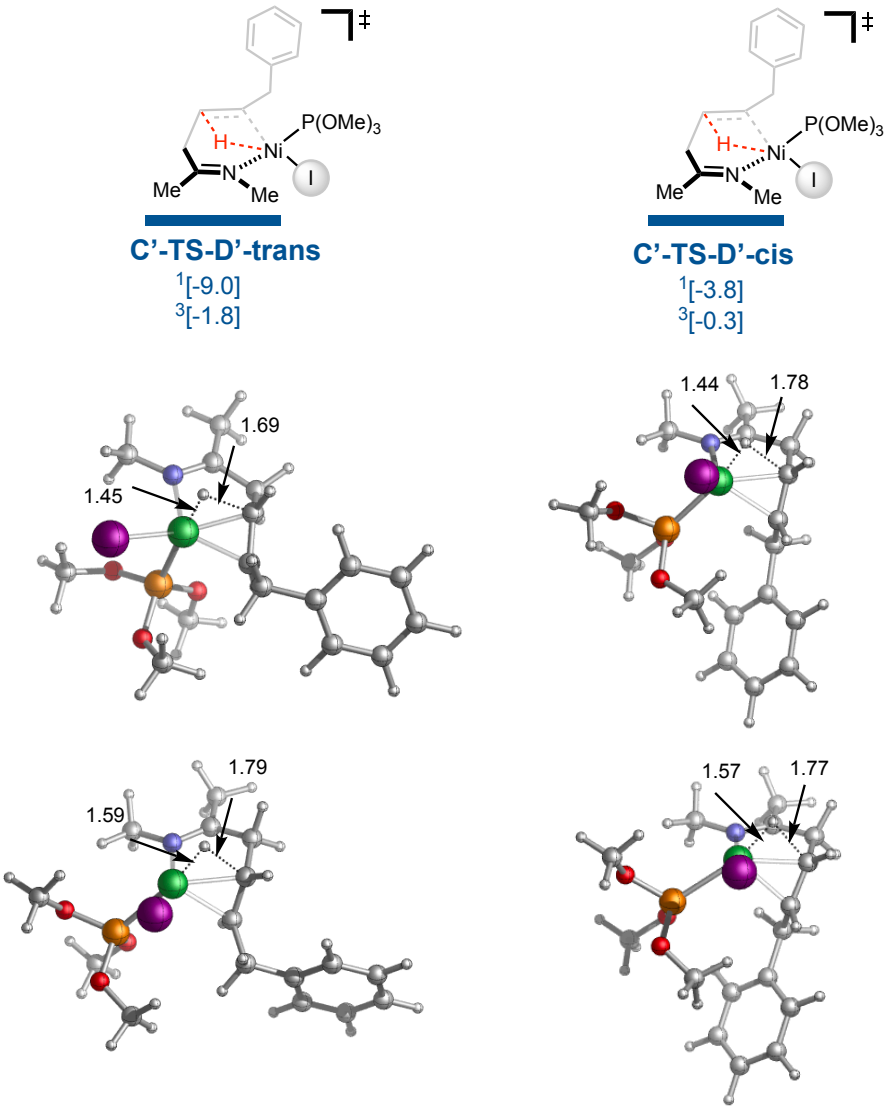


Figure A5.15 Conformers of **C'-TS-D'**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

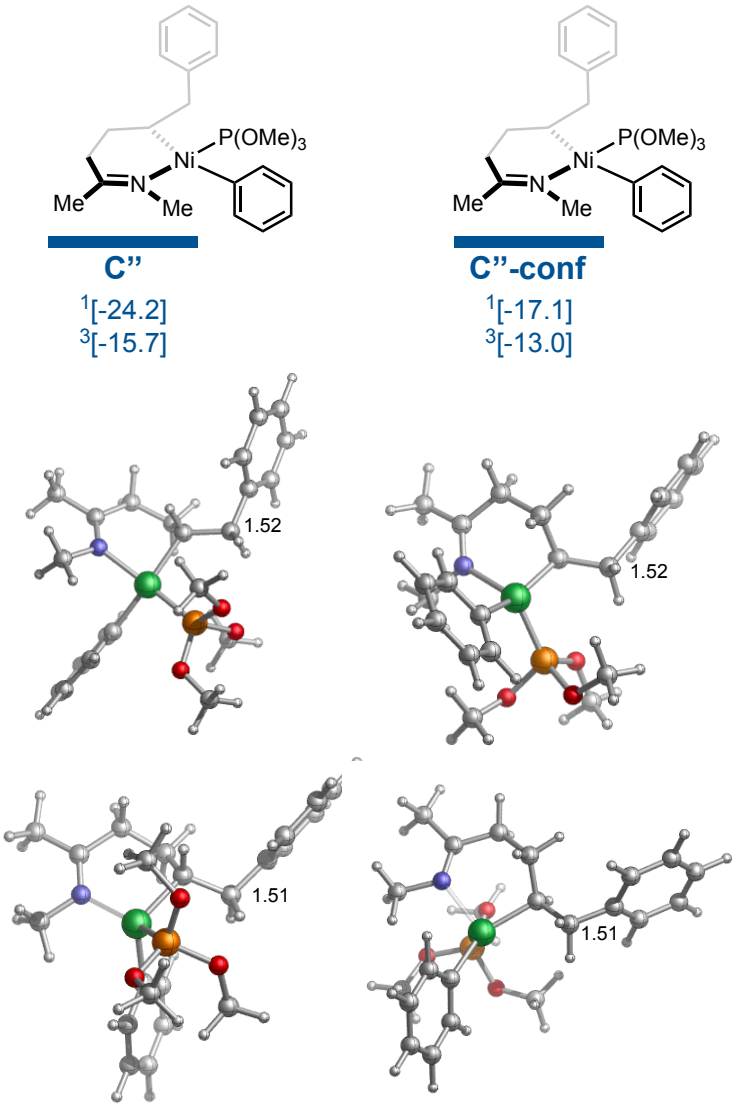


Figure A5.16 Conformers of **C''**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

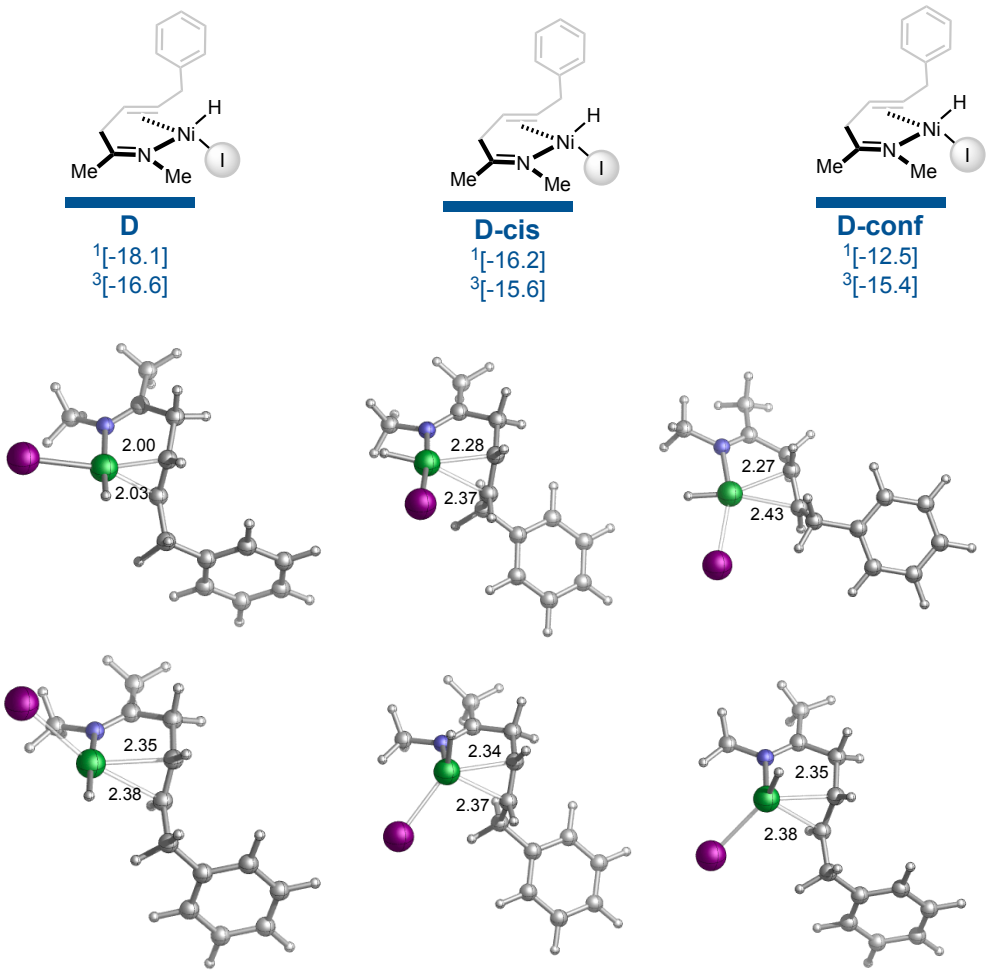


Figure A5.17 Conformers of **D**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

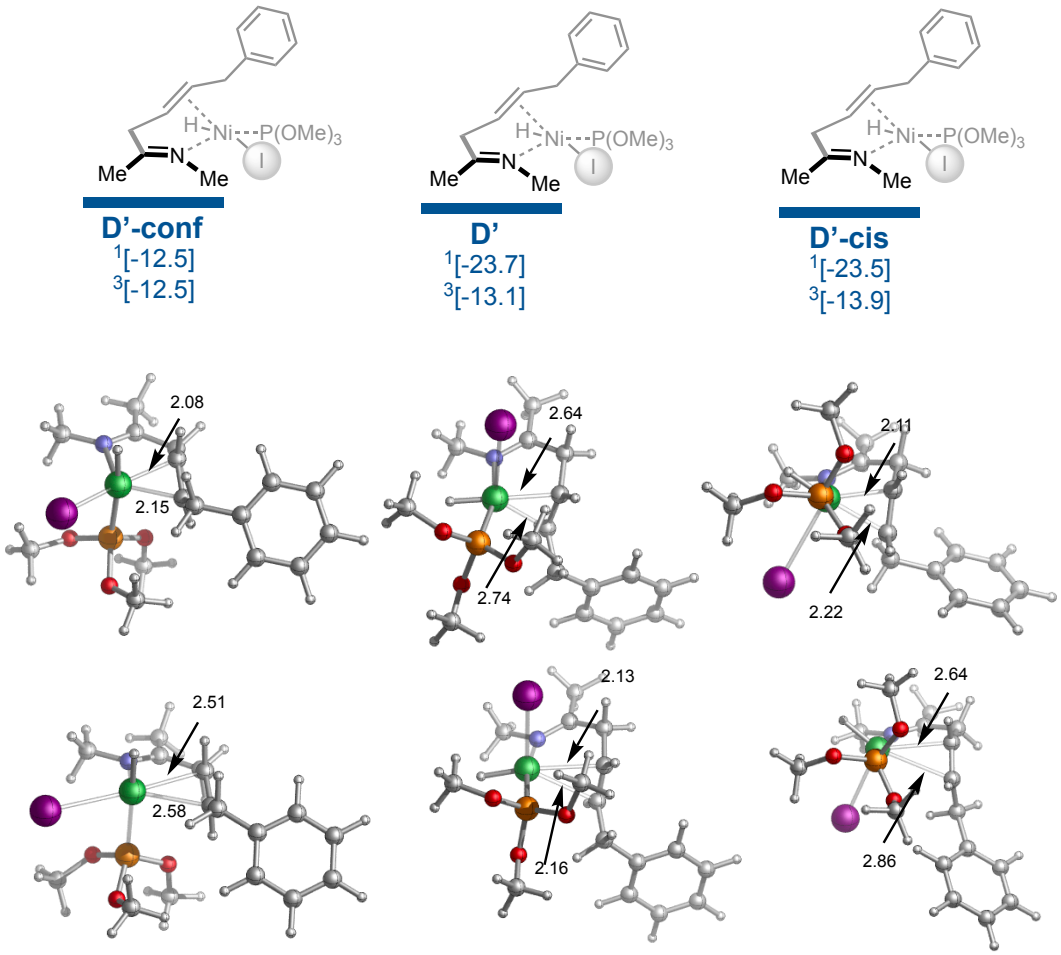


Figure A5.18 Conformers of **D'**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

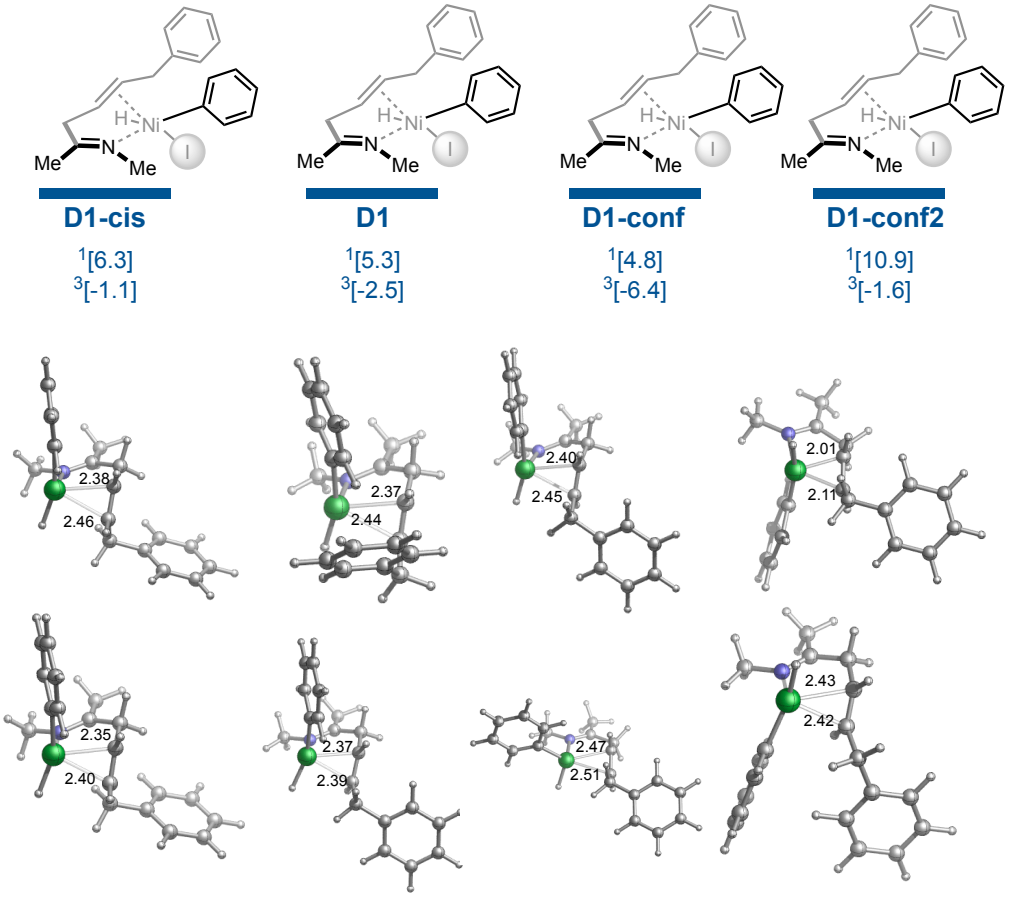


Figure A5.19 Conformers of **D1**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

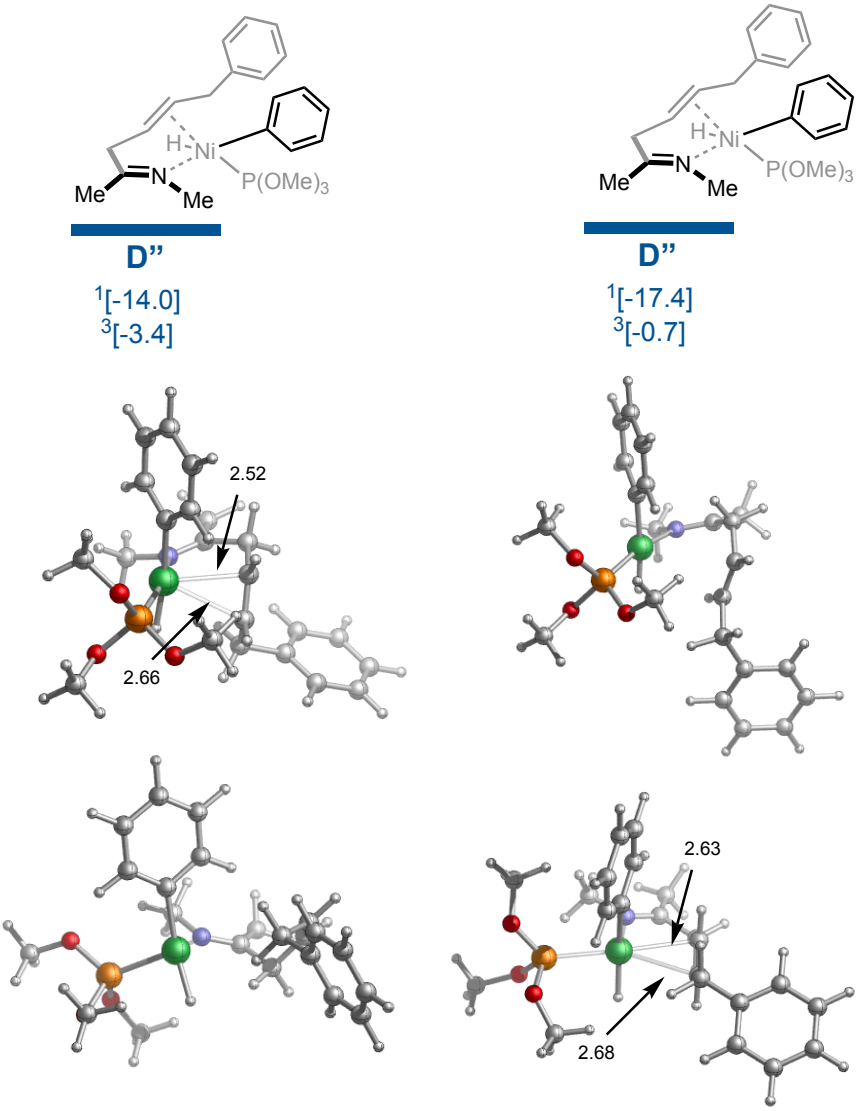


Figure A5.20 Conformers of **D’’**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

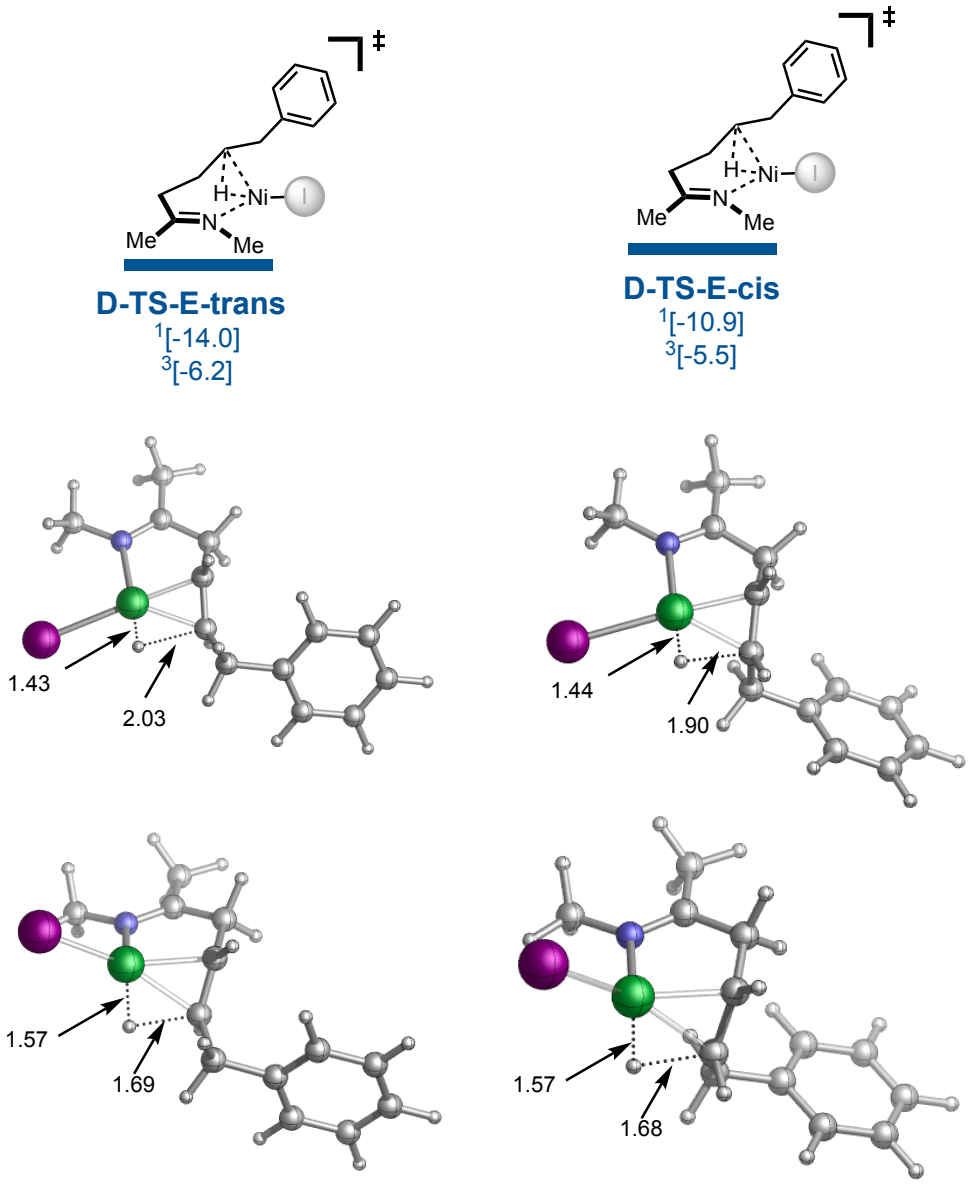


Figure A5.21 Conformers of **D-TS-E**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

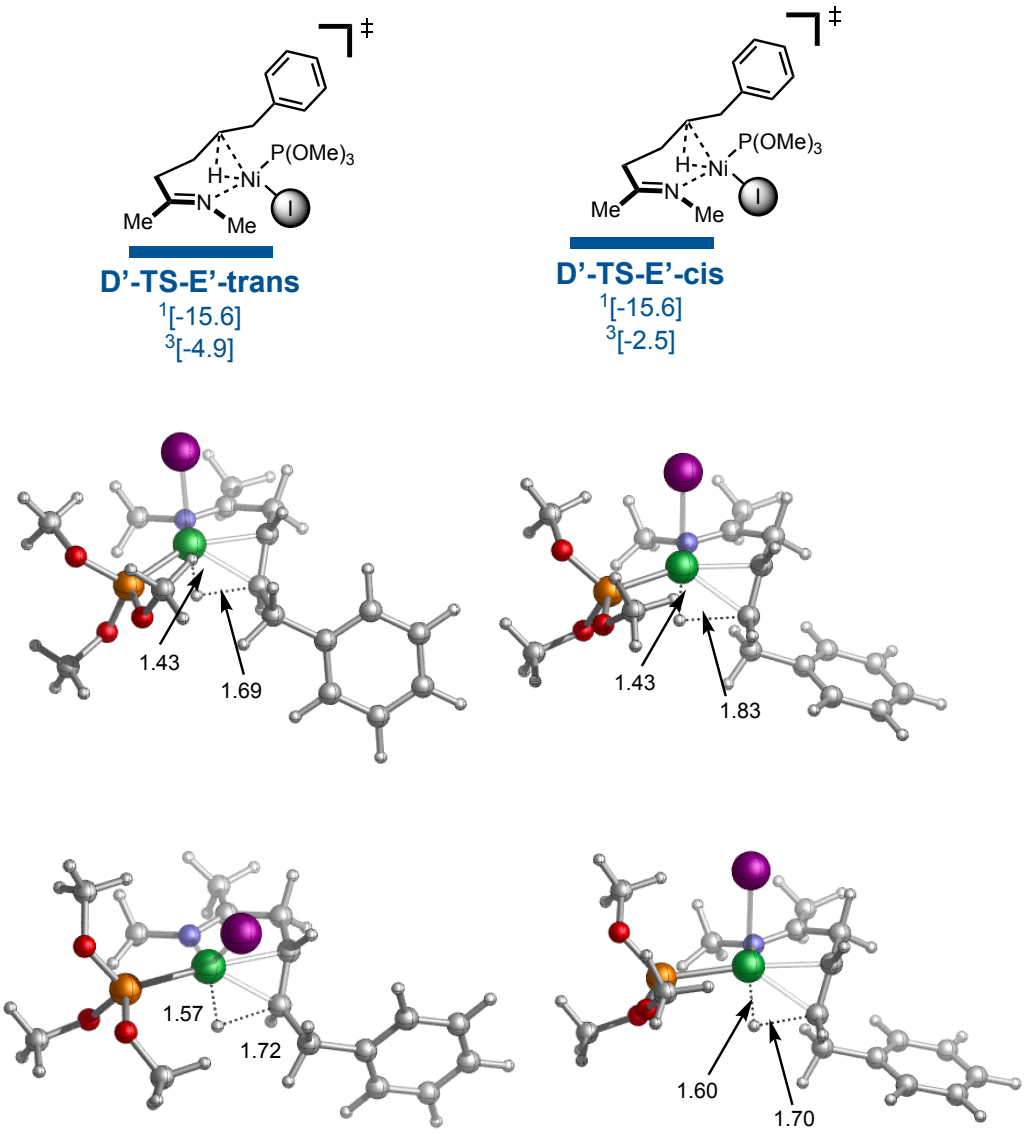


Figure A5.22 Conformers of **D'-TS-E'**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

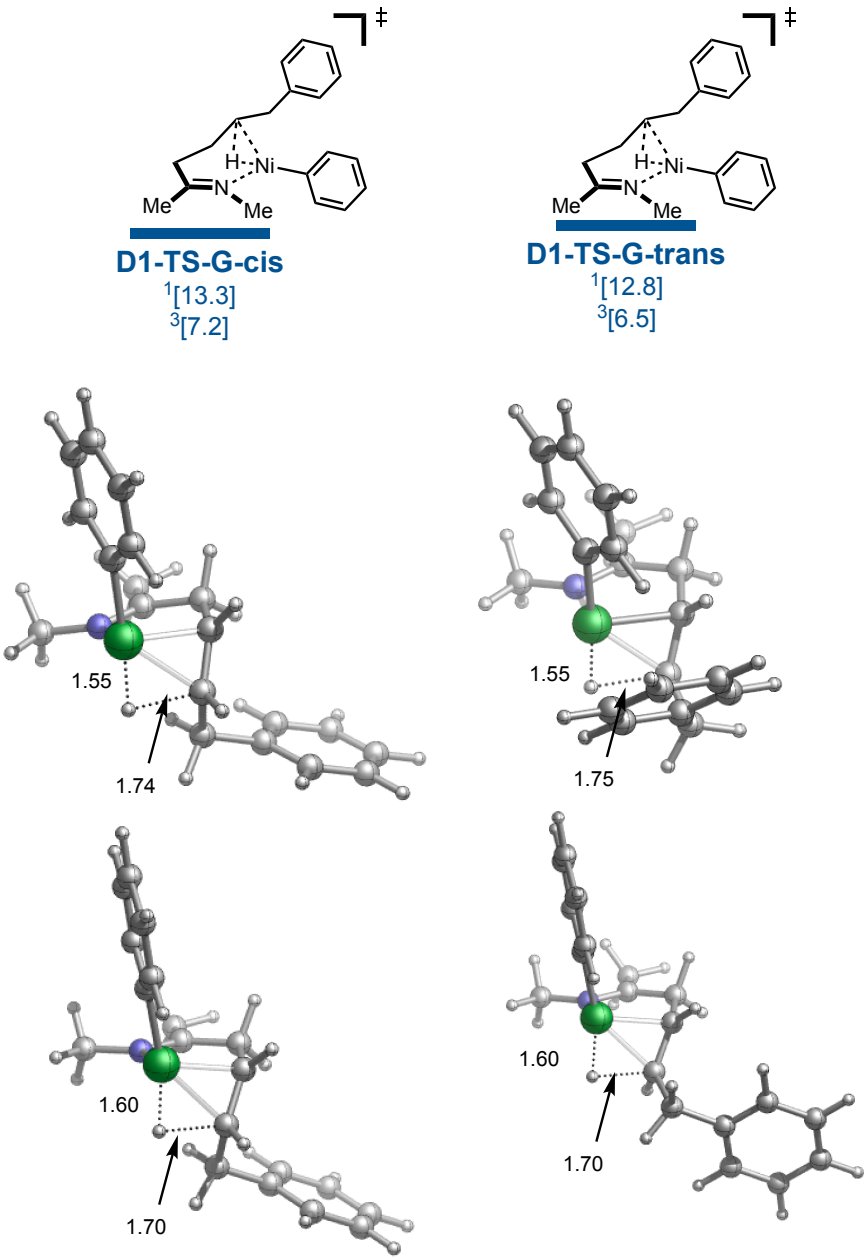


Figure A5.23 Conformers of **D1-TS-G**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

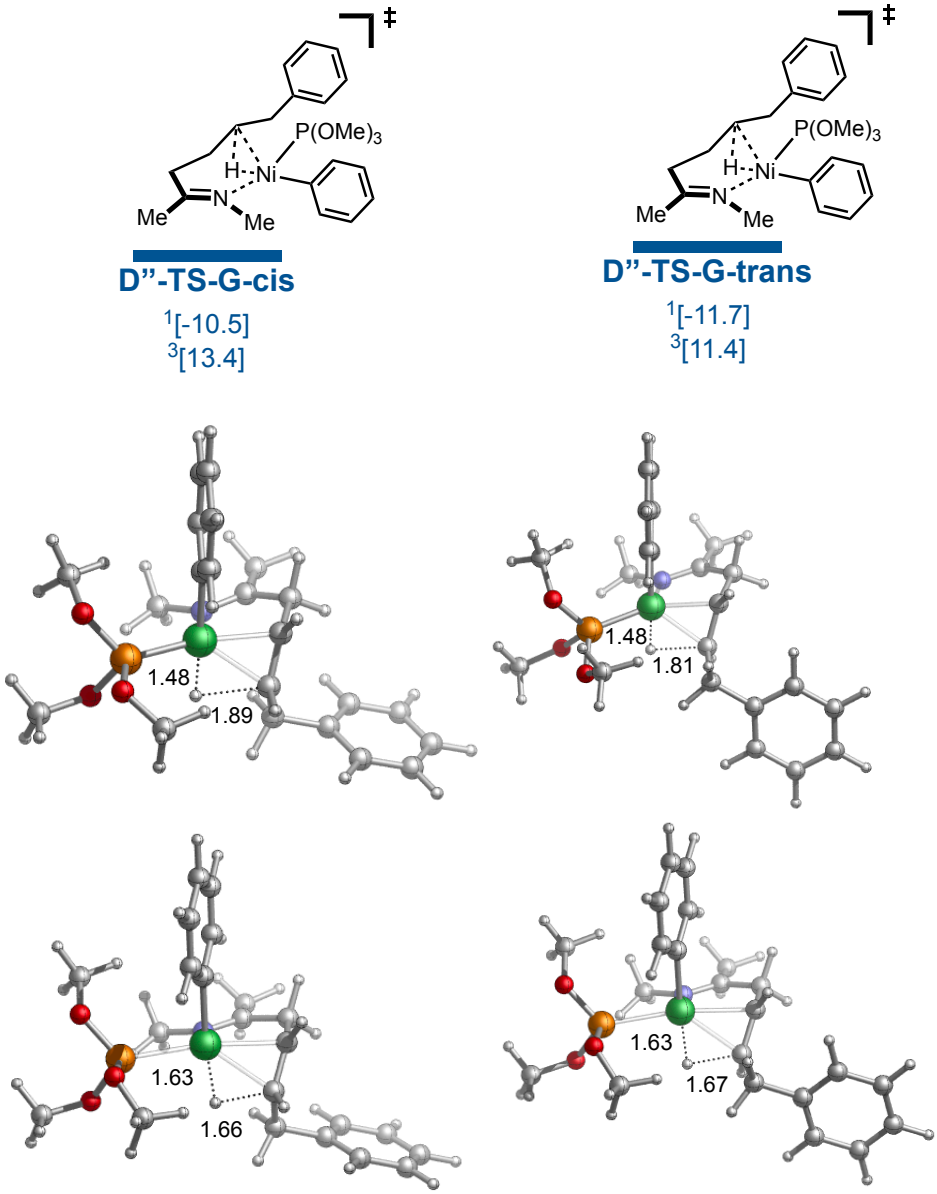


Figure A5.24 Conformers of **D''-TS-G**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

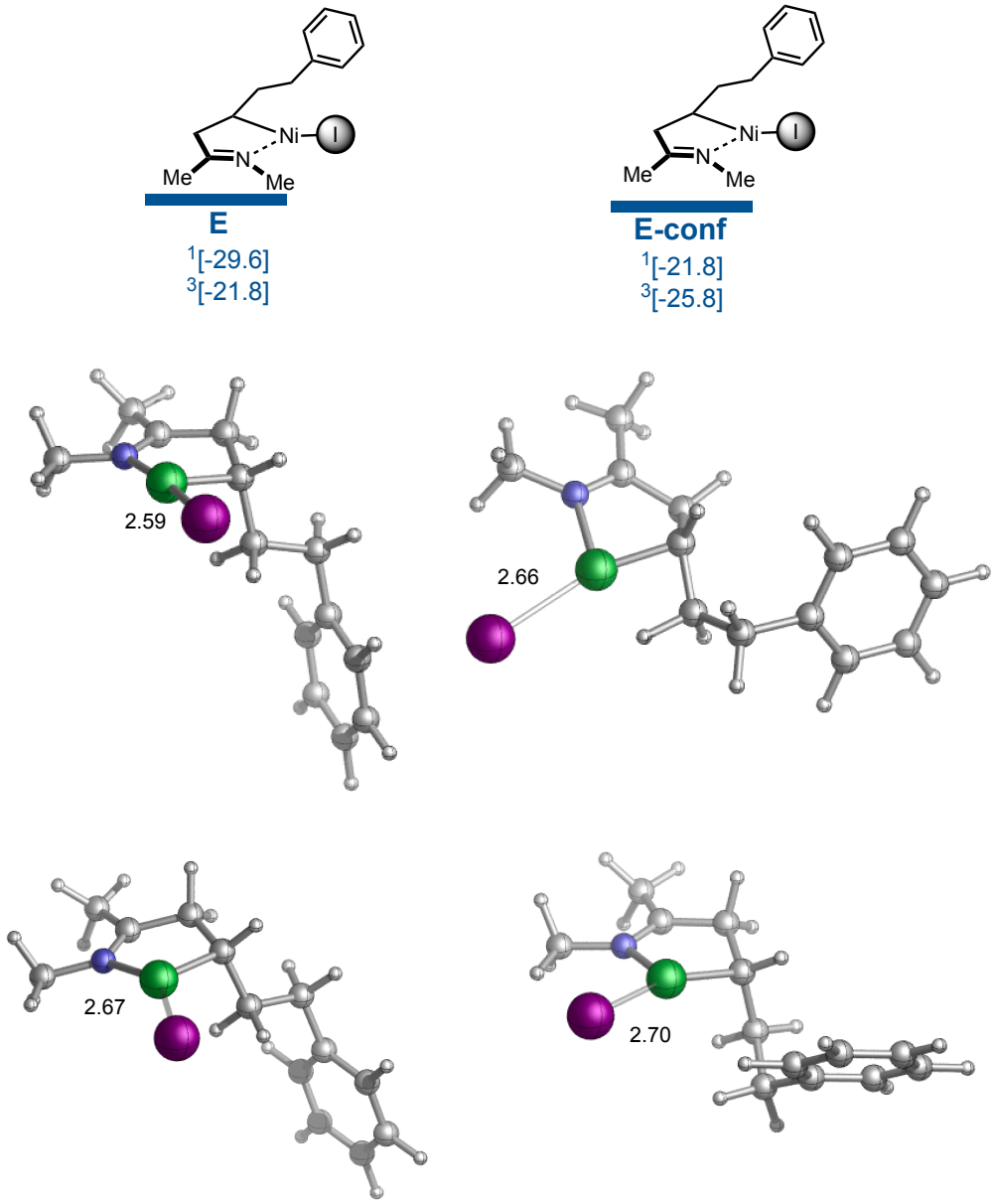


Figure A5.25 Conformers of **E**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

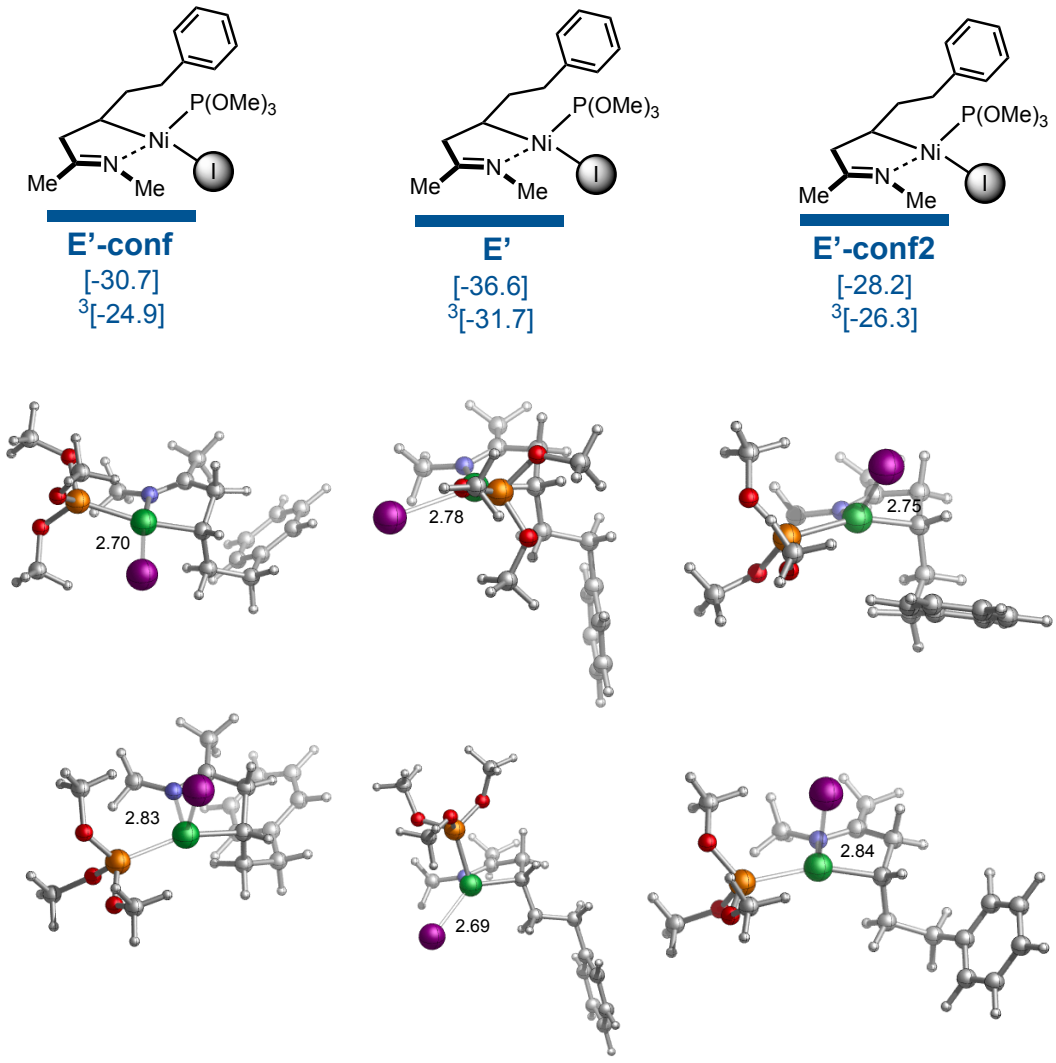


Figure A5.26 Conformers of **E'**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

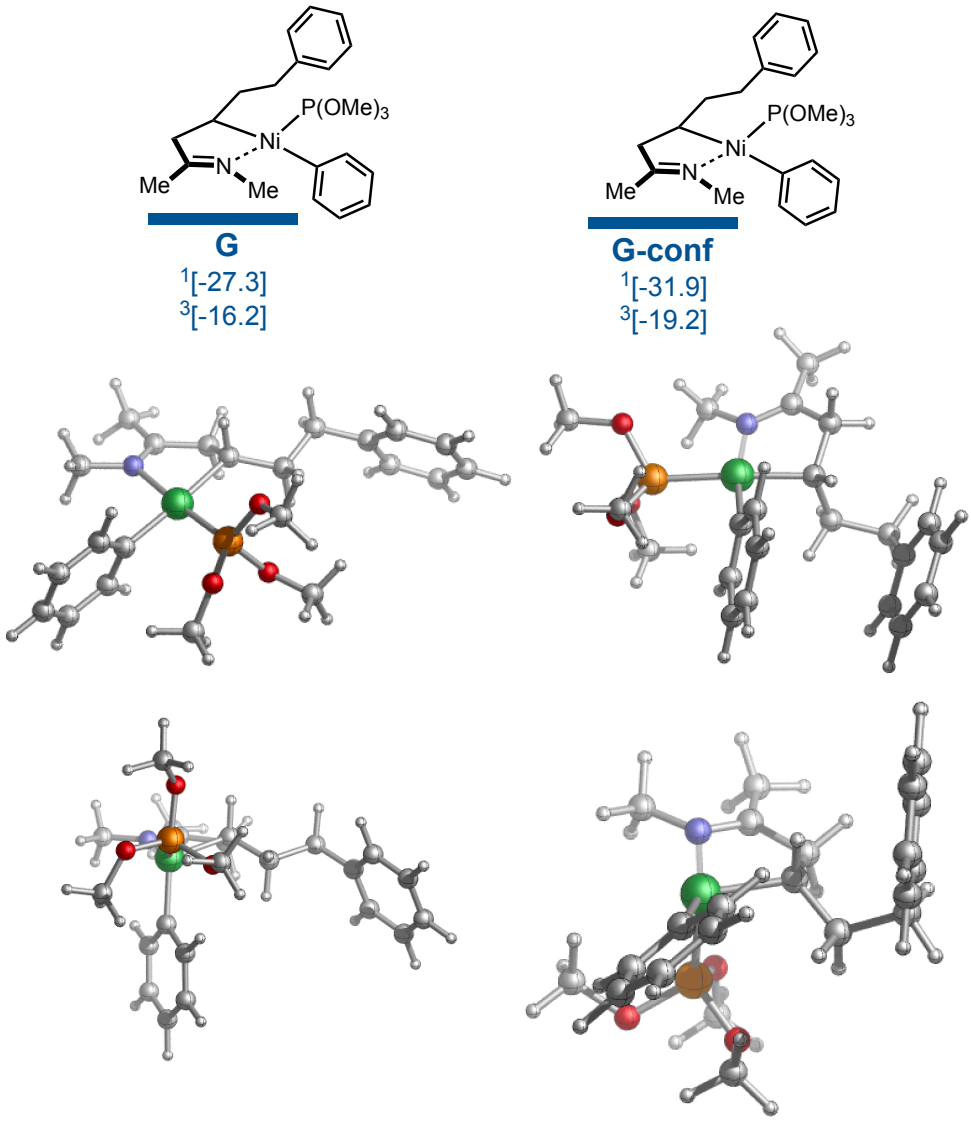


Figure A5.27 Conformers of **G**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

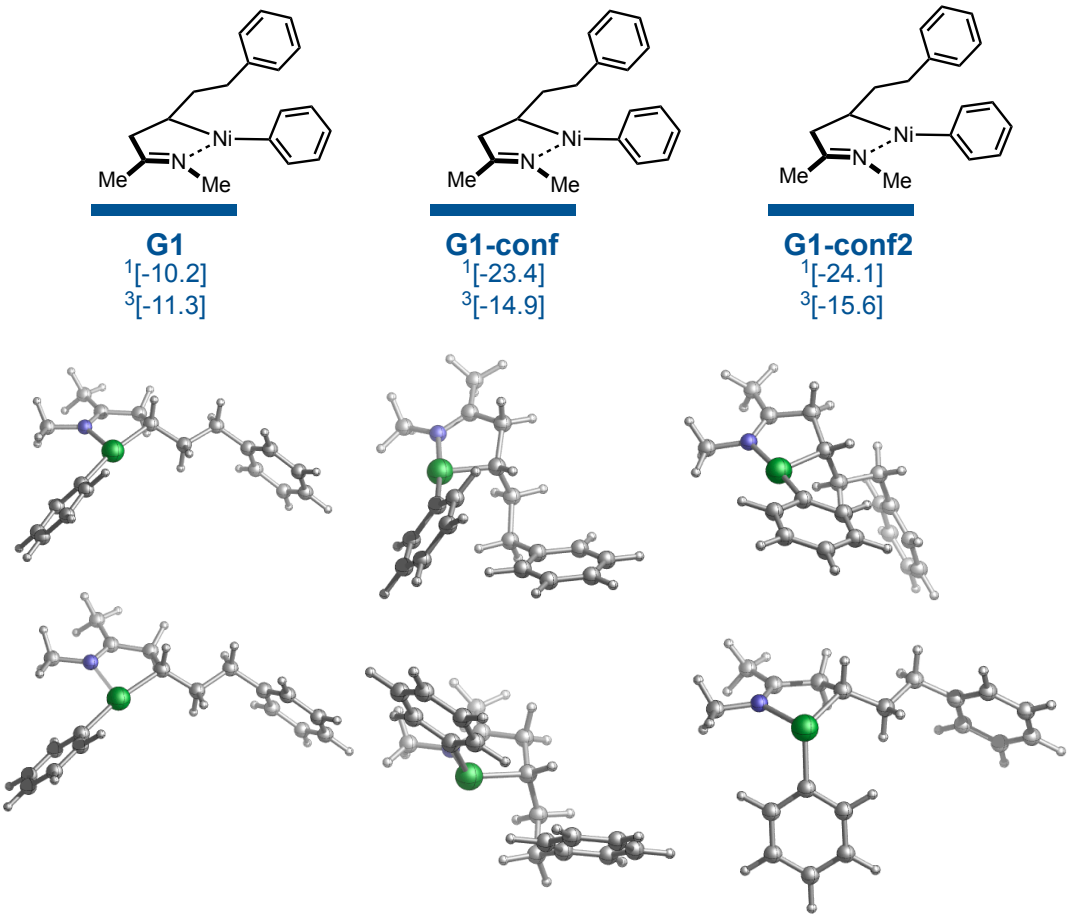


Figure A5.29 Conformers of **G1**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

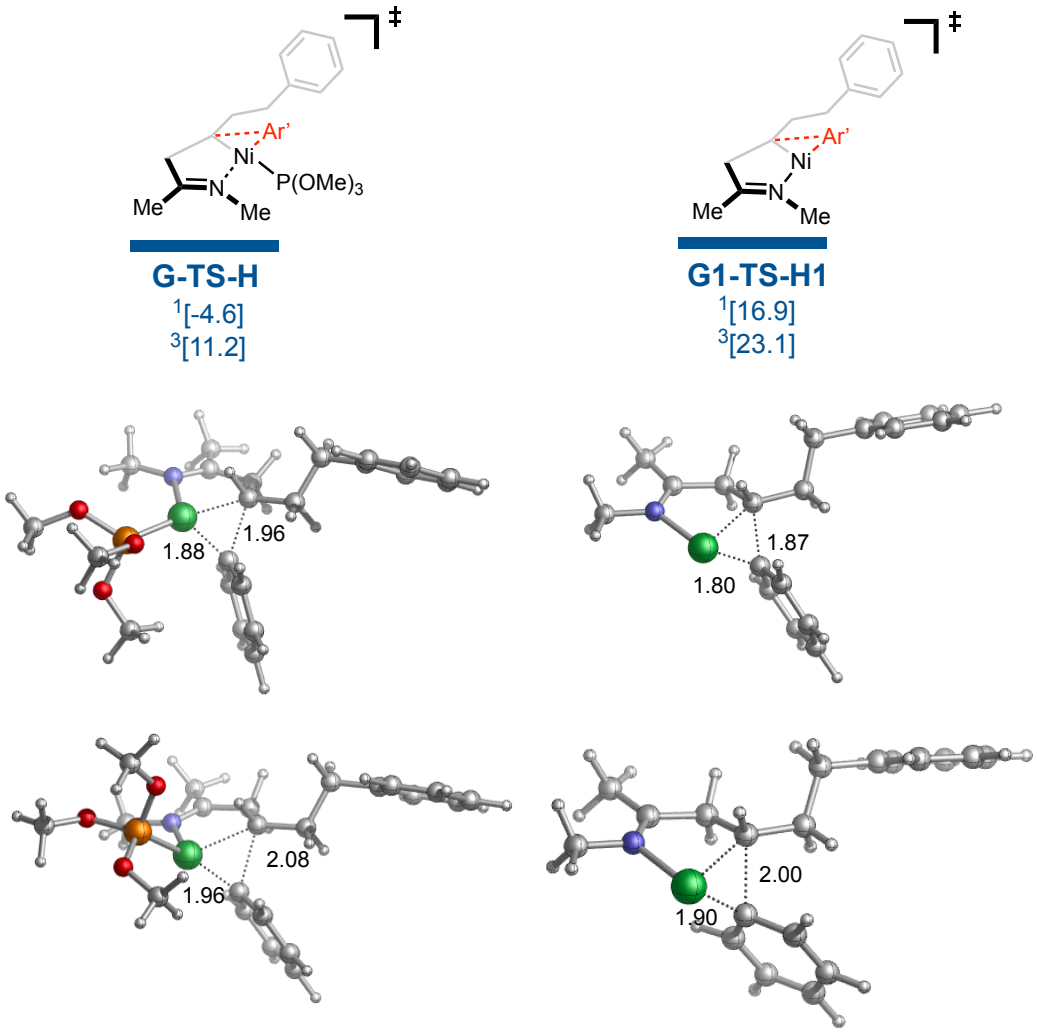


Figure A5.30 Conformers of **G-TS-H** and **G1-TS-H1**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

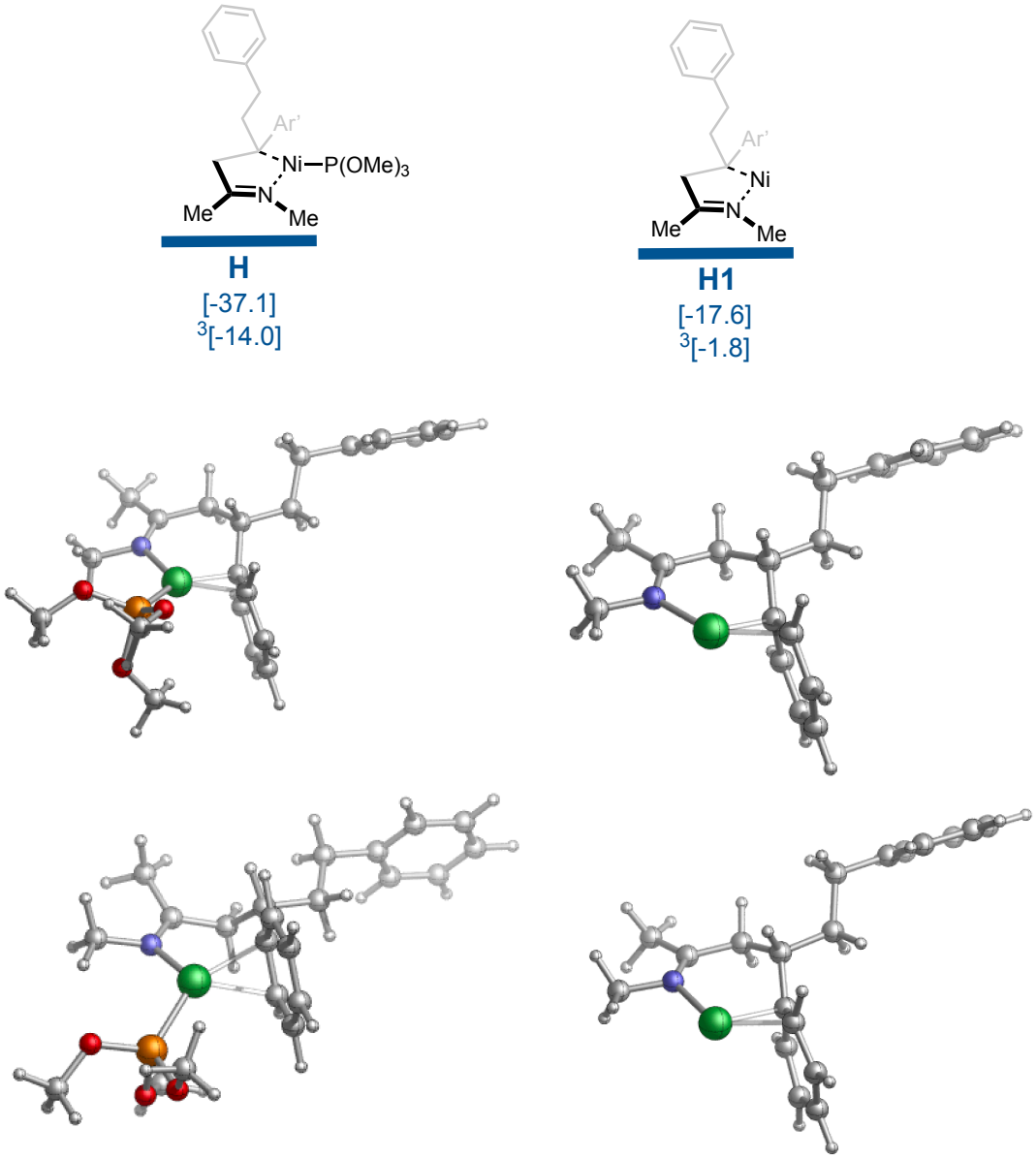


Figure A5.31 Conformers of **H** and **H1**. Singlet structures are given in the top row and triplet structures in the second row. Free energies are given at the UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

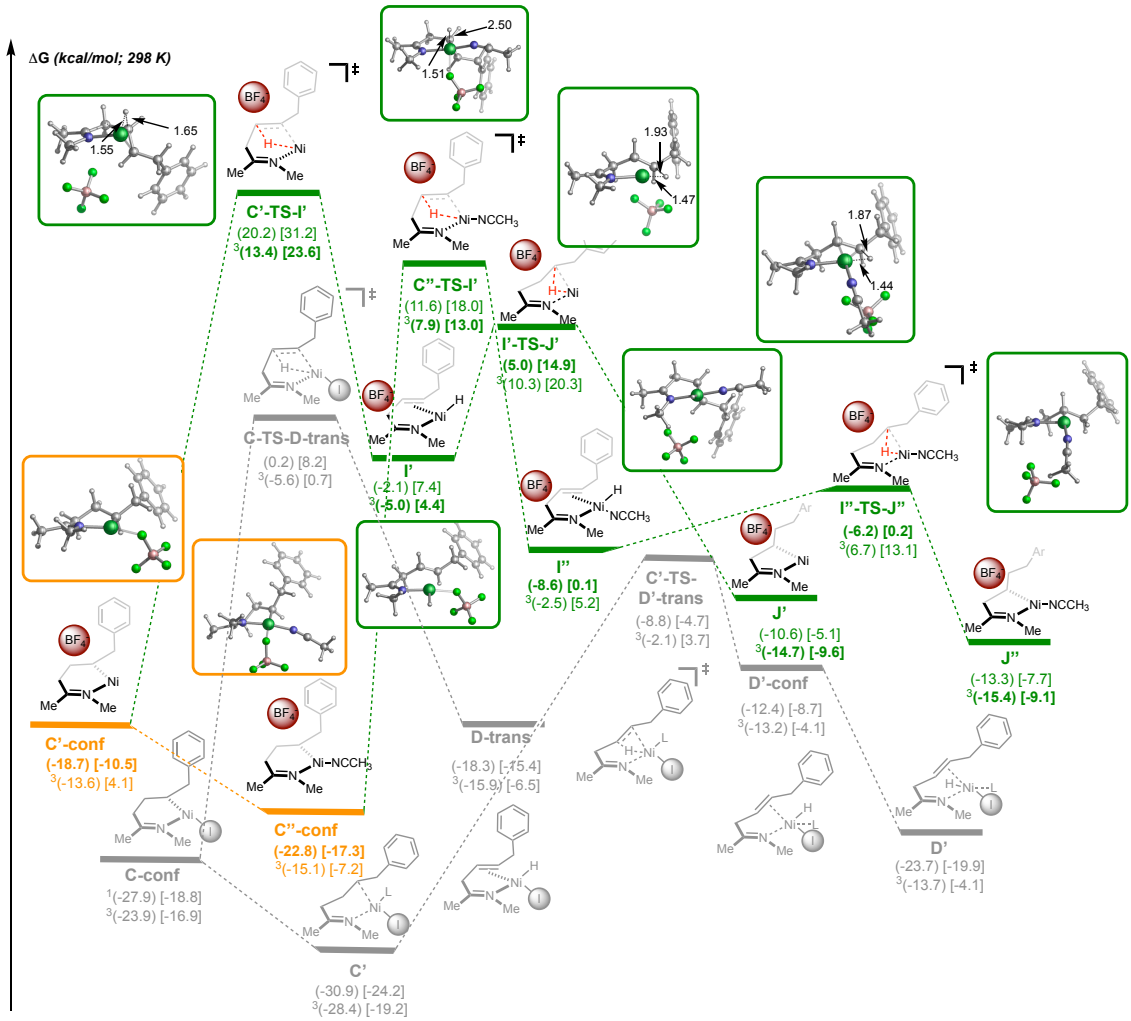


Figure A5.32 Reaction coordinate diagram showing higher energy β-hydride elimination and Ni-hydride reinsertion with $AgBF_4$ compared to the neutral system. Free energies are given at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory (parenthesis) and UM06/6-311+G(d,p)-SDD(I)-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) (brackets).

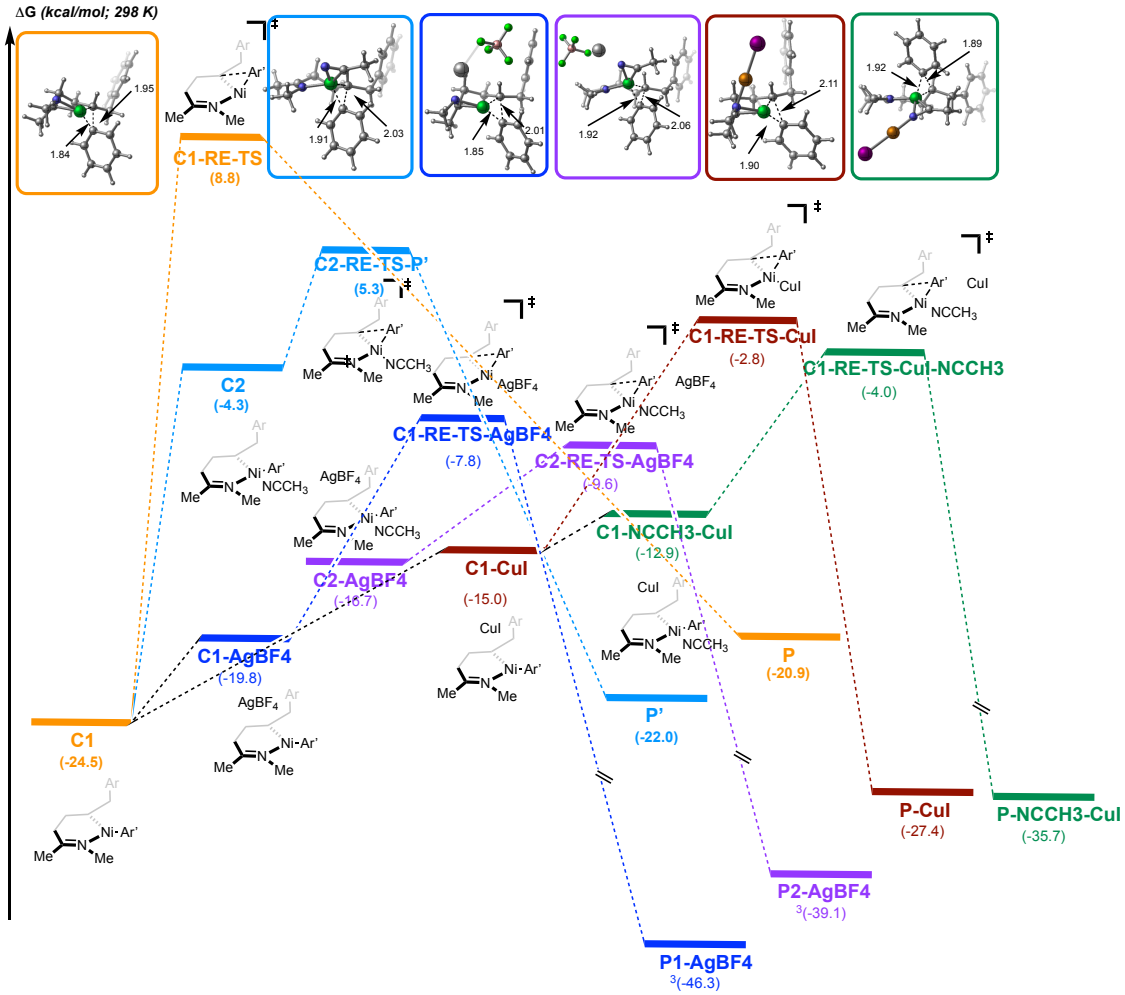


Figure A5.33 Reaction coordinate diagram summarizing the possible reductive elimination transition states to lead to 1,2-diarylation calculated at the UB3LYP-D3/def2TZVPP//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

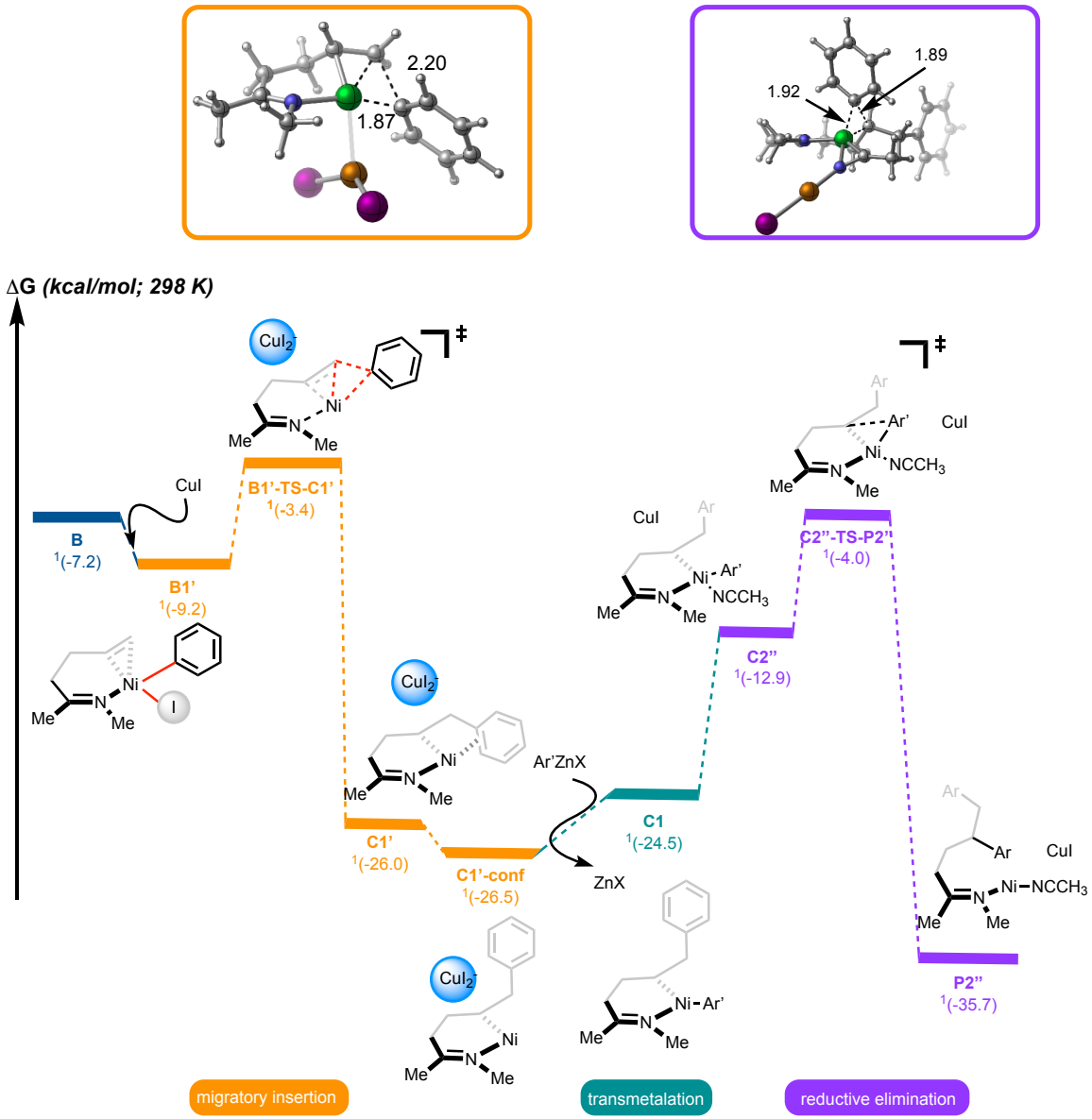


Figure A5.34 Reaction coordinate diagram of the lowest energy pathway with CuI leading to 1,2-diarylation calculated at the UB3LYP-D3/def2TZVPP//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory.

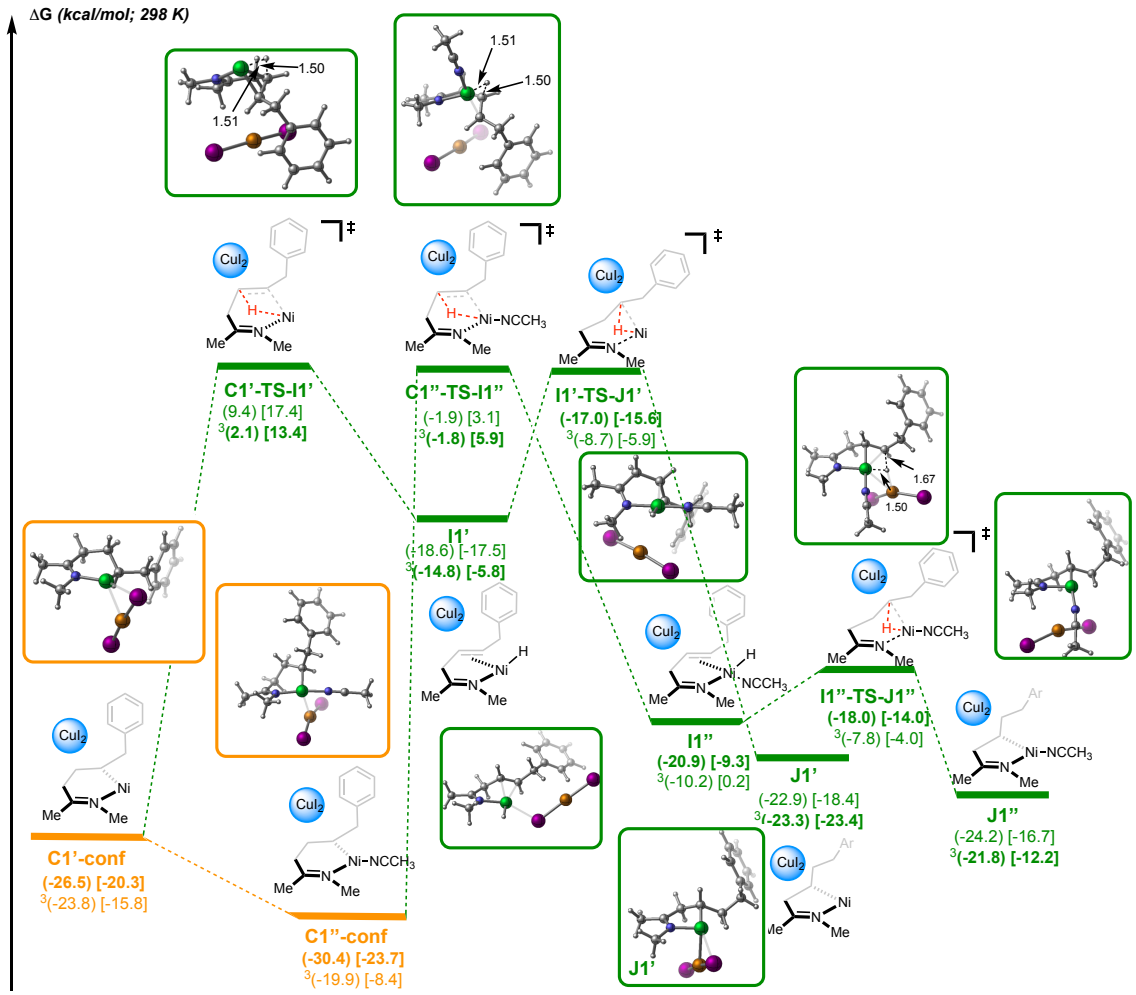


Figure A5.35 Reaction coordinate diagram showing higher energy β-hydride elimination and Ni-hydride reinsertion with CuI_2. Free energies are given at the UB3LYP-D3/def2TZVPP-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) level of theory (parenthesis) and UM06/6-311+G(d,p)-SDD(I)-CPCM(acetonitrile)//UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile) (brackets).

A5.3 Coordinates and Energies

A

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.317273 (Hartree/Particle)
Thermal correction to Energy= 0.339133
Thermal correction to Enthalpy= 0.340077
Thermal correction to Gibbs Free Energy= 0.265199
Sum of electronic and zero-point Energies= -2523.448906
Sum of electronic and thermal Energies= -2523.427046
Sum of electronic and thermal Enthalpies= -2523.426102
Sum of electronic and thermal Free Energies= -2523.500980

C	-2.70486	1.82946	0.66538
H	-2.31305	2.11837	1.66141
H	-2.31412	2.60493	-0.01689
C	-4.62876	3.46827	0.96076
H	-3.75407	4.1292	1.01508
H	-5.26229	3.81248	0.12722
H	-5.20787	3.5932	1.88909
Ni	-4.55111	-0.87549	0.51128
P	-6.0569	-2.0802	-0.28654
O	-5.65953	-3.06462	-1.57733
O	-6.71372	-3.28	0.65005
O	-7.48746	-1.43742	-0.80599
C	-5.84644	-4.20516	1.29424
H	-5.09839	-3.68671	1.91776
H	-6.46502	-4.85242	1.93286
H	-5.31262	-4.83043	0.55792
C	-4.83957	-2.52698	-2.607
H	-4.38398	-3.36575	-3.15437
H	-5.43091	-1.9199	-3.31529
H	-4.03652	-1.89513	-2.18869
C	-8.54939	-2.2356	-1.32947
H	-9.27018	-1.55572	-1.80652
H	-8.17516	-2.95162	-2.07898
H	-9.05387	-2.79605	-0.52603
C	-4.20547	2.02618	0.76117
C	-2.14671	0.45641	0.273
H	-2.35263	0.26765	-0.79542
H	-1.04294	0.52387	0.35746
C	-2.70617	-0.6734	1.10941
H	-2.59764	-0.52928	2.19684
C	-2.91132	-1.99328	0.61958
H	-2.53922	-2.27395	-0.37704
H	-2.90309	-2.83131	1.32901
N	-5.03587	1.04177	0.71701
C	-6.47423	1.26198	0.85548
H	-6.83537	0.65041	1.69655
H	-6.77322	2.30674	1.02132
H	-6.97467	0.87274	-0.04204

^{3}A

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.315573 (Hartree/Particle)
Thermal correction to Energy= 0.337962
Thermal correction to Enthalpy= 0.338907
Thermal correction to Gibbs Free Energy= 0.261499
Sum of electronic and zero-point Energies= -2523.396740
Sum of electronic and thermal Energies= -2523.374351
Sum of electronic and thermal Enthalpies= -2523.373407
Sum of electronic and thermal Free Energies= -2523.450814

C	-3.44009	1.50561	1.96787
H	-4.04225	0.91584	2.6824
H	-3.12971	2.43331	2.47534
C	-4.42112	3.32459	0.46811
H	-3.40319	3.72787	0.33644
H	-5.00709	3.56432	-0.42566
H	-4.85601	3.85804	1.33075
Ni	-4.42309	-1.02971	0.57297
P	-6.18389	-2.21967	0.08966
O	-6.29491	-2.88397	-1.43532
O	-6.45083	-3.63043	0.9092
O	-7.65809	-1.53633	0.28281
C	-5.38341	-4.57365	0.93712
H	-4.42417	-4.08285	1.19041
H	-5.61356	-5.32159	1.70883
H	-5.27296	-5.07699	-0.03823
C	-5.60742	-2.28829	-2.53191
H	-5.31208	-3.08936	-3.22586
H	-6.25843	-1.57457	-3.06499
H	-4.70377	-1.75726	-2.1799
C	-8.86744	-2.20704	-0.09037
H	-9.69059	-1.49467	0.05699
H	-8.83451	-2.51937	-1.14594
H	-9.03045	-3.09427	0.54134
C	-4.32392	1.85651	0.788
C	-2.19218	0.6763	1.58734
H	-1.62182	1.24332	0.82717
H	-1.5497	0.63	2.48399
C	-2.47283	-0.73659	1.08711
H	-2.11183	-1.53588	1.74959
C	-2.55757	-1.05253	-0.31129
H	-2.44456	-0.25261	-1.05511
H	-2.26792	-2.05196	-0.66039
N	-4.90878	0.89453	0.16008
C	-5.78656	1.10403	-0.98242
H	-6.07007	2.151	-1.1622
H	-5.29535	0.7114	-1.88608
H	-6.7022	0.51615	-0.82556

A'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.278717 (Hartree/Particle)
Thermal correction to Energy= 0.296848
Thermal correction to Enthalpy= 0.297792
Thermal correction to Gibbs Free Energy= 0.230486
Sum of electronic and zero-point Energies= -2079.892442

Sum of electronic and thermal Energies= -2079.874311
Sum of electronic and thermal Enthalpies= -2079.873367
Sum of electronic and thermal Free Energies= -2079.940674

C	-0.16286	2.36242	-2.56917
H	-0.39403	2.81338	-3.54584
H	-0.78357	1.45488	-2.4818
C	-1.09614	4.6471	-1.83276
H	-1.38372	5.27283	-0.98011
H	-0.33998	5.18418	-2.43085
H	-1.97321	4.51561	-2.48798
C	-0.5541	3.30024	-1.45135
C	1.33826	1.94907	-2.52841
H	1.45767	1.08007	-3.1942
H	1.93444	2.7691	-2.96123
C	1.88298	1.61914	-1.15132
H	2.35638	2.45563	-0.62162
C	2.11047	0.33514	-0.67508
H	1.92235	-0.54009	-1.30529
H	2.78185	0.16954	0.1742
N	-0.37489	2.87833	-0.24828
C	-0.67361	3.71037	0.91409
H	-0.15393	4.68033	0.86613
H	-1.75658	3.89608	1.00274
H	-0.34894	3.18308	1.81929
I	-0.559	-2.32082	-0.67107
Ni	0.32274	1.05478	0.03211
C	-0.16454	-0.5878	0.85522
C	0.61019	-1.00747	1.98882
C	-1.26263	0.32689	1.0534
C	0.34946	-0.48699	3.23668
H	1.42926	-1.71564	1.84436
C	-1.53862	0.78126	2.3889
H	-2.07802	0.38545	0.32552
C	-0.74152	0.40995	3.4473
H	0.9872	-0.76941	4.07922
H	-2.41746	1.41103	2.55519
H	-0.95679	0.77122	4.45611

A'-TS-B

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -65.00 cm^{-1}
Zero-point correction= 0.278896 (Hartree/Particle)
Thermal correction to Energy= 0.296427
Thermal correction to Enthalpy= 0.297371
Thermal correction to Gibbs Free Energy= 0.231242
Sum of electronic and zero-point Energies= -2079.891474
Sum of electronic and thermal Energies= -2079.873943
Sum of electronic and thermal Enthalpies= -2079.872999
Sum of electronic and thermal Free Energies= -2079.939127

C	-4.76154	0.12279	-0.4495
H	-5.06628	0.56488	-1.40923
H	-5.39149	-0.76891	-0.29452
C	-5.54457	2.44639	0.31545
H	-5.73161	3.11009	1.16662
H	-4.81533	2.92932	-0.35696
H	-6.47648	2.33631	-0.2629
C	-5.02955	1.08642	0.68572
C	-3.27189	-0.31977	-0.53034
H	-3.22326	-1.20571	-1.1818
H	-2.69762	0.47892	-1.02717
C	-2.61544	-0.62673	0.80189
H	-2.12036	0.22076	1.29177
C	-2.35468	-1.896	1.28029
H	-2.61575	-2.7859	0.70067
H	-1.64204	-2.05013	2.0965
N	-4.76168	0.6604	1.8701
C	-4.88047	1.44922	3.08511
H	-3.8719	1.60301	3.50094
H	-5.35866	2.4285	2.94562
H	-5.45065	0.86952	3.82484
I	-4.56549	-4.94323	1.74084
Ni	-4.10458	-1.17324	2.13411
C	-4.43047	-2.70215	3.11733
C	-3.70348	-2.94599	4.31432
C	-5.69057	-2.02774	3.16646
C	-4.20024	-2.47794	5.51842
H	-2.74153	-3.46121	4.27003
C	-6.19825	-1.62059	4.43914
H	-6.3953	-2.08518	2.33074
C	-5.45895	-1.82238	5.58858
H	-3.60841	-2.60859	6.429
H	-7.19844	-1.18149	4.49568
H	-5.84668	-1.50049	6.55821

B

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.280280 (Hartree/Particle)
Thermal correction to Energy= 0.298396
Thermal correction to Enthalpy= 0.299341
Thermal correction to Gibbs Free Energy= 0.232277
Sum of electronic and zero-point Energies= -2079.935026
Sum of electronic and thermal Energies= -2079.916909
Sum of electronic and thermal Enthalpies= -2079.915965
Sum of electronic and thermal Free Energies= -2079.983029

C	1.70917	2.42021	-1.53652
H	2.31806	2.9467	-0.77623
H	1.82175	3.02739	-2.44968
C	-0.29314	3.96836	-1.18834
H	0.48875	4.69531	-1.44255
H	-1.06559	4.00931	-1.97518
H	-0.77011	4.2749	-0.24506
C	0.26837	2.57248	-1.0869
C	2.29656	1.02379	-1.79966
H	1.75164	0.52926	-2.61974
H	3.33044	1.17219	-2.16209
C	2.34692	0.12852	-0.58469
H	2.78885	0.58797	0.30732
C	2.15579	-1.25647	-0.59584
H	2.05808	-1.80494	-1.53642
H	2.44366	-1.842	0.28216
N	-0.42218	1.59253	-0.61945
C	-1.79858	1.78984	-0.17196
H	-1.80805	2.29031	0.81001

H	-2.38572	2.39445	-0.87951
H	-2.27885	0.80953	-0.06757
I	-0.98601	-1.35637	-2.3997
Ni	0.40244	-0.17944	-0.36274
C	0.51198	0.03326	1.48438
C	0.20319	-1.15485	2.15969
C	0.71804	1.21316	2.20795
C	0.06232	-1.15221	3.55515
H	0.07129	-2.09139	1.60841
C	0.59095	1.20881	3.60334
H	0.96983	2.14218	1.69204
C	0.25757	0.02884	4.27902
H	-0.18973	-2.08114	4.07448
H	0.74954	2.1352	4.16267
H	0.15727	0.02867	5.3674

^{3}B

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.279304 (Hartree/Particle)
Thermal correction to Energy= 0.298168
Thermal correction to Enthalpy= 0.299113
Thermal correction to Gibbs Free Energy= 0.228142
Sum of electronic and zero-point Energies= -2079.941786
Sum of electronic and thermal Energies= -2079.922922
Sum of electronic and thermal Enthalpies= -2079.921977
Sum of electronic and thermal Free Energies= -2079.992948

C	-2.78348	0.96439	-0.02723
H	-1.84581	1.0996	0.54481
H	-2.63987	1.56344	-0.94219
C	-3.74996	3.13227	0.89721
H	-2.80504	3.4945	0.47307
H	-4.57889	3.62688	0.3635
H	-3.81026	3.44589	1.95075
C	-3.87043	1.63551	0.77117
C	-2.96436	-0.50338	-0.40562
H	-3.86149	-0.63487	-1.03299
H	-2.10126	-0.78959	-1.03243
C	-3.01684	-1.44526	0.76419
H	-2.37685	-1.20658	1.62201
C	-3.72202	-2.60154	0.7788
H	-4.30513	-2.92393	-0.0897
H	-3.64886	-3.29643	1.6194
N	-4.82902	0.97431	1.31965
C	-5.8553	1.69914	2.07617
H	-5.43649	2.08956	3.01711
H	-6.27317	2.5373	1.49799
H	-6.67517	1.01449	2.33029
I	-7.57094	-1.8594	0.85025
Ni	-5.15052	-1.01168	1.65128
C	-4.72381	-1.10434	3.57948
C	-3.72275	-0.30631	4.1644
C	-5.40648	-2.00107	4.42278
C	-3.41457	-0.39225	5.529
H	-3.16871	0.40739	3.54403
C	-5.10639	-2.09962	5.78945
H	-6.19545	-2.63731	4.00628
C	-4.10767	-1.29297	6.34728
H	-2.63277	0.24412	5.95557
H	-5.65473	-2.80602	6.42078
H	-3.87121	-1.36474	7.4127

B-TS-C

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -62.70 cm^{-1}
Zero-point correction= 0.280660 (Hartree/Particle)
Thermal correction to Energy= 0.298215
Thermal correction to Enthalpy= 0.299159
Thermal correction to Gibbs Free Energy= 0.231429
Sum of electronic and zero-point Energies= -2079.920088
Sum of electronic and thermal Energies= -2079.902532
Sum of electronic and thermal Enthalpies= -2079.901588
Sum of electronic and thermal Free Energies= -2079.969318

C	-3.66522	1.96837	0.06132
H	-3.82291	2.80164	0.77362
H	-3.38838	2.45487	-0.88804
C	-6.01396	2.0836	-0.94868
H	-6.19	1.55999	-1.90422
H	-6.98517	2.15328	-0.43563
H	-5.65686	3.09605	-1.17448
Ni	-4.18813	-0.96183	1.55674
C	-5.01088	1.31905	-0.12981
C	-2.52893	1.06322	0.53004
H	-2.30733	0.30527	-0.239
H	-1.62469	1.68984	0.63357
C	-2.78485	0.38758	1.85198
H	-3.09539	1.05048	2.67332
C	-2.17792	-0.8382	2.20397
H	-1.58126	-1.37793	1.46065
N	-5.28152	0.17384	0.39567
C	-6.60562	-0.42295	0.17641
H	-6.81891	-0.53112	-0.89827
H	-6.65308	-1.42235	0.62926
H	-7.39731	0.19195	0.63278
C	-3.70231	-2.36912	2.68385
C	-3.48726	-3.59033	2.02366
C	-4.15679	-2.3421	4.01293
C	-3.79556	-4.78744	2.68263
H	-3.09384	-3.5989	1.00271
C	-4.46328	-3.54416	4.6589
H	-4.27363	-1.38828	4.53453
C	-4.28195	-4.76536	3.99497
H	-3.64382	-5.7412	2.16992
H	-4.83651	-3.52862	5.68637
H	-4.50883	-5.70298	4.50871
I	-2.52069	-2.43845	-1.89855
H	-1.90546	-1.02111	3.24311

^{3}B-TS-C

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -406.74 cm^{-1}
Zero-point correction= 0.278099 (Hartree/Particle)
Thermal correction to Energy= 0.296140
Thermal correction to Enthalpy= 0.297084

Thermal correction to Gibbs Free Energy= 0.228574
Sum of electronic and zero-point Energies= -2079.901490
Sum of electronic and thermal Energies= -2079.883449
Sum of electronic and thermal Enthalpies= -2079.882505
Sum of electronic and thermal Free Energies= -2079.951015

C	-3.67753	1.92925	0.12465
H	-3.80756	2.70357	0.90615
H	-3.43266	2.5012	-0.78747
C	-6.06465	2.28771	-0.69186
H	-6.30528	1.97853	-1.72354
H	-7.00667	2.2823	-0.1227
H	-5.67812	3.31425	-0.72729
Ni	-4.10587	-1.18019	1.09863
C	-5.05431	1.3402	-0.09332
C	-2.49989	1.01658	0.49244
H	-2.28649	0.32758	-0.34057
H	-1.61242	1.67668	0.5714
C	-2.72107	0.25276	1.77409
H	-3.10513	0.84902	2.6128
C	-2.14314	-1.0113	2.11147
H	-1.48292	-1.4904	1.37901
N	-5.3557	0.1267	0.21179
C	-6.70316	-0.38301	-0.04891
H	-7.06324	-0.12103	-1.05603
H	-6.69775	-1.47706	0.03605
H	-7.41799	0.01902	0.6885
C	-3.42209	-2.51387	2.51025
C	-2.97181	-3.81866	2.25133
C	-4.27423	-2.29397	3.60891
C	-3.39282	-4.88538	3.04977
H	-2.30503	-3.99887	1.40382
C	-4.72137	-3.36488	4.39383
H	-4.58813	-1.27367	3.86258
C	-4.27583	-4.66189	4.11694
H	-3.04063	-5.89882	2.83668
H	-5.40204	-3.18429	5.23048
H	-4.60811	-5.49913	4.73628
I	-3.42412	-2.47616	-1.29143
H	-1.80051	-1.14614	3.1402

C

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.282504 (Hartree/Particle)
Thermal correction to Energy= 0.299219
Thermal correction to Enthalpy= 0.300163
Thermal correction to Gibbs Free Energy= 0.235367
Sum of electronic and zero-point Energies= -2079.954476
Sum of electronic and thermal Energies= -2079.937761
Sum of electronic and thermal Enthalpies= -2079.936817
Sum of electronic and thermal Free Energies= -2080.001613

C	-0.11146	3.37977	-0.26934
H	-0.27414	4.18953	0.4689
H	0.12837	3.8939	-1.21376
C	-2.44616	3.37208	-1.33003
H	-2.49276	2.85187	-2.30316
H	-3.45696	3.35157	-0.89752
H	-2.15879	4.41417	-1.51993
Ni	-0.62684	0.59499	1.3676
C	-1.43966	2.68862	-0.44752
C	1.04886	2.48482	0.15643
H	1.23503	1.72925	-0.626
H	1.96089	3.10863	0.21809
C	0.82033	1.79836	1.47871
H	0.58184	2.51557	2.2847
C	1.81687	0.7214	1.90771
H	2.47221	0.43275	1.0742
N	-1.68538	1.56519	0.13497
C	-2.96726	0.88486	-0.08757
H	-3.19438	0.80294	-1.16104
H	-2.93077	-0.13532	0.31949
H	-3.78801	1.42322	0.41241
C	0.93605	-0.46469	2.29799
C	0.97951	-1.70388	1.60873
C	-0.01276	-0.30048	3.34132
C	0.12093	-2.73832	1.96029
H	1.67792	-1.8243	0.77862
C	-0.87654	-1.36225	3.69211
H	0.00352	0.6008	3.95997
C	-0.81276	-2.56756	3.00201
H	0.16213	-3.68509	1.41693
H	-1.58652	-1.22963	4.51117
H	-1.48539	-3.38634	3.26809
I	0.60456	-1.02675	-2.45922
H	2.4503	1.03806	2.75311

^{3}C

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.281236 (Hartree/Particle)
Thermal correction to Energy= 0.299168
Thermal correction to Enthalpy= 0.300112
Thermal correction to Gibbs Free Energy= 0.230940
Sum of electronic and zero-point Energies= -2079.960487
Sum of electronic and thermal Energies= -2079.942555
Sum of electronic and thermal Enthalpies= -2079.941611
Sum of electronic and thermal Free Energies= -2080.010783

C	0.07521	3.37415	-0.12657
H	-0.09513	3.88392	0.84276
H	0.60701	4.11874	-0.74252
C	-1.92268	4.43423	-1.32611
H	-1.93242	4.36759	-2.42797
H	-2.96787	4.54423	-0.99993
H	-1.36451	5.3365	-1.04556
Ni	-1.22177	0.41177	0.2037
C	-1.28982	3.19495	-0.74781
C	0.96095	2.14119	0.07358
H	1.13245	1.66219	-0.90878
H	1.95619	2.51262	0.39579
C	0.42398	1.10991	1.0616
H	0.14295	1.62715	2.00198
C	1.44582	0.01635	1.34832
H	1.75393	-0.44095	0.39097

N	-1.88006	2.05102	-0.77495
C	-3.1942	1.91388	-1.40341
H	-3.20065	2.31266	-2.43033
H	-3.46399	0.85103	-1.44741
H	-3.96761	2.44446	-0.82347
C	1.02593	-1.1042	2.28208
C	1.80008	-2.2775	2.34792
C	-0.10819	-1.02095	3.10593
C	1.45727	-3.32767	3.20263
H	2.6853	-2.36657	1.7104
C	-0.45846	-2.07154	3.96463
H	-0.73704	-0.12912	3.06854
C	0.32234	-3.229	4.01842
H	2.07454	-4.22993	3.23029
H	-1.34902	-1.98177	4.59295
H	0.04936	-4.05016	4.68637
I	-0.84228	-1.52608	-1.63055
H	2.37807	0.46179	1.76184

C-conf

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.282145 (Hartree/Particle)
Thermal correction to Energy= 0.300031
Thermal correction to Enthalpy= 0.300975
Thermal correction to Gibbs Free Energy= 0.232023
Sum of electronic and zero-point Energies= -2079.957687
Sum of electronic and thermal Energies= -2079.939800
Sum of electronic and thermal Enthalpies= -2079.938856
Sum of electronic and thermal Free Energies= -2080.007809

C	0.18501	-1.7144	-2.88418
H	0.7507	-1.7901	-3.82553
H	-0.30365	-2.69806	-2.74484
C	-1.39447	-0.38365	-4.4408
H	-2.49012	-0.29305	-4.47768
H	-0.97603	0.57941	-4.78381
H	-1.07564	-1.15926	-5.14889
Ni	-1.21415	-0.6006	-0.22844
C	-0.90003	-0.68406	-3.05454
C	1.12024	-1.40702	-1.71727
H	1.96186	-2.1219	-1.75186
H	1.56128	-0.40721	-1.87619
C	0.46557	-1.46083	-0.34726
H	0.20406	-2.50835	-0.09521
N	-1.3547	-0.08019	-2.00906
C	-2.38544	0.95556	-2.13706
H	-2.06331	1.7498	-2.82801
H	-3.3332	0.5299	-2.50366
H	-2.57279	1.41814	-1.15722
C	2.64882	-1.63097	0.94398
C	2.64699	-2.8448	1.65352
C	3.85929	-1.18754	0.38836
C	3.81886	-3.59107	1.80672
H	1.71166	-3.20449	2.09302
C	5.03592	-1.93056	0.53921
H	3.87991	-0.24577	-0.16752
C	5.02004	-3.13599	1.24884
H	3.79654	-4.52981	2.36701
H	5.96893	-1.56505	0.1016
H	5.93817	-3.7168	1.36943
I	-2.19343	-1.19411	2.1295
C	1.35614	-0.8618	0.75452
H	0.80532	-0.85395	1.70501
H	1.58126	0.18802	0.50469

^{3}C-conf

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.281043 (Hartree/Particle)
Thermal correction to Energy= 0.299165
Thermal correction to Enthalpy= 0.300109
Thermal correction to Gibbs Free Energy= 0.229673
Sum of electronic and zero-point Energies= -2079.958732
Sum of electronic and thermal Energies= -2079.940611
Sum of electronic and thermal Enthalpies= -2079.939667
Sum of electronic and thermal Free Energies= -2080.010103

C	0.40155	-1.38466	-2.79983
H	0.97471	-1.31918	-3.73988
H	0.15254	-2.45963	-2.69668
C	-1.47689	-0.77359	-4.42699
H	-2.56077	-0.95951	-4.40898
H	-1.31533	0.17461	-4.9692
H	-0.98555	-1.57339	-4.99613
Ni	-1.00143	-0.11558	-0.13303
C	-0.9044	-0.66536	-3.03711
C	1.27078	-0.92951	-1.62567
H	2.24786	-1.44103	-1.73349
H	1.48913	0.14949	-1.74089
C	0.66068	-1.18316	-0.2537
H	0.37413	-2.25231	-0.16957
N	-1.48914	0.00117	-2.10357
C	-2.72832	0.72914	-2.38174
H	-2.65548	1.33442	-3.29886
H	-3.5762	0.03235	-2.49204
H	-2.94743	1.39437	-1.53706
C	2.81275	-1.72047	1.01408
C	2.72244	-2.97681	1.63974
C	4.03776	-1.36186	0.4268
C	3.81626	-3.84638	1.67776
H	1.77684	-3.27463	2.10343
C	5.13617	-2.22952	0.45923
H	4.13176	-0.38731	-0.06113
C	5.02975	-3.4763	1.08458
H	3.72311	-4.81633	2.17423
H	6.07962	-1.92898	-0.00492
H	5.88644	-4.15475	1.11232
I	-2.79825	0.74804	1.69036
C	1.59284	-0.82527	0.91823
H	1.0248	-0.8925	1.86182
H	1.91269	0.22691	0.819

C-TS-D

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -789.53 cm^{-1}
Zero-point correction= 0.275033 (Hartree/Particle)

Thermal correction to Energy= 0.293316
Thermal correction to Enthalpy= 0.294260
Thermal correction to Gibbs Free Energy= 0.223225
Sum of electronic and zero-point Energies= -2079.913689
Sum of electronic and thermal Energies= -2079.895406
Sum of electronic and thermal Enthalpies= -2079.894462
Sum of electronic and thermal Free Energies= -2079.965497

C	-3.46126	0.80068	0.56569
H	-3.16206	1.52623	-0.21136
H	-2.95977	-0.1458	0.29862
C	-5.46044	-0.03347	-0.83762
H	-5.98714	-0.97388	-0.6036
H	-6.18689	0.62393	-1.34202
H	-4.64135	-0.25725	-1.53304
Ni	-4.74951	1.78771	2.97029
C	-4.95621	0.60643	0.42445
C	-2.99345	1.26618	1.93523
H	-2.14183	1.95335	1.92172
H	-3.94524	2.67535	2.04197
C	-3.13157	0.44153	3.07282
H	-3.62813	-0.52987	2.95946
N	-5.72424	1.0248	1.36466
C	-7.17175	0.89858	1.26735
H	-7.56809	1.52596	0.45114
H	-7.47817	-0.1427	1.07288
H	-7.61935	1.22602	2.21369
C	-0.98691	-0.22601	4.19903
C	-0.97311	-1.56348	4.62795
C	0.18274	0.30603	3.63121
C	0.17654	-2.34877	4.49318
H	-1.87456	-1.99285	5.07537
C	1.33493	-0.47514	3.49577
H	0.19174	1.34734	3.29597
C	1.3356	-1.80708	3.92572
H	0.16871	-3.38685	4.8363
H	2.23706	-0.0408	3.05654
H	2.23583	-2.41838	3.82266
I	-6.1516	1.60185	5.16438
C	-2.25252	0.60658	4.29459
H	-2.82166	0.31783	5.19203
H	-1.99169	1.67075	4.41229

^{3}C-TS-D

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -904.94 cm^{-1}
Zero-point correction= 0.275605 (Hartree/Particle)
Thermal correction to Energy= 0.293640
Thermal correction to Enthalpy= 0.294584
Thermal correction to Gibbs Free Energy= 0.223892
Sum of electronic and zero-point Energies= -2079.924524
Sum of electronic and thermal Energies= -2079.906489
Sum of electronic and thermal Enthalpies= -2079.905545
Sum of electronic and thermal Free Energies= -2079.976237

C	-3.39891	0.48641	0.63729
H	-3.00095	1.13275	-0.16545
H	-3.00972	-0.5262	0.43295
C	-5.48402	-0.19626	-0.72987
H	-6.11343	-1.05064	-0.42886
H	-6.13309	0.50176	-1.28267
H	-4.69939	-0.56254	-1.40409
Ni	-4.58308	1.95014	2.87383
C	-4.90244	0.46971	0.48312
C	-2.91883	0.95841	1.99792
H	-1.92094	1.40646	2.0022
H	-3.4907	2.52718	1.89225
C	-3.33456	0.27759	3.16896
H	-4.01739	-0.57281	3.06089
N	-5.61077	1.0565	1.37979
C	-7.06329	1.1125	1.2828
H	-7.37824	1.71317	0.413
H	-7.50167	0.10662	1.17821
H	-7.45991	1.57943	2.19292
C	-1.45522	-0.7451	4.48677
C	-1.75489	-2.03523	4.95526
C	-0.16216	-0.49629	3.99729
C	-0.79231	-3.04961	4.93287
H	-2.75635	-2.24571	5.34259
C	0.80392	-1.50772	3.97341
H	0.09187	0.5039	3.63411
C	0.49178	-2.78962	4.44019
H	-1.04469	-4.04653	5.30433
H	1.8059	-1.29272	3.59223
H	1.24599	-3.58061	4.42372
I	-5.96305	2.91841	4.87938
C	-2.52465	0.33165	4.44849
H	-3.19733	0.21571	5.31338
H	-2.05803	1.32611	4.54179

C'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.412712 (Hartree/Particle)
Thermal correction to Energy= 0.441749
Thermal correction to Enthalpy= 0.442694
Thermal correction to Gibbs Free Energy= 0.349052
Sum of electronic and zero-point Energies= -2766.312316
Sum of electronic and thermal Energies= -2766.283279
Sum of electronic and thermal Enthalpies= -2766.282335
Sum of electronic and thermal Free Energies= -2766.375976

C	0.89703	0.65245	-3.3051
H	1.09388	1.58153	-3.86827
H	1.48569	-0.12743	-3.82577
C	-1.05699	0.2203	-4.91217
H	-1.95539	0.84616	-5.035
H	-0.29391	0.55474	-5.62659
H	-1.34689	-0.81171	-5.17166
Ni	-0.80079	-0.13687	-0.57076
C	-0.54657	0.28527	-3.49784
C	1.36033	0.78449	-1.86208
H	2.4503	0.96467	-1.88378
H	0.93423	1.70233	-1.41205
N	-1.27538	0.00471	-2.4774

C	-2.66059	-0.43086	-2.68248
H	-3.27855	0.39433	-3.07086
H	-2.71143	-1.27356	-3.38983
H	-3.09256	-0.75052	-1.727
I	-2.71314	1.73387	0.32597
P	-0.9463	-1.53601	1.04421
O	-2.39399	-2.2953	1.10129
O	-0.00411	-2.84904	0.84668
O	-0.76553	-1.15535	2.62964
C	-0.05634	-3.96589	1.74445
H	-1.03171	-4.47133	1.67735
H	0.74168	-4.65635	1.4412
H	0.11384	-3.63953	2.78227
C	-3.5404	-1.80194	1.79947
H	-4.25336	-2.63534	1.86737
H	-3.26896	-1.46926	2.81298
H	-4.00051	-0.96304	1.25551
C	-0.1619	0.0758	3.0399
H	0.88873	-0.09396	3.32185
H	-0.20917	0.82529	2.23401
H	-0.71945	0.45123	3.90959
C	1.97167	-0.38994	0.2886
H	1.61996	-1.11971	1.02794
H	1.90773	0.60423	0.75902
C	3.4163	-0.72364	-0.02526
C	3.77842	-2.05668	-0.28994
C	4.41227	0.26298	-0.09166
C	5.0957	-2.39357	-0.61181
H	3.01172	-2.83557	-0.23752
C	5.7337	-0.06943	-0.41482
H	4.15045	1.30434	0.11693
C	6.07976	-1.39873	-0.67719
H	5.35782	-3.43646	-0.80995
H	6.49509	0.71398	-0.45957
H	7.11095	-1.6602	-0.92844
C	1.06954	-0.41789	-0.96015
H	1.21058	-1.36912	-1.50334

^{3}C'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.410702 (Hartree/Particle)
Thermal correction to Energy= 0.440517
Thermal correction to Enthalpy= 0.441462
Thermal correction to Gibbs Free Energy= 0.344174
Sum of electronic and zero-point Energies= -2766.305479
Sum of electronic and thermal Energies= -2766.275664
Sum of electronic and thermal Enthalpies= -2766.274719
Sum of electronic and thermal Free Energies= -2766.372007

C	0.76201	0.08045	-3.48645
H	1.13139	0.72673	-4.30137
H	1.04586	-0.94589	-3.79394
C	-1.35398	0.17477	-4.92061
H	-1.72285	1.19133	-5.14242
H	-0.61158	-0.08625	-5.68616
H	-2.20975	-0.51125	-5.00487
Ni	-0.78522	-0.30116	-0.60499
C	-0.74505	0.14035	-3.54096
C	1.45472	0.44909	-2.17361
H	2.54032	0.49893	-2.39359
H	1.16258	1.47663	-1.88716
N	-1.45554	0.1608	-2.46893
C	-2.91223	0.26331	-2.54387
H	-3.29172	0.61218	-1.57397
H	-3.25167	0.97006	-3.31683
H	-3.3562	-0.72406	-2.75528
I	-1.29938	2.1654	0.59475
P	-1.09279	-1.73809	1.22892
O	-2.49442	-2.57706	1.25543
O	-0.01517	-2.9514	1.20877
O	-1.10159	-1.22613	2.78572
C	-0.05265	-4.03699	2.14971
H	-0.8724	-4.72822	1.90242
H	0.90993	-4.55931	2.07479
H	-0.19056	-3.66274	3.17575
C	-3.73036	-1.87466	1.08519
H	-4.5056	-2.62234	0.87155
H	-3.99631	-1.32213	2.00083
H	-3.671	-1.16513	0.24201
C	-0.02191	-0.45405	3.32644
H	0.87266	-1.08158	3.47191
H	0.22515	0.39832	2.6754
H	-0.35594	-0.07509	4.30181
C	2.04685	-0.24833	0.21867
H	1.70359	-0.90219	1.03508
H	1.90132	0.79044	0.55971
C	3.52043	-0.5157	-0.00943
C	4.01211	-1.83303	0.02919
C	4.42041	0.517	-0.32025
C	5.35669	-2.11057	-0.23265
H	3.3238	-2.64937	0.27018
C	5.76807	0.24522	-0.58607
H	4.05884	1.5491	-0.35046
C	6.24178	-1.07028	-0.54397
H	5.71791	-3.14202	-0.19134
H	6.45089	1.06537	-0.82503
H	7.29396	-1.28454	-0.74903
C	1.1731	-0.49788	-1.01581
H	1.30493	-1.54953	-1.34722

C'-TS-D'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -513.50 cm^{-1}
Zero-point correction= 0.407305 (Hartree/Particle)
Thermal correction to Energy= 0.436656
Thermal correction to Enthalpy= 0.437600
Thermal correction to Gibbs Free Energy= 0.342572
Sum of electronic and zero-point Energies= -2766.278153
Sum of electronic and thermal Energies= -2766.248802
Sum of electronic and thermal Enthalpies= -2766.247858
Sum of electronic and thermal Free Energies= -2766.342886

C	-3.8612	0.25054	0.83102
H	-3.27388	0.30031	-0.10029
H	-3.83501	-0.80059	1.17143
C	-5.82146	0.15305	-0.8288
H	-5.36651	0.81586	-1.58411
H	-5.47919	-0.86867	-1.05972

H	-6.91186	0.19106	-0.93235
Ni	-4.83857	1.26722	3.15641
C	-5.32738	0.5412	0.53396
C	-3.26165	1.14403	1.9108
H	-2.72732	2.02388	1.53169
H	-4.31709	2.37751	2.38514
N	-6.0195	1.03716	1.49318
C	-7.43832	1.32409	1.43908
H	-7.61739	2.27047	1.96982
H	-7.84829	1.39688	0.42076
H	-7.97478	0.53407	1.98807
I	-5.79904	3.22908	4.85494
P	-5.58758	-0.53313	4.14482
O	-7.18893	-0.86029	4.048
O	-5.01321	-1.87575	3.42342
O	-5.3868	-0.80669	5.74911
C	-5.42393	-3.19506	3.81217
H	-6.46536	-3.38008	3.50906
H	-4.75696	-3.90168	3.30098
H	-5.33346	-3.32561	4.90167
C	-8.14496	-0.14061	4.83538
H	-9.13633	-0.53136	4.56925
H	-7.96171	-0.30073	5.90921
H	-8.10356	0.939	4.62073
C	-4.26954	-0.25428	6.45249
H	-3.343	-0.80149	6.21347
H	-4.14322	0.81202	6.20848
H	-4.47999	-0.3586	7.5255
C	-1.92078	1.43768	4.06057
H	-2.14804	1.24731	5.11945
H	-2.07316	2.51467	3.89136
C	-0.48204	1.05288	3.77643
C	0.11411	-0.02971	4.4441
C	0.2653	1.72891	2.79802
C	1.42127	-0.42664	4.14386
H	-0.4539	-0.56608	5.21022
C	1.57324	1.33636	2.49561
H	-0.18215	2.57604	2.27006
C	2.15585	0.25541	3.16717
H	1.86916	-1.26977	4.67666
H	2.14081	1.8785	1.73449
H	3.17836	-0.0517	2.93286
C	-2.889	0.65801	3.19192
H	-2.87064	-0.42783	3.33778

^{3}C'-TS-D'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -627.13 cm^{-1}
Zero-point correction= 0.405557 (Hartree/Particle)
Thermal correction to Energy= 0.435250
Thermal correction to Enthalpy= 0.436194
Thermal correction to Gibbs Free Energy= 0.338924
Sum of electronic and zero-point Energies= -2766.266219
Sum of electronic and thermal Energies= -2766.236525
Sum of electronic and thermal Enthalpies= -2766.235581
Sum of electronic and thermal Free Energies= -2766.332851

C	-3.60742	1.37089	0.51897
H	-3.76324	2.29139	-0.07229
H	-2.76537	0.84062	0.04033
C	-5.13679	-0.05137	-0.99149
H	-6.08068	0.3465	-1.3994
H	-4.32925	0.16721	-1.70171
H	-5.25631	-1.14462	-0.91665
Ni	-5.04283	1.43105	3.12288
C	-4.85773	0.53973	0.36241
C	-3.24813	1.70442	1.94984
H	-2.70624	2.64323	2.09012
H	-4.71963	2.69259	2.21886
N	-5.6439	0.4137	1.36937
C	-6.88884	-0.33418	1.23447
H	-7.48906	-0.21281	2.14281
H	-7.48244	0.00973	0.37207
H	-6.68426	-1.40955	1.10325
I	-5.05507	3.40383	5.29552
P	-5.88603	-0.25238	4.53486
O	-7.51765	-0.40271	4.58406
O	-5.488	-1.70277	3.92714
O	-5.62054	-0.38391	6.14513
C	-6.01923	-2.93349	4.44435
H	-7.0561	-3.07348	4.10401
H	-5.38823	-3.74364	4.05603
H	-5.99269	-2.94096	5.54476
C	-8.31412	0.65588	5.1299
H	-9.36185	0.42633	4.89478
H	-8.1847	0.71339	6.22224
H	-8.04218	1.62814	4.686
C	-4.32229	-0.25337	6.73104
H	-3.65068	-1.05617	6.38553
H	-3.88375	0.72974	6.50229
H	-4.45315	-0.34476	7.81777
C	-2.08306	0.8807	4.05745
H	-2.31661	0.1554	4.84871
H	-2.23663	1.88265	4.48622
C	-0.6353	0.7065	3.63712
C	-0.0549	-0.57178	3.58154
C	0.14004	1.80934	3.24248
C	1.26145	-0.74512	3.14231
H	-0.6442	-1.44131	3.88814
C	1.45731	1.64078	2.80232
H	-0.29238	2.81321	3.28562
C	2.02295	0.36187	2.74948
H	1.69595	-1.74795	3.1093
H	2.0457	2.51255	2.50347
H	3.05267	0.22873	2.40782
C	-3.02721	0.68428	2.8871
H	-3.20601	-0.35118	2.57695

D

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.279072 (Hartree/Particle)
Thermal correction to Energy= 0.296895
Thermal correction to Enthalpy= 0.297839
Thermal correction to Gibbs Free Energy= 0.229262
Sum of electronic and zero-point Energies= -2079.944529
Sum of electronic and thermal Energies= -2079.926707
Sum of electronic and thermal Enthalpies= -2079.925762

Sum of electronic and thermal Free Energies= -2079.994340

C	0.89615	0.95175	-2.64604
H	0.67094	1.90261	-3.16
H	1.7639	0.52497	-3.18149
C	-0.54718	-0.55535	-4.17826
H	0.0994	-0.10387	-4.94182
H	-0.33594	-1.63844	-4.14728
H	-1.59879	-0.43764	-4.4809
Ni	-0.49703	0.94752	-0.20211
C	-0.29848	0.04833	-2.82709
C	1.22829	1.2015	-1.18852
H	1.67161	2.17613	-0.95508
H	-0.05298	1.82809	0.85063
N	-1.0498	-0.13902	-1.80035
C	-2.21482	-1.01073	-1.87997
H	-2.5855	-1.20082	-0.8663
H	-3.02503	-0.52912	-2.45225
H	-1.97249	-1.96992	-2.3639
I	-2.86997	1.54769	0.71481
C	2.16655	0.2818	1.01585
H	1.61191	-0.20489	1.83279
H	2.27188	1.34396	1.28365
C	3.53135	-0.3644	0.86364
C	3.80386	-1.62793	1.40947
C	4.54017	0.28156	0.12888
C	5.05504	-2.2302	1.23297
H	3.02853	-2.14496	1.98226
C	5.79121	-0.31544	-0.04849
H	4.34026	1.2647	-0.30726
C	6.05282	-1.57559	0.5036
H	5.25044	-3.21366	1.66859
H	6.56599	0.20436	-0.61831
H	7.03096	-2.04366	0.36632
C	1.37808	0.16416	-0.2688
H	1.23883	-0.86812	-0.61642

^{3}D

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.276462 (Hartree/Particle)
Thermal correction to Energy= 0.295176
Thermal correction to Enthalpy= 0.296120
Thermal correction to Gibbs Free Energy= 0.223884
Sum of electronic and zero-point Energies= -2079.938227
Sum of electronic and thermal Energies= -2079.919512
Sum of electronic and thermal Enthalpies= -2079.918568
Sum of electronic and thermal Free Energies= -2079.990805

C	0.74584	-0.40421	-2.96326
H	1.03896	0.38478	-3.67808
H	1.19423	-1.33381	-3.3549
C	-1.33546	-1.14475	-4.29364
H	-1.88452	-2.06497	-4.03162
H	-2.05781	-0.46464	-4.77224
H	-0.55339	-1.40169	-5.01914
Ni	-0.54926	0.90142	-0.57478
C	-0.75826	-0.52121	-3.05552
C	1.31569	-0.10197	-1.59649
H	2.0914	0.66734	-1.55112
H	-0.027	2.2078	-1.26068
C	1.07234	-0.83966	-0.48191
H	0.37088	-1.68106	-0.53419
N	-1.47631	-0.04402	-2.10492
C	-2.93244	-0.07702	-2.17407
H	-3.30103	0.55301	-3.00038
H	-3.30545	-1.10179	-2.33197
H	-3.3405	0.30154	-1.2292
C	2.79978	-1.88148	0.98271
C	2.43618	-2.98061	1.77594
C	4.04114	-1.90569	0.32619
C	3.29506	-4.07651	1.91626
H	1.47199	-2.9756	2.29242
C	4.90301	-2.99708	0.46664
H	4.335	-1.05727	-0.29867
C	4.53172	-4.08755	1.26267
H	2.99781	-4.92281	2.54115
H	5.86902	-2.99617	-0.04513
H	5.20526	-4.9411	1.37423
I	-1.89048	0.17367	1.67723
C	1.85538	-0.70613	0.80278
H	1.15626	-0.65992	1.6503
H	2.42056	0.23913	0.78902

D'-conf

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.408160 (Hartree/Particle)
Thermal correction to Energy= 0.437924
Thermal correction to Enthalpy= 0.438869
Thermal correction to Gibbs Free Energy= 0.342727
Sum of electronic and zero-point Energies= -2766.281480
Sum of electronic and thermal Energies= -2766.251717
Sum of electronic and thermal Enthalpies= -2766.250772
Sum of electronic and thermal Free Energies= -2766.346914

C	0.47398	-0.91322	-2.7491
H	1.03717	-0.98802	-3.69488
H	0.45215	-1.9232	-2.30559
C	-1.54774	-1.06634	-4.32851
H	-1.05348	-0.56488	-5.17735
H	-1.31393	-2.13964	-4.41776
H	-2.63171	-0.93366	-4.41898
Ni	-0.42532	0.46103	-0.48724
C	-0.97339	-0.5481	-3.04285
C	1.12944	0.06983	-1.80554
H	1.44719	1.00635	-2.27564
H	-0.12004	1.7622	-1.0188
N	-1.5871	0.12487	-2.13818
C	-2.98311	0.51091	-2.19092
H	-3.0704	1.54832	-1.83719
H	-3.44071	0.43225	-3.18835
H	-3.54436	-0.1244	-1.48762
I	-1.17108	2.04881	1.58579
P	-1.14123	-1.44997	0.45045
O	-2.75111	-1.73653	0.44836
O	-0.64593	-2.77755	-0.35559
O	-0.8389	-1.79983	2.02417
C	-1.07303	-4.10108	0.00149
H	-2.12985	-4.24935	-0.26604

H	-0.44443	-4.80293	-0.56205
H	-0.94301	-4.27409	1.08088
C	-3.65522	-1.07035	1.33698
H	-4.64621	-1.5153	1.1742
H	-3.35179	-1.2194	2.38449
H	-3.69521	0.00928	1.12446
C	0.41519	-1.45316	2.61941
H	1.21335	-2.13598	2.28414
H	0.69108	-0.41598	2.37594
H	0.29556	-1.54733	3.70714
C	2.57016	0.70993	0.19526
H	2.26002	0.80223	1.24718
H	2.50195	1.7181	-0.24199
C	3.99462	0.19396	0.1315
C	4.53074	-0.56993	1.1802
C	4.78839	0.42233	-1.00495
C	5.82742	-1.0902	1.09923
H	3.92487	-0.75706	2.07176
C	6.08515	-0.09285	-1.08901
H	4.38257	1.01151	-1.83262
C	6.6094	-0.85285	-0.03611
H	6.22861	-1.68069	1.9273
H	6.69025	0.10007	-1.97896
H	7.62333	-1.25608	-0.10041
C	1.61674	-0.20862	-0.53633
H	1.61056	-1.24876	-0.19133

^{3}D'-conf

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.406697 (Hartree/Particle)
Thermal correction to Energy= 0.437066
Thermal correction to Enthalpy= 0.438010
Thermal correction to Gibbs Free Energy= 0.338870
Sum of electronic and zero-point Energies= -2766.280469
Sum of electronic and thermal Energies= -2766.250100
Sum of electronic and thermal Enthalpies= -2766.249156
Sum of electronic and thermal Free Energies= -2766.348296

C	0.33066	-0.78579	-3.02083
H	0.71768	-0.86142	-4.05082
H	0.35748	-1.80307	-2.5936
C	-1.89484	-0.89387	-4.27015
H	-1.6605	-0.2685	-5.14877
H	-1.55771	-1.91432	-4.508
H	-2.98103	-0.90553	-4.12625
Ni	-0.47316	0.84266	-0.473
C	-1.12988	-0.3815	-3.08279
C	1.19205	0.14989	-2.21958
H	1.33957	1.14947	-2.6393
H	-0.02942	2.31104	-0.83507
N	-1.60474	0.32304	-2.12098
C	-2.99441	0.74434	-2.03554
H	-3.01595	1.78848	-1.69466
H	-3.54765	0.66029	-2.98084
H	-3.48967	0.14079	-1.25953
I	-2.31597	1.9396	1.60624
P	-1.02005	-1.30055	0.4874
O	-2.58546	-1.72196	0.34163
O	-0.2855	-2.53482	-0.29647
O	-0.78219	-1.62412	2.07395
C	-0.58984	-3.90932	-0.01435
H	-1.63829	-4.13013	-0.26658
H	0.07661	-4.52079	-0.63635
H	-0.4133	-4.13519	1.04877
C	-3.51033	-1.90838	1.42149
H	-4.49341	-2.07788	0.96193
H	-3.23257	-2.78239	2.02926
H	-3.55263	-1.01242	2.05855
C	0.32111	-1.01889	2.75808
H	1.25358	-1.57135	2.55857
H	0.44476	0.03339	2.45173
H	0.09959	-1.05417	3.833
C	2.73161	0.73314	-0.28981
H	2.25171	0.9774	0.67376
H	2.85866	1.68421	-0.82891
C	4.07174	0.0736	-0.02809
C	4.34066	-0.54817	1.20091
C	5.05084	0.02819	-1.03393
C	5.56001	-1.19794	1.42314
H	3.58714	-0.52094	1.99325
C	6.2713	-0.61741	-0.81479
H	4.8517	0.50403	-1.99861
C	6.52937	-1.23432	0.41542
H	5.75313	-1.67501	2.38758
H	7.02444	-0.63957	-1.60688
H	7.48307	-1.73977	0.58753
C	1.81835	-0.1772	-1.07013
H	1.70327	-1.19225	-0.67711

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UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.408849 (Hartree/Particle)
Thermal correction to Energy= 0.438266
Thermal correction to Enthalpy= 0.439210
Thermal correction to Gibbs Free Energy= 0.344385
Sum of electronic and zero-point Energies= -2766.300219
Sum of electronic and thermal Energies= -2766.270802
Sum of electronic and thermal Enthalpies= -2766.269857
Sum of electronic and thermal Free Energies= -2766.364683

C	2.07406	1.3428	-0.8915
H	1.82195	2.38198	-0.61673
H	3.17126	1.25206	-0.80056
C	2.5136	1.88668	-3.37422
H	3.33019	2.44761	-2.90238
H	2.95484	1.15853	-4.07392
H	1.90299	2.58787	-3.96397
Ni	-0.40496	-0.08968	-1.03413
C	1.67653	1.18935	-2.33693
C	1.3733	0.38271	0.04467
H	1.11299	0.7653	1.03665
H	-1.57498	-0.45628	-1.84861
C	1.3601	-0.97821	-0.1673
H	1.82448	-1.36973	-1.08126
N	0.60621	0.52203	-2.58552
C	0.07093	0.3565	-3.92791
H	-0.88188	0.90504	-3.9872
H	0.74302	0.70807	-4.72273

H	-0.15346	-0.70712	-4.08879
C	2.51845	-2.57079	1.33222
C	2.93826	-3.83988	0.90621
C	3.39028	-1.80418	2.12369
C	4.19629	-4.33638	1.2671
H	2.2709	-4.44714	0.28795
C	4.64627	-2.2969	2.48762
H	3.07813	-0.80991	2.45611
C	5.05404	-3.56645	2.05918
H	4.50577	-5.32878	0.92873
H	5.30987	-1.6891	3.10837
H	6.03626	-3.95306	2.34285
I	-1.35492	2.91275	-0.53191
P	-1.88674	-0.87931	0.23402
O	-3.40908	-0.30983	0.16257
O	-2.01249	-2.48383	0.03952
O	-1.70594	-0.81786	1.85554
C	-2.86353	-3.28633	0.8747
H	-3.8602	-2.82903	0.97061
H	-2.95417	-4.26549	0.38668
H	-2.41878	-3.40634	1.87349
C	-4.06923	0.03655	-1.05817
H	-5.06437	0.41022	-0.78095
H	-3.51449	0.82643	-1.58668
H	-4.18199	-0.84442	-1.70993
C	-1.8468	0.40179	2.59314
H	-2.89024	0.75109	2.56278
H	-1.55903	0.1807	3.62961
H	-1.19698	1.19149	2.18479
C	1.16878	-2.01227	0.91879
H	0.52455	-2.82514	0.55424
H	0.66072	-1.55769	1.78064

^{3}D'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.405149 (Hartree/Particle)
Thermal correction to Energy= 0.436089
Thermal correction to Enthalpy= 0.437033
Thermal correction to Gibbs Free Energy= 0.335985
Sum of electronic and zero-point Energies= -2766.277642
Sum of electronic and thermal Energies= -2766.246702
Sum of electronic and thermal Enthalpies= -2766.245758
Sum of electronic and thermal Free Energies= -2766.346805

C	2.00066	1.5104	-0.91261
H	1.60505	2.50309	-0.63476
H	3.09374	1.57627	-0.77171
C	2.59822	2.14824	-3.3252
H	3.26651	2.82011	-2.7713
H	3.22207	1.46973	-3.93129
H	1.99039	2.74603	-4.02164
Ni	-0.69525	-0.03961	-1.45029
C	1.72205	1.35678	-2.39071
C	1.44053	0.4581	0.0139
H	1.00869	0.81332	0.95506
H	-1.75642	-0.57783	-2.50018
C	1.57864	-0.8694	-0.17536
H	2.03316	-1.227	-1.10733
N	0.73712	0.63279	-2.77963
C	0.40383	0.51045	-4.19154
H	-0.26034	1.34101	-4.48559
H	1.28765	0.51858	-4.8468
H	-0.15214	-0.42329	-4.34009
C	2.52518	-2.63016	1.29892
C	2.83796	-3.92871	0.87068
C	3.42774	-1.96453	2.1453
C	4.02205	-4.55214	1.28199
H	2.14543	-4.45867	0.21046
C	4.60938	-2.58427	2.56025
H	3.19823	-0.94841	2.47932
C	4.91103	-3.88205	2.12837
H	4.24892	-5.56552	0.94034
H	5.29821	-2.05372	3.22298
H	5.83529	-4.36796	2.45138
I	-1.62324	2.64185	-0.99093
P	-1.99482	-0.88587	0.32331
O	-3.57812	-0.48025	0.36535
O	-1.98029	-2.51108	0.28528
O	-1.6566	-0.65111	1.90969
C	-2.69376	-3.31231	1.24048
H	-3.71774	-2.9334	1.38069
H	-2.73206	-4.3332	0.83817
H	-2.16966	-3.31296	2.20791
C	-4.35006	-0.29335	-0.82783
H	-5.28909	0.19185	-0.52799
H	-3.81273	0.3447	-1.54359
H	-4.57625	-1.26342	-1.29946
C	-1.82643	0.62399	2.53829
H	-2.88702	0.91958	2.53538
H	-1.4763	0.51827	3.57388
H	-1.23876	1.40388	2.02798
C	1.25609	-1.93391	0.83922
H	0.56983	-2.67297	0.39817
H	0.73348	-1.48379	1.69633

D-TS-E

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -230.60 cm^{-1}
Zero-point correction= 0.279719 (Hartree/Particle)
Thermal correction to Energy= 0.297358
Thermal correction to Enthalpy= 0.298302
Thermal correction to Gibbs Free Energy= 0.229810
Sum of electronic and zero-point Energies= -2080.236799
Sum of electronic and thermal Energies= -2080.219160
Sum of electronic and thermal Enthalpies= -2080.218216
Sum of electronic and thermal Free Energies= -2080.286708

C	0.65144	0.98657	-2.55973
H	1.31248	1.4591	-3.30578
H	0.95396	-0.0765	-2.52673
C	-1.05358	0.75572	-4.48697
H	-0.15455	0.37288	-4.98752
H	-1.86465	0.02306	-4.61034
H	-1.35835	1.68223	-5.0023
Ni	-0.94821	1.47926	-0.2717
C	-0.77064	1.03533	-3.0362
C	0.81796	1.64176	-1.20307
H	1.11534	2.6991	-1.21791

H	-0.49469	1.70191	1.06288
N	-1.65546	1.29295	-2.13394
C	-3.07071	1.37269	-2.46763
H	-3.58879	0.48499	-2.07288
H	-3.50285	2.24314	-1.95648
H	-3.2636	1.45553	-3.54579
I	-3.18168	1.48091	1.11614
C	1.8885	1.41611	1.11545
H	1.5166	1.01194	2.0682
H	1.81641	2.51301	1.1717
C	3.33054	0.99309	0.90635
C	3.86072	-0.12058	1.57585
C	4.15159	1.68397	-0.00084
C	5.17939	-0.53208	1.35074
H	3.23416	-0.67003	2.28448
C	5.46923	1.2773	-0.22806
H	3.75111	2.55069	-0.5344
C	5.98793	0.16591	0.44784
H	5.5761	-1.39998	1.88413
H	6.0949	1.83014	-0.9338
H	7.01853	-0.15288	0.27186
C	1.02838	0.9143	-0.03183
H	0.98599	-0.18264	-0.1019

^{3}D-TS-E

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -849.38 cm^{-1}
Zero-point correction= 0.275652 (Hartree/Particle)
Thermal correction to Energy= 0.293609
Thermal correction to Enthalpy= 0.294553
Thermal correction to Gibbs Free Energy= 0.224681
Sum of electronic and zero-point Energies= -2079.926030
Sum of electronic and thermal Energies= -2079.908072
Sum of electronic and thermal Enthalpies= -2079.907128
Sum of electronic and thermal Free Energies= -2079.977001

C	-3.24585	1.03995	2.31609
H	-2.92743	2.09501	2.38909
H	-2.35398	0.4956	1.94873
C	-3.89734	1.29019	-0.18021
H	-2.84346	1.59019	-0.2429
H	-4.05177	0.41155	-0.82887
H	-4.52329	2.10128	-0.58621
Ni	-5.81639	0.3064	3.5245
C	-4.29639	0.97211	1.23168
C	-3.7063	0.52103	3.65992
H	-3.50512	1.13804	4.54149
H	-5.64156	-1.24913	3.59019
C	-4.01873	-0.84306	3.85218
H	-3.7794	-1.52555	3.02758
N	-5.49397	0.64818	1.57261
C	-6.56482	0.56885	0.58763
H	-6.7301	1.54095	0.09389
H	-6.33478	-0.17463	-0.19328
H	-7.49192	0.27535	1.09526
C	-2.4441	-1.76673	5.56561
C	-1.85813	-2.97605	5.15735
C	-1.64511	-0.82885	6.23962
C	-0.50952	-3.24285	5.41568
H	-2.46764	-3.71848	4.63365
C	-0.29689	-1.09226	6.50148
H	-2.08597	0.11712	6.56604
C	0.27608	-2.30069	6.08886
H	-0.07174	-4.19125	5.09316
H	0.30799	-0.35198	7.0318
H	1.32934	-2.5085	6.29423
I	-8.08167	1.38599	4.32245
C	-3.89277	-1.46676	5.23776
H	-4.48876	-2.39022	5.28218
H	-4.31676	-0.77092	5.97828

D'-TS-E'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -465.00 cm^{-1}
Zero-point correction= 0.406742 (Hartree/Particle)
Thermal correction to Energy= 0.436208
Thermal correction to Enthalpy= 0.437152
Thermal correction to Gibbs Free Energy= 0.341490
Sum of electronic and zero-point Energies= -2766.284191
Sum of electronic and thermal Energies= -2766.254725
Sum of electronic and thermal Enthalpies= -2766.253781
Sum of electronic and thermal Free Energies= -2766.349443

C	-3.35103	1.38878	2.23746
H	-3.05681	2.44172	2.39233
H	-2.41554	0.85905	1.97788
C	-3.6633	1.78947	-0.29167
H	-2.61464	2.09149	-0.17019
H	-3.69984	0.96623	-1.02371
H	-4.2213	2.637	-0.71999
Ni	-6.00798	0.52181	3.20293
C	-4.26254	1.36219	1.0268
C	-3.95915	0.82957	3.50762
H	-3.89629	1.46077	4.39779
H	-5.68388	-0.85383	2.95757
C	-4.19781	-0.53295	3.70008
H	-3.85164	-1.22347	2.91995
N	-5.4793	1.01051	1.20632
C	-6.45829	0.97988	0.13841
H	-7.1629	1.8166	0.28067
H	-6.04069	1.04509	-0.87887
H	-7.0443	0.05258	0.22674
C	-2.97765	-1.77262	5.50222
C	-2.79856	-3.16419	5.49309
C	-1.89278	-0.95889	5.87054
C	-1.56864	-3.73169	5.84646
H	-3.63346	-3.81125	5.20878
C	-0.66363	-1.52098	6.22551
H	-2.01619	0.12786	5.87661
C	-0.49717	-2.91159	6.21399
H	-1.44881	-4.81829	5.83566
H	0.16795	-0.87244	6.51373
H	0.46357	-3.35269	6.49174
I	-6.62034	3.00781	4.05032
P	-7.79592	-0.50942	3.67012
O	-9.26124	0.24034	3.6844
O	-8.05875	-1.8366	2.76115
O	-7.88449	-1.18978	5.15933

C	-9.16984	-2.71241	2.99571
H	-10.10634	-2.14283	3.10128
H	-9.24328	-3.37949	2.12638
H	-9.00625	-3.3079	3.90696
C	-9.65149	1.02642	2.55601
H	-10.46924	1.68561	2.8784
H	-8.81391	1.64648	2.19832
H	-10.00686	0.38176	1.73481
C	-7.73834	-0.35944	6.31452
H	-8.68317	0.16181	6.53812
H	-7.46782	-1.0096	7.15755
H	-6.94637	0.39221	6.1606
C	-4.29627	-1.15227	5.08481
H	-5.09036	-1.91265	5.09856
H	-4.59437	-0.37043	5.80038

^{3}D'-TS-E'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -742.58 cm^{-1}
Zero-point correction= 0.404999 (Hartree/Particle)
Thermal correction to Energy= 0.434882
Thermal correction to Enthalpy= 0.435826
Thermal correction to Gibbs Free Energy= 0.337923
Sum of electronic and zero-point Energies= -2766.269006
Sum of electronic and thermal Energies= -2766.239123
Sum of electronic and thermal Enthalpies= -2766.238179
Sum of electronic and thermal Free Energies= -2766.336082

C	-3.41096	0.94381	2.19722
H	-3.15613	2.01829	2.17136
H	-2.48539	0.42492	1.87712
C	-4.01023	0.94482	-0.30529
H	-2.99892	1.36951	-0.35028
H	-4.00912	-0.00488	-0.86671
H	-4.7061	1.62505	-0.82077
Ni	-6.03048	0.28159	3.48576
C	-4.44026	0.71434	1.11777
C	-3.83164	0.53183	3.58359
H	-3.65806	1.24007	4.39539
H	-5.79147	-1.24717	3.77172
C	-4.13774	-0.79643	3.91228
H	-3.94786	-1.55229	3.14075
N	-5.62651	0.34484	1.45538
C	-6.63595	0.12201	0.42343
H	-7.03821	1.08568	0.06634
H	-6.23234	-0.41942	-0.44624
H	-7.46105	-0.46277	0.84259
C	-2.51215	-1.52173	5.67093
C	-1.88682	-2.73627	5.3449
C	-1.74005	-0.50871	6.26284
C	-0.52618	-2.93496	5.60217
H	-2.47508	-3.53624	4.88545
C	-0.38006	-0.70367	6.52375
H	-2.21267	0.44243	6.52333
C	0.23234	-1.91803	6.19259
H	-0.05743	-3.88812	5.34327
H	0.20374	0.09508	6.98903
H	1.29513	-2.07192	6.39649
I	-6.35829	2.03885	5.80621
P	-8.33947	-0.07345	3.56591
O	-9.45203	1.11062	3.3799
O	-8.81669	-1.2378	2.51643
O	-8.9253	-0.61439	4.99109
C	-10.17868	-1.68271	2.44139
H	-10.8476	-0.84667	2.18452
H	-10.22512	-2.44742	1.65494
H	-10.4993	-2.11908	3.40011
C	-9.1388	2.22131	2.53251
H	-9.75497	3.06957	2.8603
H	-8.07434	2.49897	2.61701
H	-9.37152	1.98984	1.4803
C	-8.19873	-1.60796	5.72126
H	-7.18577	-1.25123	5.96571
H	-8.75563	-1.7919	6.64994
H	-8.12471	-2.54901	5.1516
C	-3.97365	-1.2952	5.34246
H	-4.53957	-2.22977	5.47343
H	-4.4094	-0.5489	6.02303

E

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.280984 (Hartree/Particle)
Thermal correction to Energy= 0.298788
Thermal correction to Enthalpy= 0.299732
Thermal correction to Gibbs Free Energy= 0.230851
Sum of electronic and zero-point Energies= -2079.949597
Sum of electronic and thermal Energies= -2079.931793
Sum of electronic and thermal Enthalpies= -2079.930849
Sum of electronic and thermal Free Energies= -2079.999730

C	0.96353	-0.68038	-2.09446
H	1.85339	-0.55008	-2.73595
H	0.90958	-1.76051	-1.86461
C	-0.44395	-0.58665	-4.30566
H	0.39724	-1.17942	-4.6867
H	-1.38435	-1.12007	-4.51635
H	-0.48	0.3633	-4.86681
Ni	-0.78142	0.25776	-0.27143
C	-0.29295	-0.31375	-2.84072
C	0.99122	0.15414	-0.82037
H	1.44518	1.14675	-0.97064
H	0.13516	-0.24947	1.11717
N	-1.21793	0.22501	-2.1083
C	-2.49712	0.62714	-2.68143
H	-3.08665	-0.25722	-2.97641
H	-3.06254	1.18021	-1.92334
H	-2.35951	1.26283	-3.57062
I	-2.99527	0.33629	1.20748
C	2.20825	0.23077	1.45968
H	2.05019	-0.11468	2.49346
H	2.05986	1.32191	1.45497
C	3.60938	-0.11422	1.00878
C	4.21827	-1.30856	1.42866
C	4.30868	0.71502	0.11669
C	5.49048	-1.66587	0.97107
H	3.68799	-1.96564	2.1245
C	5.58167	0.36165	-0.34353
H	3.85276	1.65092	-0.21772

C	6.17669	-0.8313	0.08149
H	5.94876	-2.59792	1.31229
H	6.1117	1.02237	-1.03465
H	7.1719	-1.10787	-0.27596
C	1.15146	-0.41284	0.5423
H	1.24484	-1.51075	0.54456

^{3}E

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.281431 (Hartree/Particle)
Thermal correction to Energy= 0.299418
Thermal correction to Enthalpy= 0.300362
Thermal correction to Gibbs Free Energy= 0.230312
Sum of electronic and zero-point Energies= -2079.960966
Sum of electronic and thermal Energies= -2079.942979
Sum of electronic and thermal Enthalpies= -2079.942035
Sum of electronic and thermal Free Energies= -2080.012085

C	2.12706	0.09233	-2.41223
H	2.82133	0.94681	-2.52878
H	2.4901	-0.66962	-3.13103
C	0.51164	0.72845	-4.35623
H	1.41422	0.53326	-4.94951
H	-0.26578	0.00592	-4.65919
H	0.12869	1.73183	-4.60068
Ni	0.68517	0.72313	-0.11756
C	0.78219	0.59557	-2.88624
C	2.09924	-0.40312	-0.96163
H	3.08296	-0.24771	-0.487
H	0.79594	-2.05525	-1.47025
C	1.71852	-1.88337	-0.88523
H	2.50005	-2.50194	-1.37439
N	-0.07473	0.92091	-1.98119
C	-1.39171	1.44165	-2.3163
H	-1.31818	2.42704	-2.80729
H	-1.93596	0.76394	-2.99457
H	-1.97054	1.55867	-1.39103
C	2.63983	-2.17286	1.47972
C	3.82127	-2.92831	1.38467
C	2.58346	-1.14613	2.43638
C	4.91409	-2.66513	2.21636
H	3.88382	-3.73375	0.64644
C	3.67392	-0.87895	3.27181
H	1.67359	-0.54542	2.52366
C	4.8448	-1.6368	3.16432
H	5.82316	-3.26623	2.12682
H	3.60717	-0.07486	4.0099
H	5.69738	-1.43044	3.81666
I	-0.83066	1.78464	1.8543
C	1.48413	-2.4296	0.53924
H	1.29623	-3.5151	0.47444
H	0.56871	-1.97895	0.95826

E'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.411847 (Hartree/Particle)
Thermal correction to Energy= 0.441276
Thermal correction to Enthalpy= 0.442220
Thermal correction to Gibbs Free Energy= 0.347333
Sum of electronic and zero-point Energies= -2766.308219
Sum of electronic and thermal Energies= -2766.278790
Sum of electronic and thermal Enthalpies= -2766.277845
Sum of electronic and thermal Free Energies= -2766.372732

C	2.51572	0.13021	-2.58121
H	2.61887	1.22848	-2.49837
H	3.4063	-0.21489	-3.14438
C	1.28911	-0.02883	-4.87294
H	2.21225	0.46146	-5.20855
H	1.25664	-1.03378	-5.32821
H	0.42681	0.53762	-5.25439
Ni	0.49087	-0.17086	-0.74058
C	1.26935	-0.13911	-3.37497
C	2.35806	-0.51022	-1.20429
H	3.04052	-0.05979	-0.46897
H	2.09062	-2.43112	-2.17542
C	2.57084	-2.02821	-1.26745
H	3.65452	-2.22982	-1.38843
N	0.2314	-0.4509	-2.66952
C	-1.05381	-0.75492	-3.28674
H	-1.71052	0.12873	-3.2262
H	-0.96633	-1.05663	-4.33988
H	-1.53451	-1.55964	-2.71915
C	2.56748	-2.42897	1.28013
C	3.93812	-2.51701	1.58019
C	1.70058	-1.93947	2.26837
C	4.42656	-2.12844	2.831
H	4.63127	-2.89667	0.82354
C	2.1831	-1.55635	3.52466
H	0.63681	-1.84344	2.04175
C	3.54839	-1.64772	3.81114
H	5.49632	-2.2042	3.04468
H	1.48815	-1.17573	4.27813
H	3.92865	-1.34584	4.79063
I	1.08072	1.78422	1.09689
P	-1.61348	-0.51084	0.15385
O	-2.73259	0.68633	0.25618
O	-2.39237	-1.75463	-0.55456
O	-1.67594	-1.05606	1.69648
C	-3.65506	-2.24622	-0.08111
H	-4.37483	-1.42088	0.03465
H	-4.0264	-2.95368	-0.83417
H	-3.53163	-2.75956	0.88414
C	-2.67991	1.7881	-0.65626
H	-3.08442	2.66965	-0.14003
H	-1.64182	1.99878	-0.96241
H	-3.28988	1.57778	-1.54947
C	-1.67424	-0.23541	2.86842
H	-2.29308	0.66183	2.72019
H	-2.09731	-0.84137	3.68192
H	-0.64902	0.06994	3.12518
C	2.04129	-2.84823	-0.07453
H	2.29923	-3.90844	-0.24715
H	0.93951	-2.80043	-0.06447

^{3}E'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.411109 (Hartree/Particle)
Thermal correction to Energy= 0.440686
Thermal correction to Enthalpy= 0.441630
Thermal correction to Gibbs Free Energy= 0.345610
Sum of electronic and zero-point Energies= -2766.305489
Sum of electronic and thermal Energies= -2766.275912
Sum of electronic and thermal Enthalpies= -2766.274967
Sum of electronic and thermal Free Energies= -2766.370988

C	2.35138	0.51032	-2.481
H	2.50664	1.56691	-2.18973
H	3.25765	0.22261	-3.05194
C	1.37313	0.87467	-4.86328
H	2.37518	1.2908	-5.03039
H	1.2712	-0.02838	-5.49028
H	0.61917	1.59776	-5.21001
Ni	0.15805	-0.06123	-0.88236
C	1.17037	0.51575	-3.41887
C	2.10509	-0.34504	-1.23812
H	2.72851	0.01869	-0.40654
H	1.76894	-2.17226	-2.35044
C	2.3783	-1.82714	-1.49417
H	3.43566	-1.98163	-1.79911
N	0.02087	0.22719	-2.91288
C	-1.17818	0.18447	-3.73967
H	-1.53768	1.20195	-3.9683
H	-1.00558	-0.33766	-4.6944
H	-1.96919	-0.34808	-3.19692
C	2.90205	-2.4385	0.9325
C	4.15643	-3.03774	1.13575
C	2.4555	-1.50114	1.87974
C	4.93959	-2.71359	2.24914
H	4.52293	-3.77126	0.41106
C	3.23304	-1.17274	2.99428
H	1.48925	-1.01605	1.73026
C	4.48032	-1.77894	3.18403
H	5.91122	-3.19538	2.38886
H	2.86338	-0.43937	3.71615
H	5.08963	-1.52598	4.05566
I	0.39984	2.49729	0.31802
P	-2.13043	-0.31124	-0.20261
O	-3.15877	0.95974	-0.22998
O	-2.90076	-1.44313	-1.09079
O	-2.4365	-0.7559	1.3356
C	-4.26237	-1.82557	-0.83836
H	-4.92911	-0.95068	-0.8858
H	-4.54385	-2.54659	-1.61668
H	-4.35094	-2.29549	0.15313
C	-3.18994	1.82788	-1.36799
H	-3.76135	2.71931	-1.07664
H	-2.17238	2.1366	-1.65649
H	-3.68906	1.34446	-2.22335
C	-1.35475	-1.07822	2.21949
H	-0.65338	-0.23292	2.30934
H	-1.79834	-1.28465	3.20231
H	-0.80742	-1.9721	1.87943
C	2.08101	-2.75564	-0.29675
H	2.26371	-3.80025	-0.59887
H	1.00861	-2.68005	-0.04692

G

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.501278 (Hartree/Particle)
Thermal correction to Energy= 0.533521
Thermal correction to Enthalpy= 0.534465
Thermal correction to Gibbs Free Energy= 0.435042
Sum of electronic and zero-point Energies= -2986.268818
Sum of electronic and thermal Energies= -2986.236576
Sum of electronic and thermal Enthalpies= -2986.235632
Sum of electronic and thermal Free Energies= -2986.335055

C	-0.887	-2.2683	-1.8551
H	-1.00093	-1.83447	-2.86715
H	-0.55569	-3.31216	-2.02914
C	-3.23408	-3.35362	-1.6503
H	-2.86413	-3.89483	-2.53114
H	-3.35646	-4.08611	-0.83394
H	-4.22866	-2.94388	-1.8803
Ni	-0.97466	0.02149	-0.2109
C	-2.25924	-2.27942	-1.24345
C	0.09106	-1.43583	-1.01179
H	0.88962	-1.05287	-1.66365
H	-0.0593	-2.82575	0.64847
C	0.72463	-2.25176	0.12172
H	1.15561	-1.57015	0.87428
N	-2.51201	-1.33075	-0.40697
C	-3.80129	-1.23088	0.26564
H	-4.39249	-2.15699	0.23375
H	-3.63041	-0.95561	1.31491
H	-4.38378	-0.41119	-0.18284
C	3.0459	-2.48882	-0.87664
C	3.93048	-1.81863	-0.01321
C	3.26336	-2.37898	-2.25963
C	4.9919	-1.05894	-0.51303
H	3.77532	-1.88558	1.06779
C	4.3255	-1.62122	-2.76685
H	2.58423	-2.88891	-2.94885
C	5.19278	-0.95498	-1.89501
H	5.66345	-0.5423	0.17804
H	4.473	-1.5482	-3.84787
H	6.0205	-0.35914	-2.28837
C	1.84802	-3.22444	-0.32193
H	1.45988	-3.92811	-1.07702
H	2.15803	-3.83076	0.54685
P	-2.12309	1.60167	0.80914
O	-1.45278	3.04034	1.23643
O	-2.69077	1.2085	2.30481
O	-3.52335	2.04005	0.09442
C	-0.83188	3.8911	0.26728
H	-1.08372	3.59712	-0.76361
H	-1.19098	4.91718	0.43934
H	0.26077	3.84962	0.38241
C	-1.78551	0.64932	3.25766
H	-2.38156	0.28763	4.10649
H	-1.22541	-0.19777	2.82388
H	-1.06863	1.40775	3.61309
C	-4.45543	2.93852	0.71138
H	-5.01762	2.42282	1.50504

H	-3.93697	3.8085	1.14377
H	-5.14787	3.27675	-0.07131
C	0.6314	1.05142	-0.17979
C	1.18196	1.63591	-1.34088
C	1.34171	1.26447	1.02135
C	2.35521	2.39926	-1.30815
H	0.67894	1.48759	-2.3025
C	2.51997	2.02172	1.06838
H	0.96118	0.83578	1.95438
C	3.03358	2.59936	-0.0989
H	2.7461	2.83819	-2.23194
H	3.03888	2.16293	2.02209
H	3.95193	3.19244	-0.06812

^{3}G

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.498620 (Hartree/Particle)
Thermal correction to Energy= 0.531985
Thermal correction to Enthalpy= 0.532929
Thermal correction to Gibbs Free Energy= 0.427436
Sum of electronic and zero-point Energies= -2986.236971
Sum of electronic and thermal Energies= -2986.203606
Sum of electronic and thermal Enthalpies= -2986.202662
Sum of electronic and thermal Free Energies= -2986.308155

C	-0.08612	-1.56187	-2.05044
H	0.41057	-0.91064	-2.79567
H	0.01321	-2.5865	-2.46384
C	-2.39993	-1.66901	-3.23292
H	-1.79037	-2.18182	-3.98854
H	-3.1527	-2.38489	-2.86019
H	-2.94586	-0.84375	-3.71582
Ni	-0.44791	0.25048	0.04131
C	-1.54603	-1.17203	-2.09687
C	0.5455	-1.3496	-0.67316
H	1.62941	-1.17764	-0.78267
H	-0.78502	-2.65788	0.43696
C	0.3026	-2.50873	0.29971
H	0.69544	-2.23721	1.29645
N	-1.97226	-0.38362	-1.17311
C	-3.3433	0.0997	-1.14506
H	-3.43513	1.01011	-1.76239
H	-4.0738	-0.6387	-1.51201
H	-3.60655	0.36461	-0.11219
C	2.42133	-3.85418	-0.18744
C	3.22252	-4.02805	0.95452
C	3.06195	-3.58652	-1.40966
C	4.6165	-3.94125	0.87997
H	2.74364	-4.23646	1.91629
C	4.45597	-3.49927	-1.49084
H	2.45707	-3.44622	-2.30973
C	5.23979	-3.67579	-0.34515
H	5.21934	-4.08444	1.78103
H	4.93213	-3.29269	-2.45333
H	6.32922	-3.60954	-0.40663
C	0.9166	-3.88593	-0.08584
H	0.48743	-4.2222	-1.04397
H	0.61401	-4.62926	0.67147
P	-1.50336	1.43579	1.78337
O	-1.84672	3.02373	1.57006
O	-0.60892	1.68808	3.13641
O	-2.92076	0.81588	2.33284
C	-2.54943	3.42063	0.38782
H	-3.61329	3.13503	0.44365
H	-2.47643	4.51461	0.32121
H	-2.09348	2.97493	-0.51077
C	0.13905	0.58591	3.66071
H	0.51518	-0.06377	2.85071
H	0.99351	0.99725	4.21521
H	-0.4808	-0.01859	4.34268
C	-3.68104	1.45529	3.36913
H	-4.47132	0.75545	3.67184
H	-3.04293	1.68577	4.23659
H	-4.13705	2.38755	3.00079
C	0.29319	1.85358	-0.89894
C	0.04113	2.11805	-2.26182
C	1.15258	2.76035	-0.24123
C	0.60683	3.21179	-2.93218
H	-0.62822	1.453	-2.82023
C	1.73213	3.8567	-0.89568
H	1.37217	2.61686	0.82477
C	1.46018	4.08857	-2.2499
H	0.3812	3.38357	-3.9902
H	2.39318	4.53673	-0.34766
H	1.90491	4.94413	-2.76654

G1

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.369428 (Hartree/Particle)
Thermal correction to Energy= 0.391028
Thermal correction to Enthalpy= 0.391973
Thermal correction to Gibbs Free Energy= 0.314480
Sum of electronic and zero-point Energies= -2299.883380
Sum of electronic and thermal Energies= -2299.861780
Sum of electronic and thermal Enthalpies= -2299.860836
Sum of electronic and thermal Free Energies= -2299.938329

C	0.78795	3.26821	-0.58774
C	0.1342	3.91353	-1.8144
H	0.33756	3.70277	0.32969
H	-0.12538	4.98611	-1.71614
H	0.81895	3.86962	-2.68595
C	2.30251	3.40053	-0.52179
H	2.68765	2.80203	0.32572
H	2.75397	2.95712	-1.43004
C	2.84036	4.84574	-0.37332
H	2.47074	5.45012	-1.2187
H	2.41375	5.28602	0.54391
C	4.34754	4.90565	-0.32549
C	5.037	4.81797	0.89619
C	5.10311	4.98202	-1.50859
C	6.43532	4.81122	0.93698
H	4.46721	4.75736	1.82846
C	6.5013	4.97528	-1.4739
H	4.58486	5.05014	-2.47004
C	7.17386	4.8896	-0.24928
H	6.95067	4.74689	1.89928
H	7.0686	5.03982	-2.4065

H	8.26658	4.88648	-0.2196
Ni	0.30185	1.36113	-0.64697
C	-1.08869	3.13833	-2.20928
C	-2.10588	3.73145	-3.1401
H	-3.05049	3.91871	-2.6006
H	-1.75294	4.68466	-3.55427
H	-2.33982	3.04406	-3.96818
C	-2.32765	1.0958	-2.03487
H	-3.2801	1.63154	-1.89517
H	-2.28041	0.74567	-3.07982
H	-2.30563	0.21943	-1.37944
N	-1.1836	1.94503	-1.72126
C	0.1734	-0.61244	-0.54923
C	0.48041	-1.23259	0.68562
C	-0.06992	-1.49659	-1.62571
C	0.54055	-2.62502	0.84424
H	0.68039	-0.60642	1.56555
C	-0.01583	-2.89067	-1.49057
H	-0.31734	-1.08278	-2.61107
C	0.29031	-3.46305	-0.24891
H	0.77926	-3.05883	1.82125
H	-0.2126	-3.5356	-2.35374
H	0.33091	-4.55042	-0.13472

^{3}G1

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.368744 (Hartree/Particle)
Thermal correction to Energy= 0.390571
Thermal correction to Enthalpy= 0.391515
Thermal correction to Gibbs Free Energy= 0.312409
Sum of electronic and zero-point Energies= -2299.886516
Sum of electronic and thermal Energies= -2299.864690
Sum of electronic and thermal Enthalpies= -2299.863745
Sum of electronic and thermal Free Energies= -2299.942851

C	0.97327	3.12713	-0.58654
C	0.27458	3.77126	-1.7914
H	0.52282	3.5561	0.33515
H	0.05619	4.85336	-1.6882
H	0.92463	3.7099	-2.68937
C	2.47876	3.37568	-0.54646
H	2.9193	2.84324	0.31607
H	2.95623	2.93401	-1.44268
C	2.90661	4.86254	-0.45839
H	2.51449	5.402	-1.33682
H	2.42815	5.31103	0.42936
C	4.40295	5.04105	-0.38204
C	5.06543	5.07592	0.85738
C	5.18205	5.11072	-1.55039
C	6.45846	5.18182	0.92951
H	4.47759	5.02309	1.77892
C	6.57525	5.21595	-1.48459
H	4.68577	5.0851	-2.52543
C	7.22004	5.25205	-0.24263
H	6.95135	5.21256	1.90519
H	7.16034	5.27321	-2.40666
H	8.30851	5.33732	-0.18869
Ni	0.41317	1.18552	-0.60988
C	-1.00336	3.06675	-2.17463
C	-1.9755	3.74784	-3.09724
H	-2.91814	3.96012	-2.56401
H	-1.5725	4.6958	-3.47683
H	-2.23137	3.09916	-3.95022
C	-2.37917	1.11187	-2.03819
H	-3.30372	1.66905	-1.81184
H	-2.39964	0.84646	-3.10956
H	-2.36967	0.18179	-1.4569
N	-1.18983	1.88156	-1.70763
C	0.17506	-0.80882	-0.45564
C	0.34809	-1.50762	0.76183
C	-0.14692	-1.61208	-1.57443
C	0.2105	-2.89953	0.86495
H	0.59937	-0.94701	1.67115
C	-0.28534	-3.00513	-1.49557
H	-0.30142	-1.13314	-2.54941
C	-0.10707	-3.65701	-0.26903
H	0.35069	-3.39638	1.83089
H	-0.53505	-3.58534	-2.39027
H	-0.21647	-4.74325	-0.1973

G-TS-H

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -357.12 cm^{-1}
Zero-point correction= 0.499094 (Hartree/Particle)
Thermal correction to Energy= 0.531158
Thermal correction to Enthalpy= 0.532103
Thermal correction to Gibbs Free Energy= 0.431825
Sum of electronic and zero-point Energies= -2986.222674
Sum of electronic and thermal Energies= -2986.190610
Sum of electronic and thermal Enthalpies= -2986.189665
Sum of electronic and thermal Free Energies= -2986.289943

C	2.01994	2.97506	-0.75926
C	0.6887	3.38373	-1.39298
H	2.06136	3.35817	0.29054
H	0.65418	4.46799	-1.6062
H	0.58148	2.90793	-2.38558
C	3.22247	3.59732	-1.47589
H	4.15149	3.2167	-1.02927
H	3.24001	3.27707	-2.53208
C	3.27996	5.13951	-1.41055
H	2.40748	5.57928	-1.9187
H	3.22401	5.45105	-0.35357
C	4.54419	5.67754	-2.03924
C	5.72468	5.80344	-1.2873
C	4.58667	6.00804	-3.40408
C	6.91081	6.25056	-1.87836
H	5.71084	5.54991	-0.22291
C	5.7705	6.45515	-4.00045
H	3.67741	5.91562	-4.00574
C	6.93808	6.57819	-3.23889
H	7.81693	6.34608	-1.27393
H	5.78061	6.71082	-5.06348
H	7.86354	6.92979	-3.70231
Ni	1.47163	1.47755	0.53024
P	1.92514	0.09882	2.01274

O	3.47069	0.22806	2.60706
O	1.82002	-1.54376	1.76112
O	1.00918	0.12704	3.39448
C	2.49466	-2.12831	0.64911
H	3.58872	-2.02608	0.74563
H	2.23602	-3.19717	0.63456
H	2.18803	-1.66489	-0.30149
C	0.58564	-1.00011	4.16027
H	-0.03083	-0.61309	4.98499
H	-0.01673	-1.69291	3.55224
H	1.43502	-1.55892	4.58426
C	3.9593	-0.56437	3.68636
H	5.04878	-0.42303	3.7392
H	3.51349	-0.24749	4.64454
H	3.74596	-1.63491	3.5297
C	-0.53028	3.03545	-0.5802
C	-1.86974	3.54864	-1.03408
H	-2.28396	4.25143	-0.29095
H	-1.79846	4.06858	-1.99836
H	-2.59272	2.72241	-1.1296
C	-1.48304	1.91023	1.3009
H	-1.09429	1.41246	2.19775
H	-2.09821	2.7746	1.6045
H	-2.14201	1.20194	0.76793
N	-0.35756	2.30093	0.46364
C	2.48762	1.09038	-1.0005
C	1.68238	0.45408	-1.9814
C	3.86294	0.7308	-0.98235
C	2.20418	-0.5145	-2.84785
H	0.61913	0.70136	-2.05166
C	4.38219	-0.22498	-1.85078
H	4.51487	1.18005	-0.22945
C	3.55773	-0.86249	-2.79461
H	1.54267	-0.99847	-3.57337
H	5.43994	-0.49774	-1.77978
H	3.96815	-1.61327	-3.47472

^{3}G-TS-H

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -307.02 cm^{-1}
Zero-point correction= 0.371076 (Hartree/Particle)
Thermal correction to Energy= 0.392131
Thermal correction to Enthalpy= 0.393075
Thermal correction to Gibbs Free Energy= 0.316727
Sum of electronic and zero-point Energies= -2300.304494
Sum of electronic and thermal Energies= -2300.283439
Sum of electronic and thermal Enthalpies= -2300.282495
Sum of electronic and thermal Free Energies= -2300.358843

C	2.11954	2.70494	-0.78428
C	0.79582	3.3871	-1.05951
H	2.32507	2.70651	0.30361
H	0.81321	4.45183	-0.74765
H	0.60652	3.42701	-2.15014
C	3.30049	3.31639	-1.50665
H	4.19867	2.70575	-1.32533
H	3.12932	3.28348	-2.59733
C	3.62658	4.77179	-1.09342
H	2.76959	5.42722	-1.3183
H	3.77586	4.80474	-0.00066
C	4.85586	5.29349	-1.79787
C	6.13801	5.08015	-1.26268
C	4.75487	5.9432	-3.03999
C	7.28329	5.50638	-1.94295
H	6.23716	4.57486	-0.29709
C	5.89703	6.37143	-3.7247
H	3.76536	6.11711	-3.47369
C	7.16714	6.15441	-3.17823
H	8.27071	5.3344	-1.50579
H	5.79495	6.87886	-4.6879
H	8.06086	6.49029	-3.71052
Ni	1.47262	0.70733	0.21572
P	1.79224	0.03673	2.27622
O	2.61419	1.1532	3.15898
O	2.68767	-1.33283	2.52611
O	0.50722	-0.35538	3.21067
C	3.79827	-1.59393	1.66761
H	4.64052	-0.91616	1.88712
H	4.11605	-2.63066	1.84519
H	3.51563	-1.47745	0.60637
C	0.43771	-1.40221	4.18538
H	-0.60848	-1.45579	4.51692
H	0.7367	-2.36749	3.75107
H	1.07949	-1.1885	5.05449
C	3.00095	0.94809	4.5209
H	3.74565	1.71585	4.77327
H	2.13326	1.05682	5.19229
H	3.44828	-0.0489	4.66175
C	-0.4168	2.7661	-0.41826
C	-1.73717	3.46396	-0.60864
H	-1.62658	4.3738	-1.21272
H	-2.46076	2.79741	-1.1061
H	-2.17632	3.74147	0.36413
C	-1.46151	1.03423	0.83857
H	-1.13951	0.16598	1.42424
H	-2.0012	1.72387	1.50918
H	-2.1699	0.69857	0.06219
N	-0.2911	1.66654	0.23933
C	2.05992	0.81867	-1.64804
C	1.16792	0.83983	-2.77361
C	3.39401	0.36331	-1.94514
C	1.5724	0.47775	-4.05581
H	0.12332	1.12838	-2.61634
C	3.79161	-0.00724	-3.225
H	4.12361	0.30141	-1.13011
C	2.89093	0.05089	-4.30812
H	0.84505	0.50184	-4.87531
H	4.81507	-0.36312	-3.38854
H	3.20478	-0.2364	-5.315

G1-TS-H1

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -403.95 cm^{-1}
Zero-point correction= 0.368867 (Hartree/Particle)
Thermal correction to Energy= 0.389668
Thermal correction to Enthalpy= 0.390612
Thermal correction to Gibbs Free Energy= 0.316564
Sum of electronic and zero-point Energies= -2299.837164
Sum of electronic and thermal Energies= -2299.816363

Sum of electronic and thermal Enthalpies= -2299.815419
Sum of electronic and thermal Free Energies= -2299.889467

C	1.98102	2.85669	-0.84069
C	0.60943	3.38128	-1.31131
H	2.14349	3.13797	0.22171
H	0.63058	4.47547	-1.47251
H	0.39214	2.96545	-2.31351
C	3.12988	3.51176	-1.6268
H	4.07619	3.00991	-1.37103
H	2.98231	3.34393	-2.70865
C	3.31321	5.02147	-1.36262
H	2.40342	5.57385	-1.64612
H	3.45318	5.17402	-0.27891
C	4.49357	5.5837	-2.11915
C	5.7848	5.55565	-1.56522
C	4.33949	6.09283	-3.4198
C	6.88804	6.02598	-2.28502
H	5.92462	5.16222	-0.55378
C	5.4394	6.56383	-4.14435
H	3.34175	6.12211	-3.8682
C	6.71928	6.53217	-3.57893
H	7.8833	5.99957	-1.83298
H	5.29629	6.95976	-5.15347
H	7.5798	6.90226	-4.14231
Ni	1.18612	1.23045	0.1107
C	-0.58711	3.06378	-0.43885
C	-1.85553	3.84086	-0.66488
H	-1.74758	4.55912	-1.48797
H	-2.69645	3.16645	-0.89768
H	-2.13973	4.39812	0.24477
C	-1.63552	1.74156	1.24852
H	-2.45801	1.34215	0.62883
H	-1.33468	0.96715	1.96374
H	-2.03051	2.60566	1.81035
N	-0.48456	2.10438	0.4278
C	2.39997	1.06976	-1.20491
C	2.07525	0.59864	-2.50903
C	3.57619	0.53741	-0.59676
C	2.85163	-0.37087	-3.14174
H	1.18993	0.9948	-3.016
C	4.328	-0.46407	-1.2235
H	3.91347	0.93227	0.36728
C	3.9788	-0.91784	-2.50183
H	2.57269	-0.72029	-4.14108
H	5.20255	-0.88399	-0.71568
H	4.57928	-1.68283	-3.00123

^{3}G1-TS-H1

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -377.93 cm^{-1}
Zero-point correction= 0.368147 (Hartree/Particle)
Thermal correction to Energy= 0.389142
Thermal correction to Enthalpy= 0.390086
Thermal correction to Gibbs Free Energy= 0.314194
Sum of electronic and zero-point Energies= -2299.828582
Sum of electronic and thermal Energies= -2299.807588
Sum of electronic and thermal Enthalpies= -2299.806644
Sum of electronic and thermal Free Energies= -2299.882535

C	1.98493	2.9366	-0.659
C	0.65448	3.37517	-1.26149
H	2.04063	3.27286	0.39573
H	0.6189	4.47237	-1.40256
H	0.55955	2.96993	-2.2888
C	3.17928	3.51344	-1.40373
H	4.1057	3.07937	-0.99734
H	3.13981	3.19727	-2.46145
C	3.31343	5.05229	-1.34015
H	2.43059	5.53252	-1.79223
H	3.33794	5.36238	-0.28149
C	4.55809	5.53317	-2.04727
C	5.78654	5.61631	-1.3693
C	4.53414	5.84355	-3.41782
C	6.9537	6.00201	-2.03667
H	5.82562	5.37763	-0.30208
C	5.69841	6.22942	-4.09023
H	3.5874	5.78342	-3.96332
C	6.9142	6.31015	-3.40147
H	7.89773	6.06471	-1.48847
H	5.65596	6.47055	-5.15592
H	7.82478	6.61377	-3.92446
Ni	1.21945	1.22346	0.62286
C	-0.59564	2.98725	-0.51738
C	-1.89578	3.61629	-0.93694
H	-2.64461	2.84433	-1.17804
H	-2.31441	4.2205	-0.11419
H	-1.7653	4.26602	-1.81182
C	-1.69493	1.69062	1.16723
H	-2.42137	1.18422	0.50927
H	-1.39227	0.98568	1.95307
H	-2.20585	2.54602	1.63932
N	-0.5114	2.11358	0.42746
C	2.31714	0.97597	-0.90716
C	1.73337	0.53782	-2.15195
C	3.71979	0.6596	-0.76074
C	2.47163	-0.10764	-3.13828
H	0.6636	0.70136	-2.3186
C	4.44598	0.00653	-1.74818
H	4.22764	0.93927	0.1685
C	3.84179	-0.38738	-2.96156
H	1.96885	-0.42505	-4.05924
H	5.50337	-0.22129	-1.57077
H	4.4165	-0.90148	-3.73616

H

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.502384 (Hartree/Particle)
Thermal correction to Energy= 0.534303
Thermal correction to Enthalpy= 0.535247
Thermal correction to Gibbs Free Energy= 0.435781
Sum of electronic and zero-point Energies= -2986.274720
Sum of electronic and thermal Energies= -2986.242801
Sum of electronic and thermal Enthalpies= -2986.241857
Sum of electronic and thermal Free Energies= -2986.341323

C	2.48151	3.16842	-0.88263

C	1.06044	3.71695	-1.06889
H	2.78702	3.39485	0.15488
H	1.04574	4.79172	-0.8192
H	0.77545	3.6883	-2.13825
C	3.48464	3.88359	-1.81407
H	4.47021	3.40905	-1.67377
H	3.20033	3.69297	-2.86449
C	3.63584	5.39875	-1.58991
H	2.68325	5.9092	-1.80305
H	3.86358	5.5805	-0.52549
C	4.72237	5.99452	-2.45541
C	6.05733	6.02518	-2.0178
C	4.43298	6.4792	-3.74207
C	7.07272	6.52752	-2.8382
H	6.30204	5.65208	-1.01866
C	5.44474	6.98209	-4.56684
H	3.39904	6.46354	-4.09999
C	6.76984	7.00795	-4.11744
H	8.10434	6.54632	-2.47639
H	5.19704	7.35772	-5.56337
H	7.56164	7.40281	-4.7593
Ni	1.72602	0.91635	0.56588
P	1.79327	-0.4116	2.16266
O	3.27427	-0.57835	2.88758
O	1.39181	-2.00108	1.85724
O	0.80975	-0.22785	3.49037
C	1.76005	-2.56304	0.60141
H	2.8442	-2.76037	0.55173
H	1.21481	-3.51165	0.48844
H	1.50358	-1.88945	-0.23401
C	0.03516	-1.24601	4.1182
H	-0.55682	-0.75925	4.90753
H	-0.64655	-1.73253	3.40285
H	0.66776	-2.02336	4.57699
C	3.48167	-1.43292	4.00898
H	4.56322	-1.47122	4.20464
H	2.9707	-1.04267	4.90547
H	3.11824	-2.45449	3.80718
C	-0.08419	3.09217	-0.30113
C	-1.40516	3.81838	-0.45749
H	-1.7497	4.22371	0.50788
H	-1.31056	4.65674	-1.15996
H	-2.19083	3.14438	-0.83278
C	-1.04908	1.44946	1.14935
H	-0.73893	1.32244	2.1959
H	-1.986	2.02387	1.10985
H	-1.23415	0.43715	0.75643
N	0.06912	2.0308	0.40987
C	2.57714	1.656	-1.07016
C	2.03548	1.03623	-2.2523
C	3.5649	0.88971	-0.33
C	2.46773	-0.19708	-2.69722
H	1.2686	1.5683	-2.82266
C	4.06026	-0.34126	-0.87704
H	4.21528	1.40956	0.38614
C	3.5169	-0.88614	-2.01861
H	2.02257	-0.63714	-3.59436
H	4.87609	-0.85329	-0.35733
H	3.88297	-1.84043	-2.40731

^{3}H

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.499378 (Hartree/Particle)
Thermal correction to Energy= 0.532225
Thermal correction to Enthalpy= 0.533169
Thermal correction to Gibbs Free Energy= 0.428713
Sum of electronic and zero-point Energies= -2986.236675
Sum of electronic and thermal Energies= -2986.203828
Sum of electronic and thermal Enthalpies= -2986.202884
Sum of electronic and thermal Free Energies= -2986.307340

C	2.93959	3.28986	-0.47199
C	1.38096	3.40598	-0.37267
H	3.37072	3.89429	0.34504
H	1.0719	4.36404	-0.814
H	0.94895	2.61158	-1.01109
C	3.45854	3.86819	-1.80726
H	4.50719	3.55696	-1.95112
H	2.88937	3.42049	-2.64134
C	3.3938	5.40271	-1.90594
H	2.35764	5.74601	-1.75787
H	3.99035	5.83531	-1.08489
C	3.90604	5.91076	-3.23393
C	5.27168	6.18145	-3.42378
C	3.038	6.07008	-4.32723
C	5.75639	6.60238	-4.6666
H	5.9628	6.06313	-2.58374
C	3.51742	6.49062	-5.57217
H	1.97121	5.86357	-4.19818
C	4.88004	6.7583	-5.74657
H	6.82222	6.81185	-4.79168
H	2.82405	6.61228	-6.40878
H	5.25646	7.08923	-6.71798
Ni	2.10785	0.7261	0.89632
P	1.24029	-1.21461	1.39991
O	0.79431	-1.50888	2.95505
O	2.04335	-2.6	1.00316
O	-0.13816	-1.58476	0.58615
C	3.29281	-2.8453	1.65147
H	3.1383	-3.25496	2.66398
H	3.84296	-3.5775	1.04413
H	3.89566	-1.92428	1.72283
C	-0.76224	-0.60109	-0.24651
H	-1.82008	-0.88212	-0.3458
H	-0.68347	0.40698	0.19155
H	-0.29559	-0.58431	-1.24543
C	0.01484	-2.65516	3.31651
H	-0.01818	-2.69404	4.41385
H	-1.00856	-2.57211	2.91849
H	0.47253	-3.58104	2.93208
C	0.8352	3.29742	1.01483
C	0.47332	4.54736	1.77084
H	1.26701	4.84238	2.49243
H	0.32982	5.39587	1.08559
H	-0.44893	4.44074	2.3673
C	0.3903	1.94958	2.95236
H	0.49893	0.90958	3.28614
H	0.88715	2.59434	3.70214
H	-0.68862	2.20248	2.98016
N	0.94922	2.09868	1.61686
C	3.45318	1.8715	-0.30895
C	2.9439	0.80034	-1.12493
C	4.6744	1.63643	0.39333
C	3.67291	-0.41898	-1.22521
H	2.11496	0.97501	-1.81341

C	5.37891	0.44655	0.27164
H	5.0747	2.44465	1.01246
C	4.86781	-0.59802	-0.5485
H	3.27552	-1.21838	-1.85575
H	6.31573	0.30733	0.81614
H	5.41425	-1.53956	-0.63957

H1

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.371619 (Hartree/Particle)
Thermal correction to Energy= 0.392367
Thermal correction to Enthalpy= 0.393311
Thermal correction to Gibbs Free Energy= 0.319819
Sum of electronic and zero-point Energies= -2299.893810
Sum of electronic and thermal Energies= -2299.873063
Sum of electronic and thermal Enthalpies= -2299.872118
Sum of electronic and thermal Free Energies= -2299.945610

C	2.4307	2.98316	-1.0383
C	1.01384	3.59271	-1.12603
H	2.75442	3.06201	0.01432
H	1.06296	4.66002	-0.8563
H	0.67633	3.59588	-2.18136
C	3.43955	3.78992	-1.88356
H	4.39647	3.24089	-1.87489
H	3.10761	3.80554	-2.93682
C	3.70234	5.23039	-1.40857
H	2.77618	5.82379	-1.46988
H	3.99425	5.20657	-0.34465
C	4.78154	5.90994	-2.21973
C	6.1348	5.79554	-1.85894
C	4.46288	6.62518	-3.38646
C	7.13966	6.38014	-2.63675
H	6.40254	5.24256	-0.95346
C	5.46384	7.21136	-4.16825
H	3.41444	6.72519	-3.68337
C	6.80752	7.09073	-3.79589
H	8.18615	6.28281	-2.3352
H	5.19343	7.76689	-5.07036
H	7.59111	7.55021	-4.40393
Ni	1.41674	0.68614	-0.10114
C	-0.12226	2.9987	-0.31163
C	-1.3255	3.89116	-0.1277
H	-1.41868	4.20573	0.92686
H	-1.24904	4.79738	-0.74278
H	-2.26076	3.37106	-0.38923
C	-1.21396	1.28976	0.94155
H	-1.49546	1.97134	1.76185
H	-2.10005	1.14915	0.29911
H	-0.95063	0.31675	1.3753
N	-0.0779	1.79463	0.16598
C	2.45404	1.50277	-1.41749
C	2.05932	1.11381	-2.75832
C	3.30116	0.54272	-0.69163
C	2.38403	-0.11445	-3.29423
H	1.48365	1.82075	-3.36385
C	3.60441	-0.71937	-1.29175
H	3.95337	0.88891	0.12347
C	3.15106	-1.06245	-2.55399
H	2.04656	-0.36743	-4.30455
H	4.23875	-1.41958	-0.73677
H	3.38534	-2.0392	-2.98549

^{3}H1

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.371229 (Hartree/Particle)
Thermal correction to Energy= 0.392326
Thermal correction to Enthalpy= 0.393270
Thermal correction to Gibbs Free Energy= 0.317356
Sum of electronic and zero-point Energies= -2299.867581
Sum of electronic and thermal Energies= -2299.846485
Sum of electronic and thermal Enthalpies= -2299.845541
Sum of electronic and thermal Free Energies= -2299.921455

C	2.39782	2.98298	-1.1349
C	0.9894	3.57628	-1.26634
H	2.68073	3.05988	-0.06913
H	1.01557	4.65203	-1.02336
H	0.64886	3.54927	-2.31839
C	3.43366	3.80058	-1.93918
H	4.39182	3.25603	-1.90603
H	3.13208	3.82609	-3.00132
C	3.67509	5.23592	-1.43562
H	2.75101	5.82916	-1.52383
H	3.92701	5.1972	-0.36207
C	4.78336	5.92634	-2.19654
C	6.12258	5.80092	-1.78965
C	4.50802	6.66337	-3.36065
C	7.15594	6.39624	-2.52037
H	6.35637	5.23096	-0.88529
C	5.53787	7.26033	-4.09538
H	3.47114	6.77213	-3.69289
C	6.86705	7.12866	-3.67758
H	8.19072	6.29025	-2.18346
H	5.30132	7.83293	-4.99632
H	7.67302	7.59651	-4.24884
Ni	1.46426	0.54223	0.08847
C	-0.11566	2.99245	-0.42036
C	-1.40738	3.77103	-0.41139
H	-1.57485	4.22228	0.58174
H	-1.39429	4.57906	-1.15435
H	-2.26813	3.11551	-0.61579
C	-1.04299	1.42953	1.1182
H	-0.66176	0.60868	1.74328
H	-1.4335	2.22084	1.77867
H	-1.87976	1.04096	0.51396
N	0.04362	1.91091	0.26196
C	2.48345	1.5147	-1.5175
C	1.83958	0.98109	-2.65
C	3.34761	0.62799	-0.7475
C	2.11065	-0.31324	-3.11454
H	1.11987	1.59655	-3.19734
C	3.77352	-0.60439	-1.37004
H	4.02963	1.08056	-0.01784
C	3.14925	-1.07323	-2.50619
H	1.58838	-0.69781	-3.99397
H	4.56991	-1.18674	-0.89712
H	3.44495	-2.0333	-2.94001

B’

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.296728 (Hartree/Particle)
Thermal correction to Energy= 0.318380
Thermal correction to Enthalpy= 0.319324
Thermal correction to Gibbs Free Energy= 0.244471
Sum of electronic and zero-point Energies= -2492.642692
Sum of electronic and thermal Energies= -2492.621040
Sum of electronic and thermal Enthalpies= -2492.620096
Sum of electronic and thermal Free Energies= -2492.694949

C	-3.99254	1.36994	0.17785
H	-4.44477	1.51018	1.17664
H	-3.92974	2.36588	-0.28036
C	-5.81982	1.15839	-1.66052
H	-5.47976	0.87731	-2.66925
H	-6.85479	0.80074	-1.54301
H	-5.80323	2.25134	-1.57274
Ni	-4.08128	-1.644	1.06984
C	-4.91279	0.50858	-0.65825
C	-2.574	0.78033	0.28916
H	-2.23299	0.55982	-0.72908
H	-1.91756	1.55657	0.7154
C	-2.42386	-0.44797	1.15309
H	-2.27021	-0.2713	2.22551
C	-2.09909	-1.70329	0.6349
H	-2.02643	-1.82776	-0.45098
N	-4.87023	-0.76875	-0.49732
C	-5.65163	-1.65728	-1.35742
H	-5.39513	-1.48033	-2.41169
H	-5.41515	-2.7024	-1.11091
H	-6.73437	-1.5056	-1.21599
C	-3.80094	-2.53865	2.68185
C	-3.67623	-3.93743	2.68517
C	-4.00527	-1.85671	3.89153
C	-3.79556	-4.65147	3.88449
H	-3.48817	-4.47469	1.75039
C	-4.12154	-2.57266	5.09095
H	-4.08389	-0.76499	3.90415
C	-4.0174	-3.9689	5.08713
H	-3.70828	-5.74171	3.88089
H	-4.29015	-2.03832	6.03022
H	-4.10035	-4.52576	6.0242
H	-1.62588	-2.46326	1.26196
B	-2.90883	-0.11093	-3.46423
F	-1.94589	-0.05882	-4.4752
F	-2.99075	1.13813	-2.81771
F	-4.16925	-0.42296	-4.02141
F	-2.56157	-1.10122	-2.52421

B’-TS-C’

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -146.53 cm^{-1}
Zero-point correction= 0.296185 (Hartree/Particle)
Thermal correction to Energy= 0.316971
Thermal correction to Enthalpy= 0.317916
Thermal correction to Gibbs Free Energy= 0.245916
Sum of electronic and zero-point Energies= -2492.647190
Sum of electronic and thermal Energies= -2492.626404
Sum of electronic and thermal Enthalpies= -2492.625460
Sum of electronic and thermal Free Energies= -2492.697459

C	-3.05596	1.54247	-0.56825
H	-3.09825	2.50057	-0.01487
H	-2.55163	1.78851	-1.51759
C	-5.22285	2.14191	-1.78609
H	-6.11861	2.55931	-1.29972
H	-4.58054	2.97021	-2.10995
H	-5.56491	1.5897	-2.67705
Ni	-4.24795	-1.29759	0.63258
C	-4.49068	1.20002	-0.87003
C	-2.24311	0.51086	0.21058
H	-1.94318	-0.3109	-0.45911
H	-1.30981	0.99933	0.54474
C	-2.96151	-0.05735	1.41286
H	-3.45718	0.66606	2.07389
C	-2.59556	-1.30647	1.957
H	-1.74548	-1.84482	1.52753
N	-5.06373	0.17728	-0.34102
C	-6.4856	-0.06832	-0.60255
H	-6.63276	-0.31988	-1.66272
H	-6.83061	-0.91832	-0.00306
H	-7.09382	0.8125	-0.34648
C	-3.95049	-2.9054	1.61936
C	-3.35831	-4.00978	0.98884
C	-4.85709	-3.10353	2.67155
C	-3.7024	-5.30531	1.38514
H	-2.6551	-3.84652	0.1692
C	-5.2095	-4.40365	3.05651
H	-5.286	-2.24331	3.19404
C	-4.63042	-5.50555	2.4168
H	-3.24874	-6.16449	0.88312
H	-5.92855	-4.5539	3.86657
H	-4.89482	-6.51995	2.72639
H	-2.74275	-1.47484	3.02415
B	-4.31119	-2.45402	-2.08862
F	-4.41886	-3.68827	-2.70004
F	-4.82011	-1.43453	-2.88501
F	-5.09593	-2.49595	-0.85435
F	-2.98698	-2.18054	-1.7188

C’

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.297706 (Hartree/Particle)
Thermal correction to Energy= 0.318911
Thermal correction to Enthalpy= 0.319855
Thermal correction to Gibbs Free Energy= 0.246031
Sum of electronic and zero-point Energies= -2492.674053
Sum of electronic and thermal Energies= -2492.652848
Sum of electronic and thermal Enthalpies= -2492.651904

Sum of electronic and thermal Free Energies= -2492.725728

C	0.13591	2.74597	-0.74022
H	-0.15588	3.65997	-0.18577
H	0.46103	3.08195	-1.73444
C	-2.00239	2.26421	-2.09001
H	-1.90467	1.43359	-2.80849
H	-3.06206	2.34416	-1.80569
H	-1.6893	3.19421	-2.58037
Ni	-0.40474	0.27276	1.31603
C	-1.12387	1.93622	-0.91863
C	1.28703	2.03003	-0.03819
H	1.57921	1.16683	-0.65285
H	2.15313	2.71917	-0.00458
C	0.96659	1.56585	1.35966
H	0.62262	2.3869	2.01424
C	1.97481	0.63297	2.03538
H	2.76945	0.33239	1.33812
N	-1.42591	0.99809	-0.08874
C	-2.65028	0.20938	-0.27456
H	-2.62998	-0.28792	-1.25371
H	-2.72071	-0.56908	0.50095
H	-3.54755	0.84294	-0.19366
C	1.14256	-0.58826	2.42494
C	1.27553	-1.83696	1.76473
C	0.12855	-0.44322	3.40755
C	0.44838	-2.90413	2.09748
H	2.01591	-1.93774	0.96949
C	-0.70179	-1.53583	3.74084
H	0.05871	0.48204	3.98541
C	-0.54387	-2.75366	3.08669
H	0.55932	-3.85926	1.57925
H	-1.4631	-1.41766	4.51469
H	-1.19099	-3.5971	3.33854
H	2.44295	1.08471	2.9246
B	0.40352	-0.63729	-2.61946
F	1.05917	-1.4114	-3.58373
F	0.66958	0.72622	-2.84786
F	-0.98866	-0.85116	-2.70708
F	0.85736	-0.99916	-1.33478

C'-conf

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.297563 (Hartree/Particle)
Thermal correction to Energy= 0.319065
Thermal correction to Enthalpy= 0.320009
Thermal correction to Gibbs Free Energy= 0.244313
Sum of electronic and zero-point Energies= -2492.675370
Sum of electronic and thermal Energies= -2492.653869
Sum of electronic and thermal Enthalpies= -2492.652924
Sum of electronic and thermal Free Energies= -2492.728620

C	0.55111	-0.85766	-3.31958
H	1.06514	0.09688	-3.51297
H	1.00156	-1.58417	-4.02425
C	-1.22896	0.27723	-4.80066
H	-1.92162	-0.15508	-5.53836
H	-1.72752	1.16211	-4.36742
H	-0.32331	0.61795	-5.318
Ni	-1.58399	-2.91102	-2.02681
C	-0.89374	-0.70162	-3.71121
C	0.77296	-1.30266	-1.8771
H	1.85882	-1.25839	-1.67422
H	0.30641	-0.56519	-1.20004
C	0.24812	-2.68802	-1.55108
H	0.74862	-3.44983	-2.1819
N	-1.79692	-1.40154	-3.11289
C	-3.21099	-1.24845	-3.47614
H	-3.53406	-0.20047	-3.38122
H	-3.3921	-1.58226	-4.5101
H	-3.839	-1.85342	-2.80719
C	1.85225	-3.21511	0.34233
C	2.53401	-4.41228	0.05839
C	2.56301	-2.17168	0.95669
C	3.88602	-4.5607	0.38165
H	1.985	-5.2293	-0.41667
C	3.91695	-2.31677	1.28166
H	2.0478	-1.23412	1.1852
C	4.58416	-3.5123	0.99416
H	4.39807	-5.50074	0.15771
H	4.45177	-1.49288	1.76223
H	5.64118	-3.62802	1.24793
C	0.40057	-3.05891	-0.06664
H	-0.12089	-4.00463	0.12394
H	-0.0803	-2.28211	0.55087
B	-1.25123	-5.88649	-1.81292
F	-1.87179	-4.66577	-1.22209
F	-2.1879	-6.8919	-1.71183
F	-0.94666	-5.57461	-3.12742
F	-0.11118	-6.15448	-1.07117

C1

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.370980 (Hartree/Particle)
Thermal correction to Energy= 0.392035
Thermal correction to Enthalpy= 0.392979
Thermal correction to Gibbs Free Energy= 0.318419
Sum of electronic and zero-point Energies= -2299.904933
Sum of electronic and thermal Energies= -2299.883878
Sum of electronic and thermal Enthalpies= -2299.882934
Sum of electronic and thermal Free Energies= -2299.957494

C	0.20533	-1.55543	-2.8354
H	0.82218	-1.59351	-3.74811
H	-0.26251	-2.55635	-2.75455
C	-1.39688	-0.34292	-4.46004
H	-2.49671	-0.32647	-4.50232
H	-1.04475	0.63078	-4.84443
H	-1.0262	-1.12539	-5.13496
Ni	-1.24457	-0.49057	-0.19191
C	-0.89671	-0.55164	-3.05677
C	1.08071	-1.26907	-1.61728
H	1.96119	-1.9354	-1.6752
H	1.47495	-0.24073	-1.70663
C	0.40999	-1.43602	-0.25374
H	0.14442	-2.50291	-0.11154
N	-1.36015	0.09383	-2.04237
C	-2.40337	1.10264	-2.23545

H	-2.1098	1.85127	-2.98848
H	-3.35198	0.64207	-2.5586
H	-2.58382	1.6292	-1.28822
C	2.62712	-1.82016	0.96073
C	2.59238	-3.12367	1.48772
C	3.85342	-1.3359	0.47756
C	3.74259	-3.91672	1.53163
H	1.64538	-3.51723	1.86958
C	5.00927	-2.12477	0.51829
H	3.90176	-0.32474	0.06267
C	4.95834	-3.41973	1.04494
H	3.69237	-4.926	1.94972
H	5.95336	-1.72562	0.1371
H	5.85961	-4.03748	1.07862
C	1.35464	-1.00008	0.88443
H	0.8215	-1.08003	1.84063
H	1.61063	0.06447	0.7515
C	-1.74313	-1.00381	1.54326
C	-2.53777	-0.03298	2.19896
C	-1.59951	-2.24103	2.20771
C	-3.15383	-0.27974	3.43467
H	-2.68705	0.95189	1.73696
C	-2.20647	-2.50153	3.44215
H	-0.98869	-3.02741	1.74994
C	-2.98921	-1.51897	4.06401
H	-3.75838	0.49917	3.9109
H	-2.07243	-3.47605	3.92321
H	-3.46315	-1.71747	5.02962

C1'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.389068 (Hartree/Particle)
Thermal correction to Energy= 0.417693
Thermal correction to Enthalpy= 0.418637
Thermal correction to Gibbs Free Energy= 0.326333
Sum of electronic and zero-point Energies= -2871.095449
Sum of electronic and thermal Energies= -2871.066824
Sum of electronic and thermal Enthalpies= -2871.065880
Sum of electronic and thermal Free Energies= -2871.158184

C	0.48242	1.95201	-1.35336
H	0.13831	2.33444	-0.38036
H	0.87245	2.80665	-1.92973
C	-0.62053	1.39495	-3.60506
H	0.42432	1.30758	-3.93109
H	-1.20707	0.60826	-4.09559
H	-1.0011	2.37294	-3.95087
Ni	-0.67799	-0.62674	-1.41656
C	-0.69556	1.34126	-2.09987
C	1.56525	0.89534	-1.10428
H	2.02844	0.58571	-2.0571
H	2.3754	1.32519	-0.48707
C	0.94655	-0.3151	-0.416
H	0.42905	-0.00248	0.51134
N	-1.85588	1.14989	-1.44368
C	-3.08291	0.8896	-2.21315
H	-3.87907	0.56896	-1.53071
H	-3.40961	1.80882	-2.72676
H	-2.95303	0.10351	-2.97492
C	2.9523	-0.96475	0.97628
C	4.278	-0.67083	0.61969
C	2.56504	-0.78198	2.31518
C	5.19586	-0.21197	1.57241
H	4.59555	-0.80318	-0.41892
C	3.4769	-0.32151	3.26867
H	1.53207	-0.98319	2.60337
C	4.79776	-0.03463	2.90168
H	6.22448	0.00871	1.27404
H	3.15127	-0.17993	4.30306
H	5.51162	0.32571	3.64717
C	1.94195	-1.42103	-0.05971
H	2.46555	-1.76088	-0.9653
H	1.38228	-2.28666	0.32646
C	0.10249	-2.0988	-2.24049
C	-0.26861	-3.38297	-1.79519
C	0.8786	-2.00208	-3.41025
C	0.10439	-4.53078	-2.50733
H	-0.84964	-3.49553	-0.87375
C	1.25824	-3.14709	-4.1222
H	1.19999	-1.02131	-3.77185
C	0.87115	-4.41587	-3.67298
H	-0.19764	-5.51846	-2.14599
H	1.86026	-3.04879	-5.03057
H	1.17114	-5.31057	-4.22529
Ag	-2.11193	1.57923	0.67698
B	-0.43564	1.09506	3.10789
F	0.47121	1.70977	2.24206
F	-0.61173	-0.25017	2.76691
F	-0.06653	1.24398	4.42846
F	-1.72745	1.74839	2.89991

C2'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.435877 (Hartree/Particle)
Thermal correction to Energy= 0.469099
Thermal correction to Enthalpy= 0.470043
Thermal correction to Gibbs Free Energy= 0.366776
Sum of electronic and zero-point Energies= -3003.736030
Sum of electronic and thermal Energies= -3003.702809
Sum of electronic and thermal Enthalpies= -3003.701865
Sum of electronic and thermal Free Energies= -3003.805131

C	1.79851	1.6635	-0.75941
H	1.49797	2.12413	0.20081
H	2.52392	2.36193	-1.20453
C	0.25524	2.90738	-2.40405
H	0.92412	3.72975	-2.12162
H	0.38816	2.70594	-3.48138
H	-0.78235	3.22627	-2.24288
Ni	0.02913	-1.11926	-0.57547
C	0.55934	1.6615	-1.61736
C	2.48417	0.31756	-0.52237
H	2.79822	-0.12134	-1.48234
H	3.41752	0.53327	0.02979
C	1.71687	-0.71457	0.28384
H	1.22188	-0.23107	1.14795
N	-0.19387	0.62107	-1.64342
C	-1.41236	0.63641	-2.45247

H	-1.91705	-0.33643	-2.38417
H	-2.10598	1.41531	-2.09667
H	-1.18811	0.82884	-3.51463
C	3.47951	-1.44031	1.93363
C	4.84371	-1.17054	1.7418
C	2.93835	-1.26424	3.21932
C	5.64757	-0.73904	2.80358
H	5.28214	-1.30392	0.74868
C	3.73667	-0.83345	4.28252
H	1.87666	-1.47001	3.38633
C	5.09635	-0.56801	4.07758
H	6.70855	-0.53703	2.6339
H	3.29768	-0.70638	5.27572
H	5.72254	-0.23161	4.90791
C	2.58856	-1.86776	0.78404
H	3.1957	-2.25885	-0.04468
H	1.94404	-2.69186	1.11735
C	0.95883	-2.29327	-1.75952
C	1.1395	-3.66473	-1.50186
C	1.29518	-1.82578	-3.04414
C	1.61827	-4.53834	-2.48711
H	0.9161	-4.06922	-0.51271
C	1.776	-2.69246	-4.03531
H	1.18303	-0.76506	-3.28189
C	1.93897	-4.05471	-3.7608
H	1.74362	-5.60054	-2.25614
H	2.02595	-2.29897	-5.02536
H	2.31736	-4.73283	-4.53056
N	-1.4966	-1.01115	0.73396
C	-0.8891	-2.06926	0.7783
C	-0.89954	-3.37096	1.4896
H	-1.67434	-3.38125	2.2705
H	-1.08948	-4.18175	0.77041
H	0.08321	-3.56096	1.94528
Ag	-2.23564	0.89542	1.13222
B	-2.04264	3.83513	0.35191
F	-2.2154	5.16971	0.64875
F	-2.59133	3.50062	-0.88775
F	-0.69991	3.45531	0.41749
F	-2.75288	3.04265	1.35803

C2'-TS-P2'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -277.18 cm^{-1}
Zero-point correction= 0.435999 (Hartree/Particle)
Thermal correction to Energy= 0.468431
Thermal correction to Enthalpy= 0.469376
Thermal correction to Gibbs Free Energy= 0.367640
Sum of electronic and zero-point Energies= -3003.725069
Sum of electronic and thermal Energies= -3003.692637
Sum of electronic and thermal Enthalpies= -3003.691693
Sum of electronic and thermal Free Energies= -3003.793428

C	-4.37175	0.58295	0.96429
H	-4.7796	0.74917	1.97895
H	-3.69241	1.42482	0.77019
C	-5.72152	1.91453	-0.8121
H	-4.98415	2.68291	-0.54905
H	-5.61968	1.68864	-1.88757
H	-6.73113	2.31949	-0.65307
Ni	-6.22039	-2.00326	1.04874
C	-5.53485	0.66259	0.00143
C	-3.55358	-0.71925	0.9481
H	-3.16547	-0.91368	-0.06348
H	-2.66343	-0.52886	1.57055
C	-4.23563	-1.95842	1.51949
H	-4.80087	-1.64827	2.42349
N	-6.33227	-0.34185	-0.08457
C	-7.45378	-0.2943	-1.02095
H	-8.05273	-1.20748	-0.9156
H	-8.09928	0.57817	-0.83129
H	-7.09439	-0.23481	-2.06212
C	-2.42988	-2.54925	3.1997
C	-1.07319	-2.21428	3.0722
C	-3.03715	-2.40683	4.45988
C	-0.34029	-1.75048	4.17135
H	-0.58446	-2.31897	2.09931
C	-2.31065	-1.94317	5.55973
H	-4.09362	-2.6657	4.57942
C	-0.95716	-1.61197	5.41859
H	0.7162	-1.49636	4.05119
H	-2.80058	-1.84272	6.53188
H	-0.38699	-1.24984	6.27792
C	-3.24353	-3.02758	2.01303
H	-2.57582	-3.33287	1.19323
H	-3.80575	-3.91975	2.31847
C	-5.03743	-3.08192	-0.01135
C	-5.11362	-4.47677	0.19431
C	-4.68394	-2.63851	-1.30162
C	-4.88944	-5.38166	-0.84696
H	-5.35487	-4.86665	1.18297
C	-4.44661	-3.54265	-2.34288
H	-4.61498	-1.57162	-1.51032
C	-4.54979	-4.92024	-2.12412
H	-4.97788	-6.45457	-0.6546
H	-4.18469	-3.16162	-3.334
H	-4.36378	-5.6264	-2.93731
N	-7.94317	-2.07208	1.93197
C	-7.22967	-3.01757	2.25849
C	-7.27438	-4.21354	3.1356
H	-8.13773	-4.18221	3.81781
H	-7.34236	-5.11755	2.50944
H	-6.34219	-4.29123	3.71475
Ag	-9.03527	-0.30218	2.1181
B	-8.69679	2.71464	1.48437
F	-8.8876	3.9824	1.99444
F	-8.8708	2.6809	0.10031
F	-7.44638	2.19824	1.83605
F	-9.7026	1.82839	2.07211

P2'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.439787 (Hartree/Particle)
Thermal correction to Energy= 0.472173
Thermal correction to Enthalpy= 0.473117
Thermal correction to Gibbs Free Energy= 0.371577
Sum of electronic and zero-point Energies= -3003.783773
Sum of electronic and thermal Energies= -3003.751388

Sum of electronic and thermal Enthalpies= -3003.750444
Sum of electronic and thermal Free Energies= -3003.851983

C	1.00587	0.71922	0.21235
H	0.3624	0.02913	0.77965
H	0.92434	1.7055	0.69606
C	0.96699	2.0631	-1.97833
H	1.76229	2.59698	-1.44255
H	1.35868	1.73054	-2.9528
H	0.14163	2.76503	-2.1683
Ni	-1.12776	-1.5516	-0.71613
C	0.44951	0.89742	-1.17902
C	2.47443	0.24445	0.26839
H	3.05076	0.69399	-0.55871
H	2.93421	0.626	1.19245
C	2.65016	-1.28942	0.2491
H	2.19905	-1.675	1.17914
N	-0.44287	0.08797	-1.63355
C	-1.02369	0.34335	-2.95185
H	-1.81545	-0.39087	-3.14764
H	-1.45756	1.35464	-3.00079
H	-0.26517	0.24372	-3.74616
C	4.89193	-1.23242	1.48866
C	5.75268	-0.12419	1.4441
C	4.70631	-1.88325	2.72069
C	6.41036	0.32303	2.59564
H	5.90869	0.39529	0.49434
C	5.35965	-1.43981	3.87407
H	4.04178	-2.75096	2.77374
C	6.21524	-0.33298	3.81549
H	7.07782	1.18703	2.5387
H	5.20399	-1.96191	4.82196
H	6.72866	0.01406	4.71588
C	4.14563	-1.69989	0.25976
H	4.63372	-1.30622	-0.64639
H	4.19578	-2.79911	0.19514
C	1.90634	-1.9325	-0.90509
C	0.83081	-2.81655	-0.64461
C	2.20795	-1.61967	-2.23148
C	0.06062	-3.34241	-1.7043
H	0.66929	-3.17229	0.37645
C	1.44842	-2.14549	-3.29091
H	3.02907	-0.93379	-2.45461
C	0.37442	-2.99143	-3.03505
H	-0.69581	-4.10445	-1.50631
H	1.69895	-1.87681	-4.32009
H	-0.21748	-3.39939	-3.85744
N	-2.7335	-1.10487	0.14264
C	-2.46383	-2.30386	0.30786
C	-3.07908	-3.46608	1.00322
H	-4.01283	-3.19416	1.52058
H	-3.28411	-4.26561	0.27357
H	-2.36341	-3.8811	1.73056
Ag	-3.27515	0.9071	0.13318
B	-2.1609	3.71895	-0.59691
F	-2.21508	5.06793	-0.31083
F	-2.03722	3.48519	-1.96658
F	-1.13726	3.08091	0.10857
F	-3.41827	3.10962	-0.16115

B1’

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.282296 (Hartree/Particle)
Thermal correction to Energy= 0.304826
Thermal correction to Enthalpy= 0.305770
Thermal correction to Gibbs Free Energy= 0.225132
Sum of electronic and zero-point Energies= -3731.759420
Sum of electronic and thermal Energies= -3731.736890
Sum of electronic and thermal Enthalpies= -3731.735946
Sum of electronic and thermal Free Energies= -3731.816584

C	-3.77928	1.51233	-0.13849
H	-4.24903	1.88908	0.78948
H	-3.64448	2.39493	-0.78228
C	-5.80237	1.22649	-1.69468
H	-5.48247	1.11769	-2.74631
H	-6.78185	0.73908	-1.58929
H	-5.90373	2.29838	-1.48071
Ni	-3.79423	-1.59195	0.87655
C	-4.76023	0.5945	-0.82184
C	-2.41739	0.87493	0.14107
H	-2.03647	0.4401	-0.79541
H	-1.71839	1.67577	0.4385
C	-2.38093	-0.16295	1.2284
H	-2.5666	0.19542	2.2499
C	-1.75398	-1.39618	1.05413
H	-1.3656	-1.67778	0.06834
N	-4.65421	-0.68216	-0.67184
C	-5.53839	-1.58438	-1.4177
H	-5.48162	-1.37504	-2.49747
H	-5.2093	-2.6207	-1.26425
H	-6.58474	-1.48723	-1.08662
C	-3.70044	-2.60204	2.41901
C	-3.66645	-3.99305	2.23245
C	-3.95989	-2.06181	3.68577
C	-3.95027	-4.84207	3.31032
H	-3.41676	-4.41216	1.2526
C	-4.23595	-2.91766	4.76049
H	-3.96021	-0.97913	3.83955
C	-4.23275	-4.30533	4.57244
H	-3.93552	-5.92594	3.16562
H	-4.4515	-2.49834	5.74717
H	-4.43897	-4.97051	5.41493
H	-1.3666	-1.96199	1.90319
Cu	-2.4764	-1.75643	-2.61047
I	-2.33869	-4.144	-1.81699
I	-2.52334	0.39227	-3.92206

B1’-TS-C1’

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -95.03 cm^{-1}
Zero-point correction= 0.281958 (Hartree/Particle)
Thermal correction to Energy= 0.303931
Thermal correction to Enthalpy= 0.304875
Thermal correction to Gibbs Free Energy= 0.225156
Sum of electronic and zero-point Energies= -3731.756805
Sum of electronic and thermal Energies= -3731.734833

Sum of electronic and thermal Enthalpies= -3731.733888
Sum of electronic and thermal Free Energies= -3731.813608

C	-2.89005	1.27033	-0.76503
H	-2.88099	2.32426	-0.42668
H	-2.35999	1.27861	-1.73151
C	-4.98737	1.79384	-2.11704
H	-5.39828	1.13163	-2.89655
H	-5.82918	2.38034	-1.71513
H	-4.27137	2.48266	-2.58164
Ni	-4.29497	-1.25074	0.81295
C	-4.34045	0.97127	-1.03731
C	-2.14205	0.38502	0.23392
H	-1.79779	-0.53381	-0.26549
H	-1.23427	0.92901	0.55143
C	-2.95079	0.02593	1.45148
H	-3.49131	0.84613	1.94207
C	-2.71277	-1.14574	2.19569
H	-1.83961	-1.75687	1.95635
N	-5.00516	0.10072	-0.35675
C	-6.44056	-0.0703	-0.59909
H	-6.61092	-0.53479	-1.58271
H	-6.86453	-0.74103	0.15703
H	-6.97353	0.89155	-0.55629
C	-3.92861	-2.88667	1.63145
C	-3.15876	-3.85862	0.9574
C	-4.90756	-3.28014	2.55929
C	-3.44582	-5.21798	1.14445
H	-2.33065	-3.55596	0.31342
C	-5.18694	-4.63815	2.73275
H	-5.46464	-2.52788	3.12387
C	-4.46229	-5.60525	2.0232
H	-2.86659	-5.97092	0.60444
H	-5.97121	-4.94551	3.42926
H	-4.68065	-6.66567	2.17029
H	-3.03691	-1.19184	3.23793
Cu	-4.60672	-3.05069	-1.04102
I	-7.00934	-3.89823	-0.84464
I	-2.83153	-2.27074	-2.734

C1'

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.284299 (Hartree/Particle)
Thermal correction to Energy= 0.306139
Thermal correction to Enthalpy= 0.307083
Thermal correction to Gibbs Free Energy= 0.228004
Sum of electronic and zero-point Energies= -3731.790191
Sum of electronic and thermal Energies= -3731.768351
Sum of electronic and thermal Enthalpies= -3731.767407
Sum of electronic and thermal Free Energies= -3731.846486

C	0.09257	2.56755	-1.00209
H	-0.07148	3.5531	-0.52328
H	0.36374	2.7995	-2.04528
C	-2.28136	2.45782	-1.95822
H	-2.50707	1.72298	-2.74991
H	-3.22737	2.67559	-1.43897
H	-1.91907	3.37639	-2.43648
Ni	-0.41559	0.08924	1.07287
C	-1.25472	1.89279	-1.01558
C	1.22692	1.81884	-0.31236
H	1.48797	0.91829	-0.89212
H	2.12816	2.46072	-0.33418
C	0.91698	1.42186	1.11039
H	0.55175	2.26954	1.7164
C	1.93706	0.54523	1.83876
H	2.72597	0.20521	1.15442
N	-1.51657	0.90269	-0.2331
C	-2.85444	0.29873	-0.23554
H	-3.17771	0.04064	-1.25418
H	-2.85377	-0.63206	0.34774
H	-3.58422	0.99248	0.21173
C	1.13082	-0.66231	2.3186
C	1.39295	-1.97718	1.8573
C	0.0427	-0.46003	3.20852
C	0.60373	-3.04474	2.26885
H	2.22318	-2.13754	1.16676
C	-0.75581	-1.55252	3.61416
H	-0.11202	0.51772	3.6728
C	-0.47949	-2.8319	3.14184
H	0.81511	-4.04934	1.89646
H	-1.58162	-1.38557	4.30897
H	-1.10149	-3.6747	3.45228
H	2.40796	1.06349	2.69012
Cu	1.1902	-1.80685	-1.36015
I	-1.10711	-2.80347	-1.59017
I	3.64643	-1.2799	-1.61158

C1'-conf

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.284201 (Hartree/Particle)
Thermal correction to Energy= 0.306437
Thermal correction to Enthalpy= 0.307381
Thermal correction to Gibbs Free Energy= 0.225667
Sum of electronic and zero-point Energies= -3731.784261
Sum of electronic and thermal Energies= -3731.762026
Sum of electronic and thermal Enthalpies= -3731.761082
Sum of electronic and thermal Free Energies= -3731.842796

C	0.40873	-0.47948	-2.83017
H	0.57649	0.61045	-2.79162
H	1.26708	-0.88023	-3.40378
C	-0.87686	0.0211	-4.9868
H	-1.0663	-0.6625	-5.82845
H	-1.70097	0.7539	-4.96294
H	0.05645	0.56619	-5.17625
Ni	-1.80701	-2.68637	-1.8095
C	-0.80422	-0.72633	-3.68282
C	0.38545	-1.08625	-1.43386
H	1.38386	-0.93343	-0.98532
H	-0.31894	-0.53609	-0.78469
C	0.0459	-2.56668	-1.43404
H	0.55192	-3.08836	-2.26672
N	-1.70769	-1.56601	-3.31051
C	-2.87977	-1.84042	-4.14905
H	-3.23119	-0.94601	-4.68245
H	-2.63489	-2.62745	-4.87931

H	-3.71307	-2.20097	-3.52731
C	1.83912	-3.37428	0.16132
C	2.63366	-4.27738	-0.56663
C	2.45984	-2.55196	1.11367
C	4.01058	-4.36046	-0.34318
H	2.16086	-4.9224	-1.31398
C	3.83884	-2.63342	1.3415
H	1.85457	-1.84486	1.68814
C	4.61873	-3.53797	0.61371
H	4.61211	-5.07264	-0.9145
H	4.30386	-1.98917	2.09253
H	5.69505	-3.60443	0.7922
C	0.35214	-3.28925	-0.11659
H	-0.0472	-4.31208	-0.16774
H	-0.16725	-2.78764	0.71486
Cu	-1.6498	-5.14606	-2.16697
I	-0.13905	-6.03988	-3.9556
I	-3.15924	-4.41643	-0.22099

C1''

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.374128 (Hartree/Particle)
Thermal correction to Energy= 0.398838
Thermal correction to Enthalpy= 0.399782
Thermal correction to Gibbs Free Energy= 0.314439
Sum of electronic and zero-point Energies= -3951.726957
Sum of electronic and thermal Energies= -3951.702247
Sum of electronic and thermal Enthalpies= -3951.701303
Sum of electronic and thermal Free Energies= -3951.786645

C	0.64276	2.05153	-1.65651
H	0.4129	2.50685	-0.68052
H	1.0007	2.85491	-2.31937
C	-0.80382	1.54735	-3.72491
H	-1.5043	0.80645	-4.13015
H	-1.17781	2.55295	-3.98978
H	0.17028	1.41338	-4.21438
Ni	-0.55351	-0.5402	-1.64202
C	-0.63949	1.4594	-2.23052
C	1.70737	0.96338	-1.46613
H	2.0836	0.61905	-2.44434
H	2.5782	1.37528	-0.92335
C	1.09723	-0.21127	-0.71351
H	0.61553	0.15033	0.21997
N	-1.67601	1.25517	-1.3952
C	-3.03008	1.05343	-1.93409
H	-3.06712	0.35674	-2.78699
H	-3.67078	0.65285	-1.13873
H	-3.4456	2.01939	-2.26422
C	3.05793	-0.85451	0.7186
C	4.3914	-0.55804	0.39611
C	2.6315	-0.65277	2.04345
C	5.2781	-0.08011	1.36846
H	4.73921	-0.70457	-0.63058
C	3.51207	-0.17422	3.01746
H	1.59336	-0.87039	2.31209
C	4.84116	0.11423	2.68285
H	6.31366	0.14205	1.09689
H	3.16059	-0.02594	4.04212
H	5.53166	0.48801	3.44333
C	2.0747	-1.32308	-0.33619
H	2.61201	-1.67197	-1.23029
H	1.50222	-2.18161	0.04668
C	0.19326	-2.00243	-2.52245
C	-0.13912	-3.29424	-2.06885
C	0.90853	-1.88843	-3.72857
C	0.21429	-4.43285	-2.80496
H	-0.67472	-3.41988	-1.12186
C	1.26831	-3.024	-4.46609
H	1.19553	-0.90073	-4.10142
C	0.92149	-4.30038	-4.00603
H	-0.0568	-5.4267	-2.43609
H	1.82278	-2.91242	-5.40272
H	1.20601	-5.18771	-4.5781
Cu	-1.60072	1.45558	0.53343
I	-1.43676	1.58965	3.01094

C2''

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.421193 (Hartree/Particle)
Thermal correction to Energy= 0.450556
Thermal correction to Enthalpy= 0.451500
Thermal correction to Gibbs Free Energy= 0.356431
Sum of electronic and zero-point Energies= -4084.370722
Sum of electronic and thermal Energies= -4084.341360
Sum of electronic and thermal Enthalpies= -4084.340416
Sum of electronic and thermal Free Energies= -4084.435484

C	-3.688	0.94932	0.38864
H	-3.3713	1.45555	1.32021
H	-3.127	1.45446	-0.41656
C	-5.48745	2.70835	-0.11273
H	-4.61098	3.36157	-0.0135
H	-5.86095	2.77909	-1.14853
H	-6.28419	3.07853	0.55077
Ni	-5.67064	-1.65413	0.6759
C	-5.14404	1.27524	0.18559
C	-3.30941	-0.52896	0.42957
H	-3.48923	-0.98581	-0.56096
H	-2.21489	-0.58539	0.57136
C	-3.96302	-1.3565	1.53514
H	-4.0833	-0.75504	2.44768
N	-6.02379	0.34244	0.25033
C	-7.43055	0.64097	-0.00154
H	-7.57637	0.88366	-1.06776
H	-8.04108	-0.23881	0.23921
H	-7.7957	1.48616	0.60318
C	-1.94578	-2.40818	2.63079
C	-0.69082	-2.44617	2.00316
C	-2.00007	-2.08476	3.99806
C	0.47978	-2.16964	2.71971
H	-0.62895	-2.70002	0.94099
C	-0.8343	-1.8083	4.71742
H	-2.971	-2.05256	4.50165
C	0.41174	-1.84861	4.07918
H	1.44789	-2.20686	2.21312
H	-0.89685	-1.56272	5.78096
H	1.32455	-1.63298	4.64042

C	-3.22692	-2.6575	1.85992
H	-3.00294	-3.19701	0.92646
H	-3.88748	-3.30025	2.45822
C	-6.33949	-1.8907	2.43956
C	-6.79744	-0.75663	3.13685
C	-6.55055	-3.14848	3.03199
C	-7.47455	-0.87498	4.35712
H	-6.61632	0.24054	2.72798
C	-7.22722	-3.27442	4.25357
H	-6.18654	-4.05429	2.54429
C	-7.69578	-2.13732	4.9201
H	-7.82394	0.02444	4.87306
H	-7.38517	-4.26747	4.68482
H	-8.22034	-2.23287	5.87458
N	-5.75364	-2.53853	-1.17641
C	-5.6147	-3.30963	-0.24024
C	-5.51719	-4.76749	0.02046
H	-4.72173	-4.97752	0.74804
H	-6.46596	-5.11878	0.45478
H	-5.32433	-5.31436	-0.9142
Cu	-5.69158	-1.09324	-2.36241
I	-5.51499	0.86472	-3.89116

C2''-TS-P2''

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Imaginary frequency = -255.80 cm^{-1}
Zero-point correction= 0.421601 (Hartree/Particle)
Thermal correction to Energy= 0.450178
Thermal correction to Enthalpy= 0.451122
Thermal correction to Gibbs Free Energy= 0.356875
Sum of electronic and zero-point Energies= -4084.354614
Sum of electronic and thermal Energies= -4084.326037
Sum of electronic and thermal Enthalpies= -4084.325092
Sum of electronic and thermal Free Energies= -4084.419340

C	-3.65632	1.15644	0.9869
H	-3.63838	1.57839	2.01035
H	-2.96167	1.79074	0.41108
C	-5.44305	2.79353	0.11935
H	-4.62799	3.50035	0.32019
H	-5.74054	2.88915	-0.93782
H	-6.31696	3.08647	0.72451
Ni	-5.37328	-1.54351	0.72963
C	-5.03844	1.37678	0.42833
C	-3.13257	-0.27871	0.97978
H	-3.17349	-0.67711	-0.04804
H	-2.05576	-0.22207	1.21758
C	-3.70618	-1.28753	2.0088
H	-3.50289	-0.83402	2.9856
N	-5.81961	0.3716	0.26508
C	-7.16404	0.57508	-0.26714
H	-7.12184	0.87305	-1.32837
H	-7.72355	-0.36621	-0.20831
H	-7.71689	1.35019	0.28766
C	-1.54961	-2.49635	2.59473
C	-0.3813	-2.40279	1.82291
C	-1.4319	-2.44707	3.99496
C	0.87229	-2.26425	2.43055
H	-0.4546	-2.44063	0.7323
C	-0.18294	-2.30783	4.60612
H	-2.33311	-2.52296	4.61123
C	0.97535	-2.21525	3.82432
H	1.77078	-2.1945	1.81169
H	-0.11161	-2.27533	5.69656
H	1.95322	-2.10761	4.30062
C	-2.91614	-2.61262	1.95118
H	-2.811	-2.92965	0.90366
H	-3.4745	-3.40401	2.46564
C	-5.46835	-1.4917	2.64922
C	-6.03583	-0.33551	3.2394
C	-5.79953	-2.73552	3.22955
C	-6.93711	-0.42766	4.29846
H	-5.77028	0.65107	2.86277
C	-6.70978	-2.82799	4.28871
H	-5.36436	-3.65311	2.8361
C	-7.28807	-1.67694	4.82964
H	-7.36655	0.48679	4.71695
H	-6.9654	-3.81307	4.68866
H	-7.99411	-1.74764	5.66065
N	-6.00512	-2.48743	-0.81561
C	-5.52088	-3.25869	0.01543
C	-5.32756	-4.72269	0.17387
H	-4.31401	-4.94231	0.53955
H	-6.03211	-5.09301	0.93655
H	-5.50852	-5.25753	-0.77114
Cu	-6.82533	-1.9147	-2.39641
I	-7.90709	-1.06808	-4.48015

P2''

UB3LYP-D3/def2SVP-LANL2DZ(I)-CPCM(acetonitrile)
Zero-point correction= 0.422664 (Hartree/Particle)
Thermal correction to Energy= 0.451713
Thermal correction to Enthalpy= 0.452657
Thermal correction to Gibbs Free Energy= 0.358535
Sum of electronic and zero-point Energies= -4084.409771
Sum of electronic and thermal Energies= -4084.380722
Sum of electronic and thermal Enthalpies= -4084.379778
Sum of electronic and thermal Free Energies= -4084.473900

C	-0.16521	3.49405	0.43729
H	-0.19152	4.08513	1.36558
H	0.38115	4.10451	-0.30502
C	-2.57028	4.37536	0.39925
H	-2.37814	5.33558	-0.11461
H	-3.61903	4.10161	0.22115
H	-2.45424	4.54204	1.47744
Ni	-2.2269	1.44432	-0.00262
C	-1.59908	3.31159	-0.07086
C	0.62484	2.20698	0.67909
H	0.63772	1.61171	-0.25333
H	1.6811	2.45601	0.8652
C	0.12457	1.29769	1.83341
H	0.56963	1.69262	2.76315
N	-1.75886	2.74929	-1.32272
C	-2.84691	3.17132	-2.21112
H	-2.56428	4.0967	-2.74195
H	-3.01829	2.38491	-2.95892
H	-3.79887	3.35138	-1.68908

C	2.17194	-0.20617	1.5712
C	2.83346	-0.32938	0.33882
C	2.94716	-0.10704	2.73911
C	4.23098	-0.3497	0.27364
H	2.24741	-0.40554	-0.58128
C	4.34392	-0.12703	2.67844
H	2.44771	-0.01461	3.70839
C	4.99195	-0.24735	1.44306
H	4.72612	-0.44603	-0.69654
H	4.92943	-0.05141	3.59873
H	6.08384	-0.26414	1.39379
C	0.66378	-0.13855	1.64357
H	0.23722	-0.55096	0.71506
H	0.30374	-0.7667	2.47427
C	-1.39209	1.32869	2.05755
C	-1.91439	2.3301	2.93871
C	-2.26557	0.25761	1.70493
C	-3.23556	2.33725	3.33884
H	-1.23684	3.10468	3.30571
C	-3.63336	0.29995	2.10365
H	-1.87601	-0.68118	1.30893
C	-4.12117	1.32838	2.88959
H	-3.59776	3.12348	4.0062
H	-4.28967	-0.51779	1.79577
H	-5.17177	1.34441	3.18939
N	-2.85046	0.01386	-1.12356
C	-3.03097	-0.80088	-1.9272
C	-3.17766	-1.80112	-2.96941
H	-4.02188	-1.54536	-3.62696
H	-2.24916	-1.82366	-3.56293
H	-3.35169	-2.79323	-2.52735
I	0.85228	-0.12046	-3.4527
Cu	-0.48161	1.56411	-2.17142

Appendix 6: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 6 (Impact of Ligands and Metals on the Formation of Metallacyclic Intermediates and a Nontraditional Mechanism for Group VI Alkyne Metathesis Catalysts)

A6.1 Methods

All optimizations of intermediates and transition states were calculated using restricted B3LYP-D3/def2SVP-LANL2DZ(M) level of the theory[245] in implicit solvent (benzene) using CPCM as solvation model[246] as implemented in Gaussian09. Frequency calculations, at the same level of theory, were used to obtain thermal corrections (at 298K) and to characterize optimized structures as transition states (only a single imaginary frequency) or intermediate (if no imaginary frequencies were found). Intrinsic reaction coordinate (IRCs) calculations were undertaken to ensure transition states connected illustrated ground states. Single point energy calculations using B3LYP-D3/def2TZVP-SDD(M) with solvent corrections calculated in implicit solvent (benzene) using CPCM were also performed on all structures.[247] For comparison, single point energy calculations with restricted PBEPBE/def2TZVP-SDD(M) were calculated with solvent corrections calculated in implicit solvent (benzene) using CPCM as a solvation model. All reported charges are from Mulliken population analysis.[248] All 3-D structures were generated using CYLview.[249] Noncovalent interaction (NCI) analysis, also known as reduce density gradient (RDG) method, was performed on Multiwfn to study the possible effect of noncovalent interaction in the metallatetrahedrane intermediates.[250] Extension distance of

0 Bohr, medium quality grid (totally about 512000 points) were set by default. Further visualization of the color-filled RDG isosurface was realized by VMD, where RDG isosurface and color range were set as 0.5, and -0.035 to 0.2, respectively.[251] The energy decomposition analysis calculations were performed using the second-generation absolutely localized molecular orbitals[252] (ALMO-EDA) method implemented in Q-Chem 5.0.[253] The HF/6-311G(d,p) method was used as employed by Liu.[254] This method decomposes the through-space interaction energies between the ligand and substrate into the energetic components including the Pauli repulsion energy (ΔE_{Pauli}), the electrostatic energy (ΔE_{elstat}), the polarization energy (ΔE_{pol}) and the charge transfer energy (ΔE_{ct}.) Distortion energies (ΔE_{dist}), or the energy required to distort the geometry of the starting intermediate to the transition state geometry as described by the distortion-interaction model,[255] were calculated using the B3LYP-D3/defTZVP-SDD(M)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(M)-CPCM(benzene)level of theory in Gaussian 09.

The computational method of B3LYP-D3/def2TZVP-SDD(M)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(M)-CPCM(benzene) was chosen as it provides an excellent balance between accuracy and computational cost, all while reproducing structural features from x-ray crystal structures. Pseudopotentials such as LANL2DZ and SDD are very commonly used on the metal center to reduce computational cost while maintaining the accuracy of the calculation.[256] Furthermore, pseudopotentials such as used LANL2DZ and SDD have been shown to be effective in describing Mo and W compounds.[257]

A6.2 Supplementary Figures

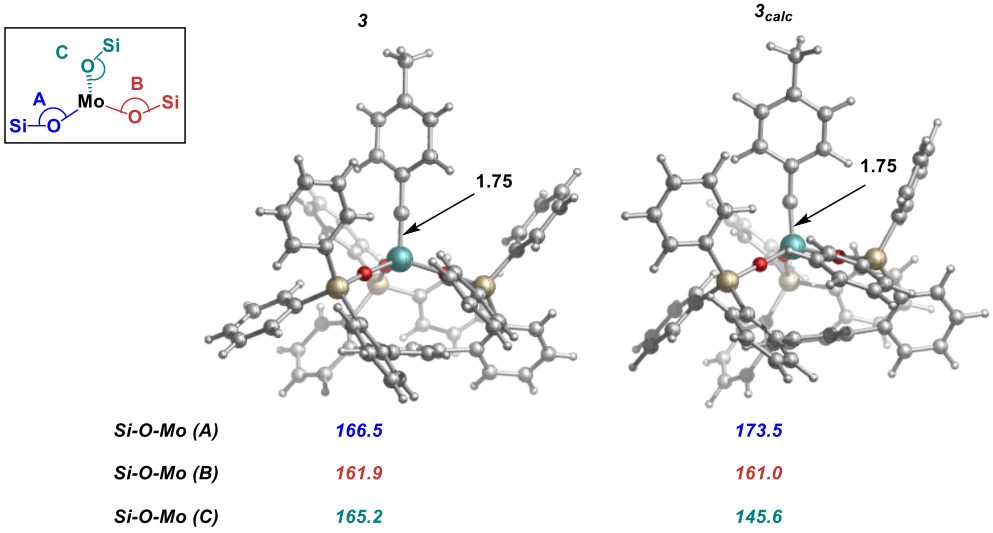


Figure A6.1 Experimental structure of **3** and computed structure $\mathbf{3}_{\mathbf{Calc}}$ optimized at the B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM (benzene) level of theory. Key bond lengths and angles are given for comparison.

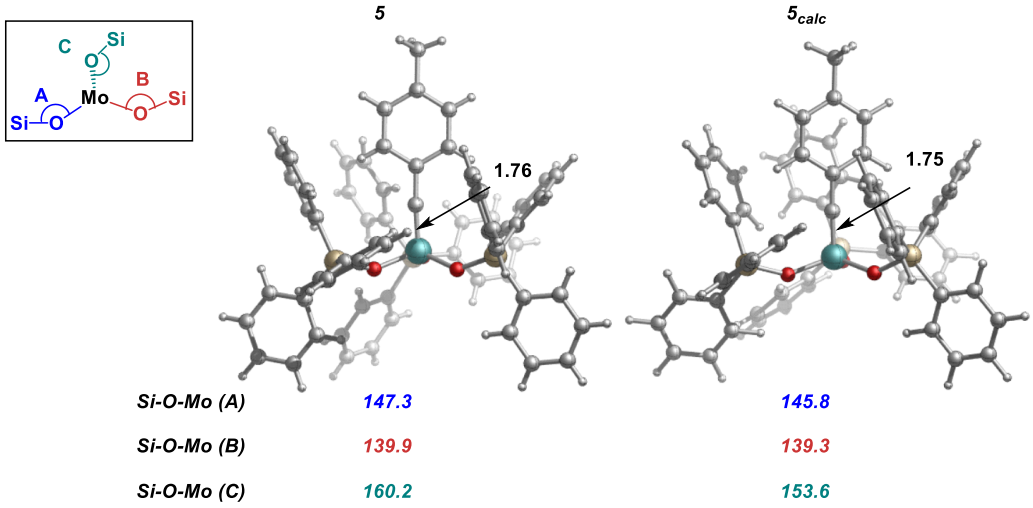
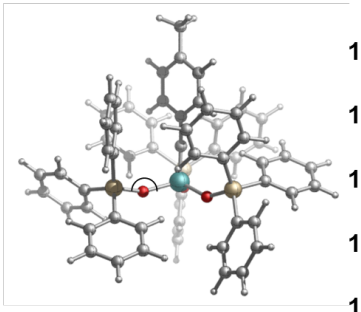
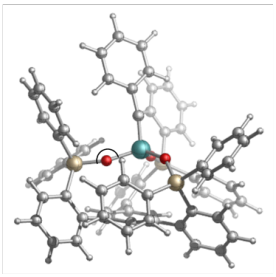


Figure A6.2 Experimental structure of **5** and computed structure $\mathbf{5}_{\mathbf{Calc}}$ optimized at the B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM (benzene) level of theory. Key bond lengths and angles are given for comparison.

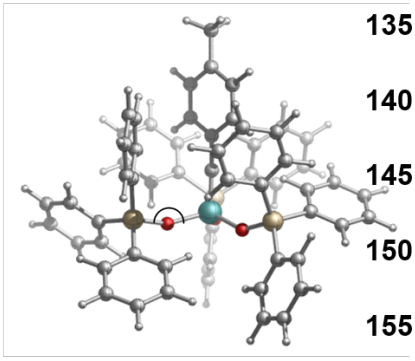


Si-O-Mo angle	C-13 Shift
135	314.61
140	315.63
145	313.94
150	314.05
155	314.81
160	313.61
165	313.85
170	314.55
175	314.80



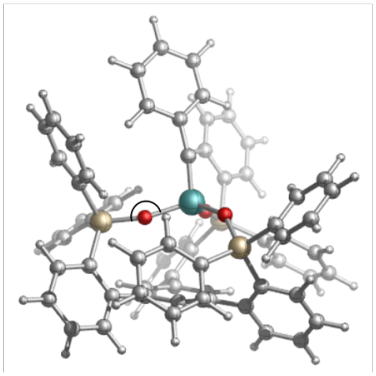
Si-O-Mo angle	C-13 Shift
135	334.59
140	333.21
145	331.59
150	330.40
155	329.98
160	330.04
165	330.04
170	331.01
175	331.72

Figure A6.3 Predicted ^{13}C chemical shifts of **5** (left) and **3** (right) as a function of a single-fixed Mo-O-Si bond angle computed at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene) level of theory relative to a TMS standard.



Si-O-Mo angle (^{o})	Mulliken Charge on C1	Mulliken Charge on Mo	Mulliken Charge on O (constrained angle)
135	-0.99	1.92	-0.98
140	-0.96	1.96	-0.96
145	-0.95	1.93	-0.95
150	-0.92	1.92	-0.92
155	-0.94	1.94	-0.94
160	-0.89	1.89	-0.89
165	-0.94	1.87	-0.94
170	-0.90	1.89	-0.90
175	-0.87	1.89	-0.87

Figure A6.4 Mulliken charges of **5** as a function of a single-fixed Mo-O-Si bond angle computed at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene) level of theory with the Si-O-Mo angle constrained. As the Mo-O-Si bond angle increases and the sp-character of the oxygen atom increases, the alkyne carbon loses electron density and the Mo atom gains electron density through donation from the oxygen atom.



Si-O-Mo angle (°)	Mulliken Charge on C1	Mulliken Charge on Mo	Mulliken Charge on O (constrained angle)
135	-0.68	1.87	-0.68
140	-0.67	1.87	-0.67
145	-0.66	1.87	-0.66
150	-0.65	1.87	-0.65
155	-0.64	1.87	-0.64
160	-0.61	1.86	-0.61
165	-0.58	1.83	-0.58
170	-0.53	1.78	-0.53
175	-0.52	1.77	-0.52

Figure A6.5 Mulliken charges of **3** as a function of a single-fixed Mo-O-Si bond angle computed at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene) level of theory with the Si-O-Mo angle constrained. As the Mo-O-Si bond angle increases and the sp-character of the oxygen atom increases, the alkyne carbon loses electron density and the Mo atom gains electron density through donation from the oxygen atom.

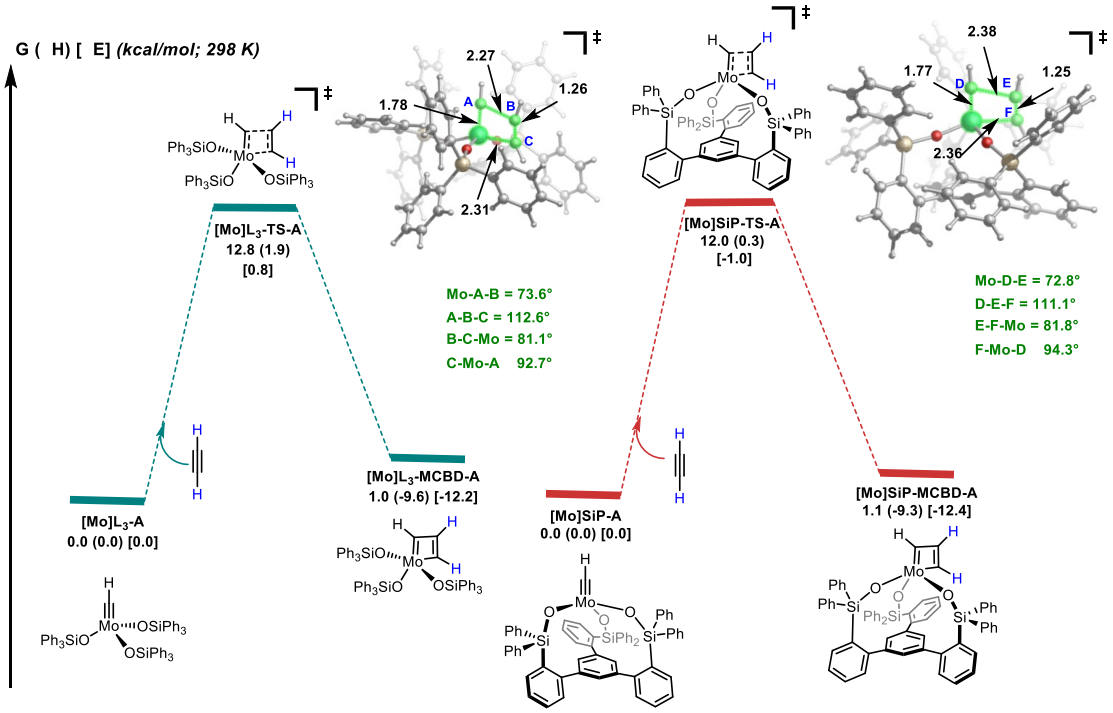
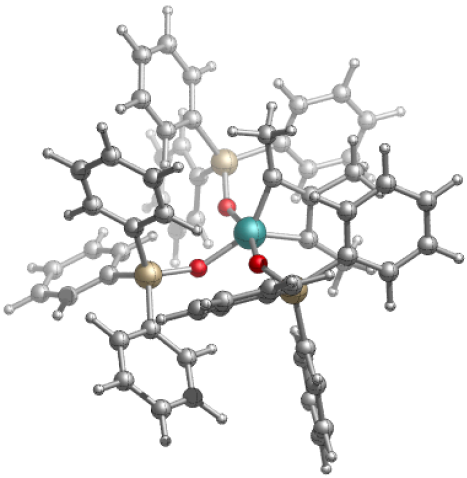
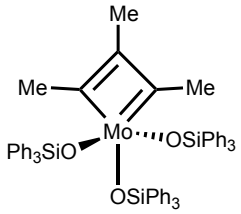


Figure A6.6 Energetics of MCBD formation with the acetylene substrate via [2+2] cycloaddition for [Mo]L_3 (left, green) and [Mo]SiP (right, red) computed at the B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ level of theory. Free energies are given as well as enthalpies (parenthesis) and the Hartree-Fock (HF) energy (brackets). The barriers to MCBD formation for [Mo]L_3 and [Mo]SiP are very similar, with the barrier 0.8 kcal/mol lower in free energy for the [Mo]SiP complex.





MCBD1-comp

	MCBD1-comp
Mo1-C1	1.920
Mo-O$_{Avg}$	1.991
O-Si$_{Avg}$	1.653
C1-C2	1.426
C2-C3	1.466
C3-Mo1	1.889
Mo1-C1-C2	79.18
C1-C2-C3	119.51
C2-C3-Mo1	79.32
C3-Mo1-C1	81.98
Mo-O-Si$_{Avg}$	143.71

Figure A6.7 List of Bond lengths and angles for **MCBD1-comp**, optimized using B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene).

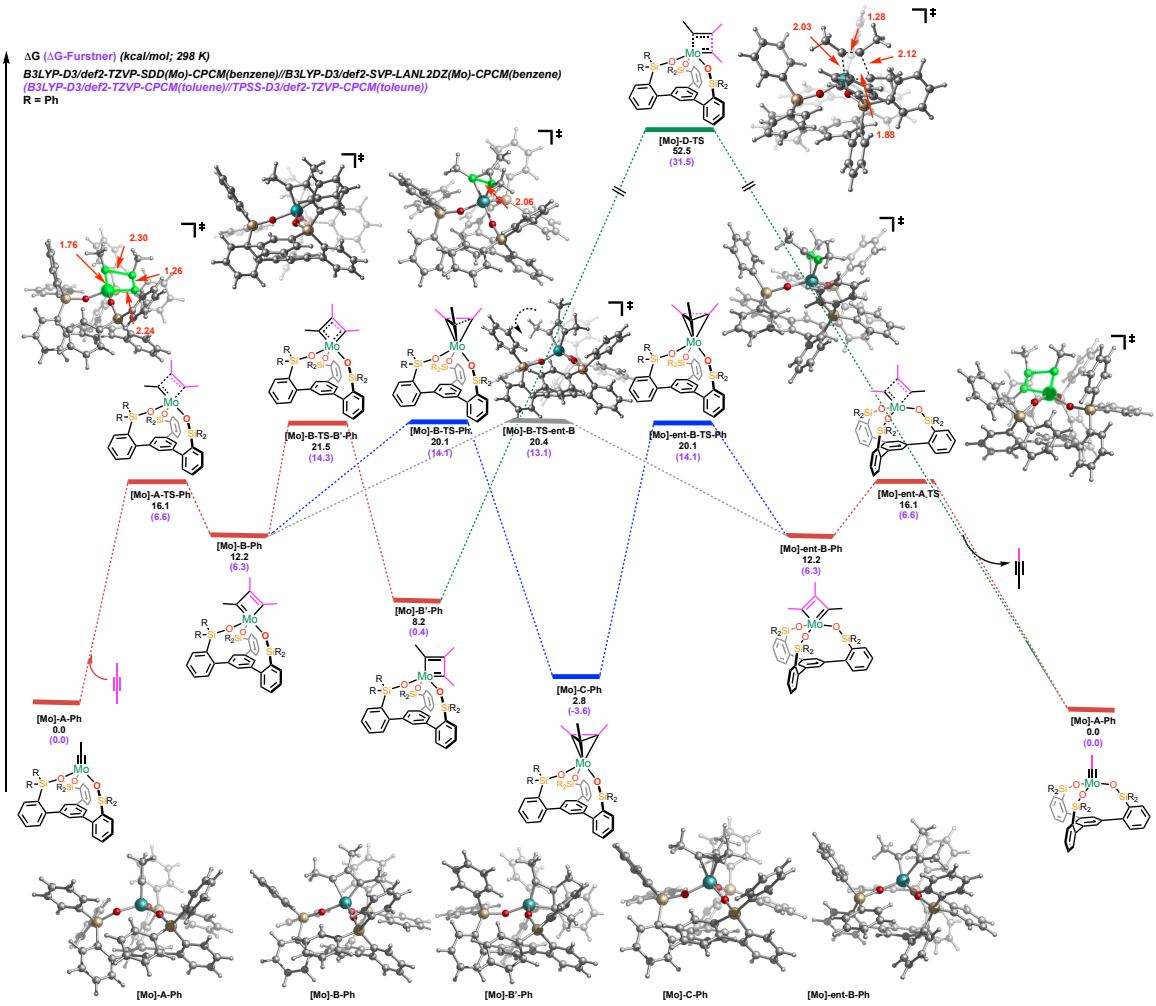
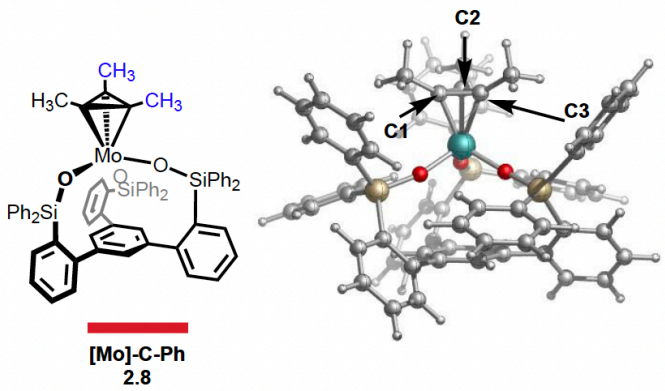


Figure A6.8 Energetics (free energies; kcal/mol) of MCBD and MT_d formation via [2+2] cycloaddition for molybdenum with **SiP^{Ph}** ligands computed in our work at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)// B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)level of theory compared to that computed by Furstner/Neese at the B3LYP-D3/def2TZVP-CPCM(toluene)// TPSS-D3/def2TZVP-CPCM(toluene) level of theory.



	[Mo]-C-Ph	MTd1
Mo-C1	2.093	2.064
Mo-C2	2.094	2.065
Mo-C3	2.094	2.064
C1-C2	1.453	1.445
C2-C3	1.454	1.458
C3-C1	1.451	1.458
Mo-C1-C2	69.65	69.2
C1-C2-C3	59.89	60.3
C2-C3-Mo	69.64	69.0
C3-Mo-C1	40.54	41.4

Figure A6.9 List of Bond Lengths (Å) and Angles (°) for computed metallatetrahedrane **[Mo]-C-Ph** compared to the analogous isolated structure **MTd1.**

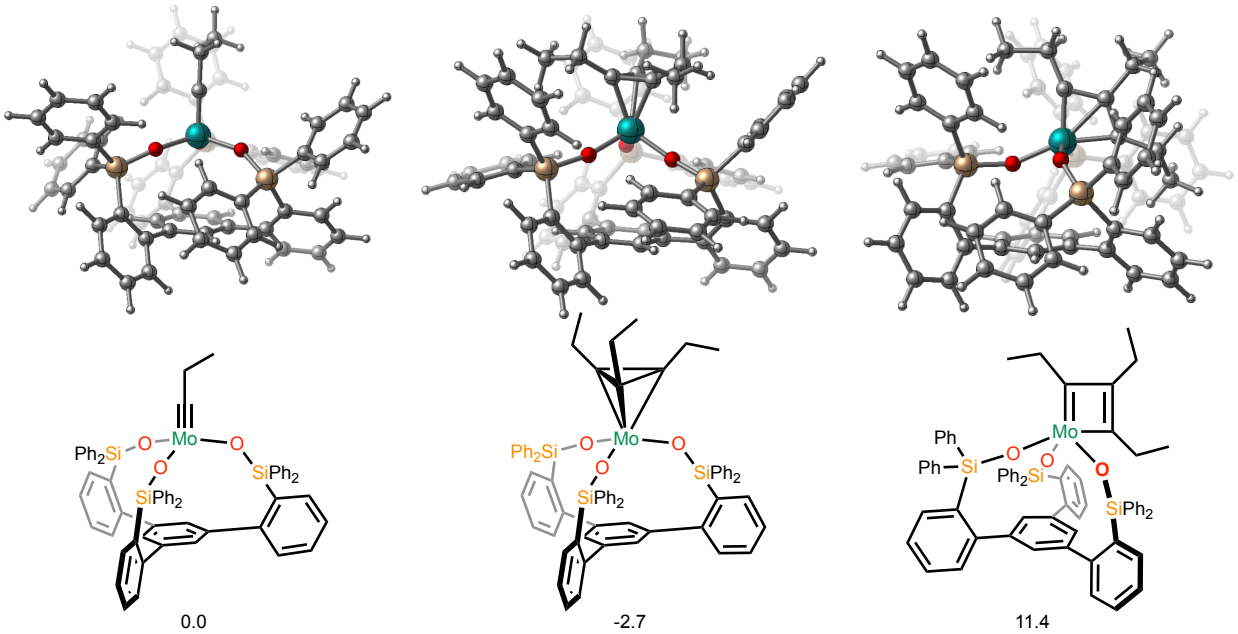


Figure A6.10 Energetics of MCBD and MT_d formation for molybdenum with **SiP^{Ph}** ligand and 3-hexyne substrate. Free energies (kcal/mol) are computed at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)// B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)level of theory.

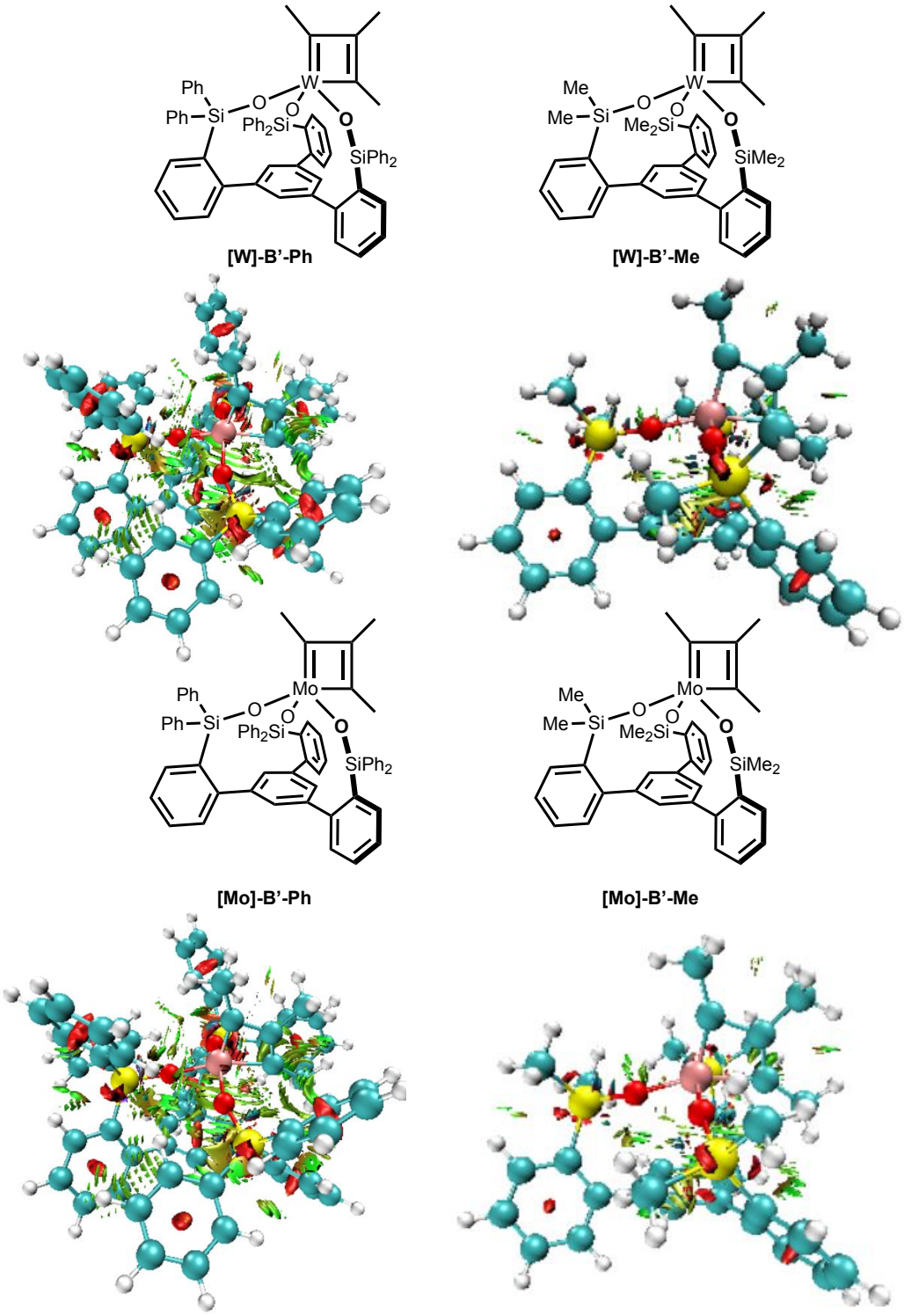


Figure A6.11 NCI plots showing the comparison between metallacyclobutadienes in the tungsten (top) and molybdenum (bottom) systems with both the SiP^{Ph} and SiP^{Me} ligands.

Key C-H···π noncovalent stabilizing interactions visible in the NCI plots of the SiP^{Ph} metallatetrahedranes are no longer present in the MCBD structures.

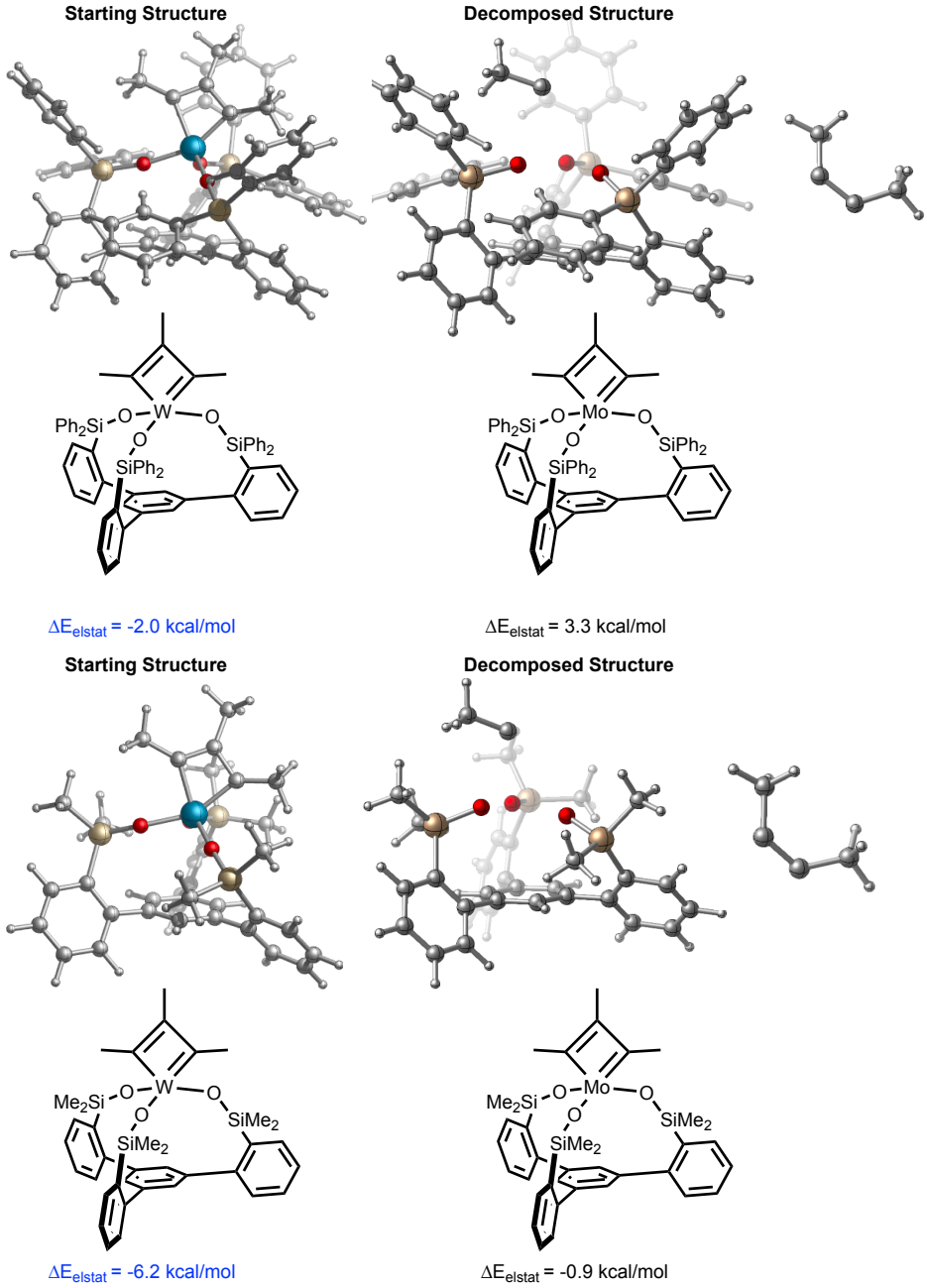


Figure A6.12 Electrostatic energies for the MCBD intermediates, [W]-B and [Mo]-B, computed by the second-generation ALMO-EDA method using HF/6-311G(d,p) with the shown decomposed intermediates from the given starting structure. The electrostatic energies are lower for [W]-B than [Mo]-B and thus the electrostatic energy likely contributes to tungsten's preference to form the MCBD.

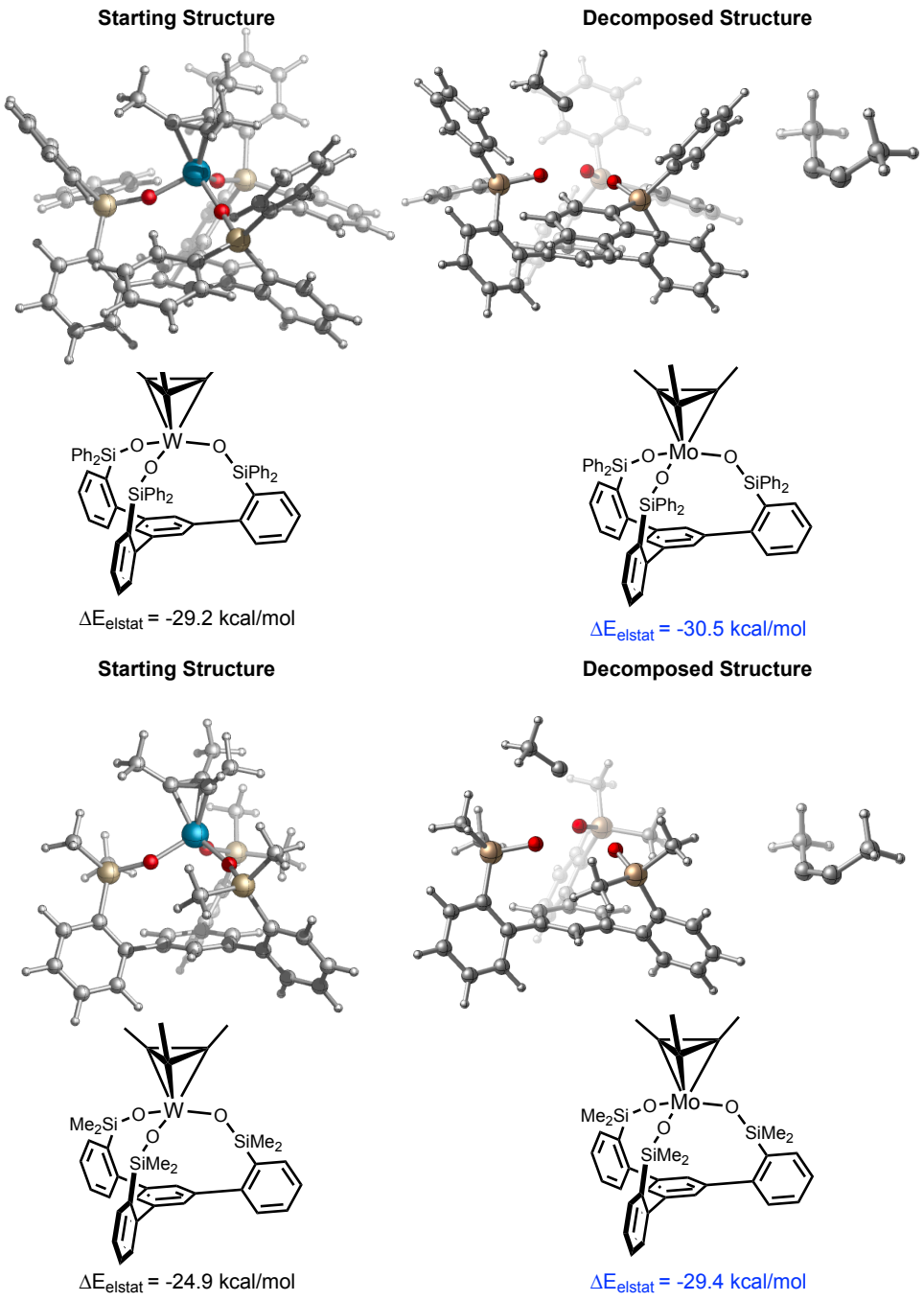


Figure A6.13 Electrostatic energies for the MTd intermediates, [W]-C and [Mo]-C, computed by the second-generation ALMO-EDA method using HF/6-311G(d,p) with the shown decomposed intermediates from the given starting structure. The electrostatic energies are lower for [Mo]-C than [W]-C and thus the electrostatic energy likely contributes to molybdenum's preference to form the MTd.

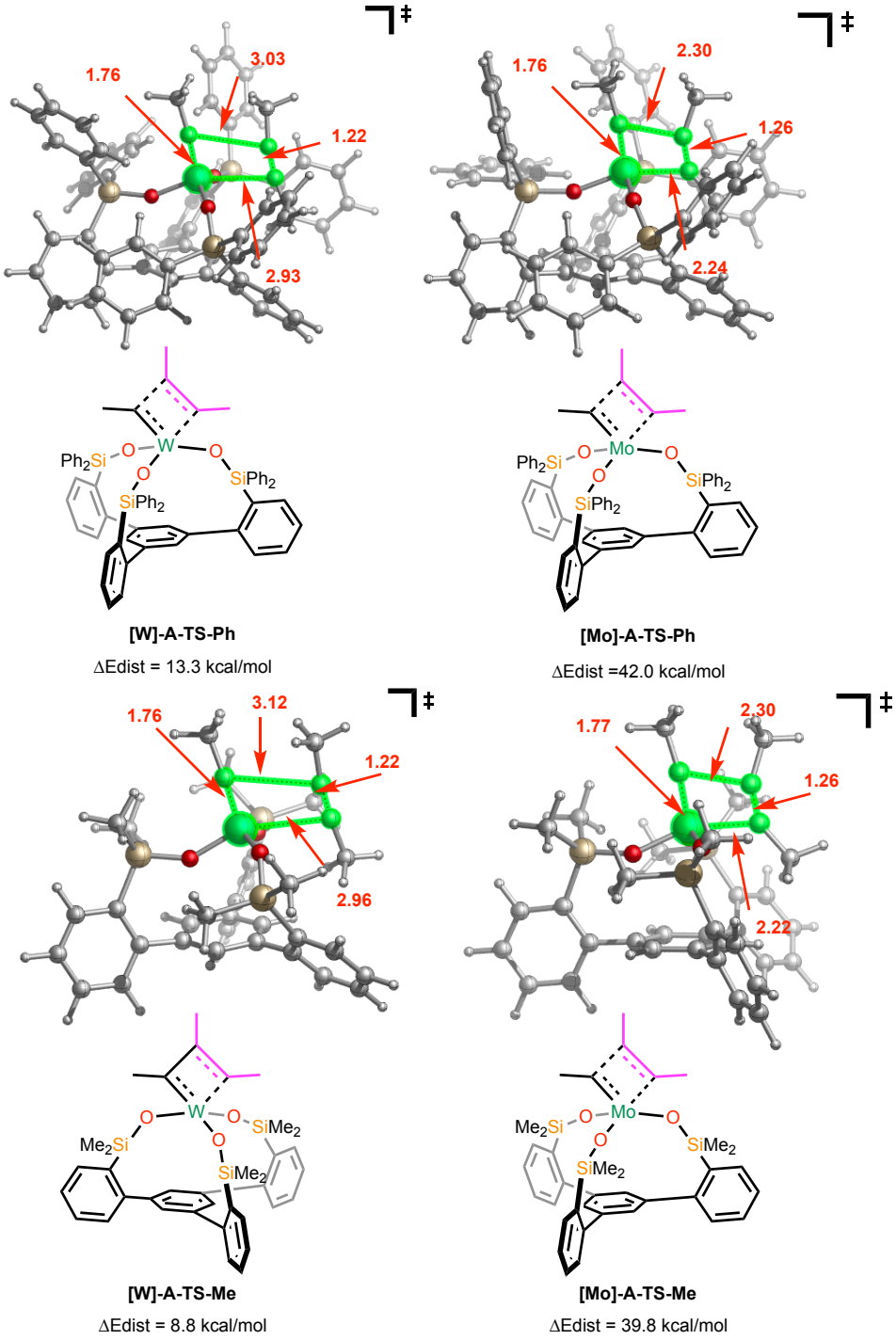


Figure A6.14 Distortion energies for the formation of the MCBD intermediates, [W]-B and [Mo]-B, computed at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)// B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene) level of theory. The low

distortion energy required to form [W]-B compared to that required to form [Mo]-B provides insight into the preference for the MCBD in the case of tungsten.

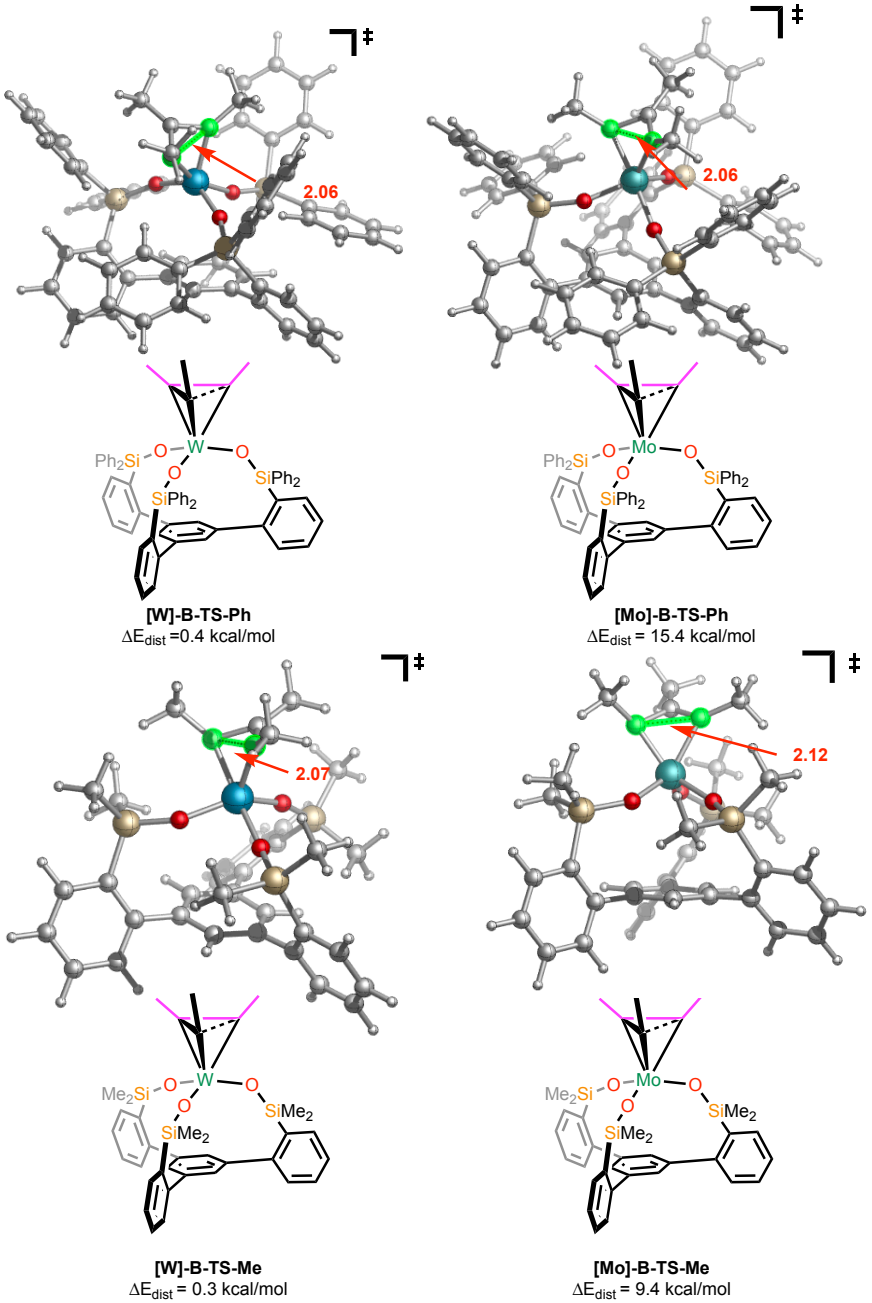


Figure A6.15 Distortion energies for the formation of the MTd intermediates, [W]-C and [Mo]-C, computed at the B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)// B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene) level of theory. In this case, the distortion energy to form [W]-C is lower than that to form [Mo]-C, and therefore the distortion energy does not control the preferred formation of the MTd intermediate in the molybdenum case.

A6.3 Coordinates and Energies

3_{calc}

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 0.998704 (Hartree/Particle)
Thermal correction to Energy= 1.064236
Thermal correction to Enthalpy= 1.065180
Thermal correction to Gibbs Free Energy= 0.890796
Sum of electronic and zero-point Energies= -3781.479020
Sum of electronic and thermal Energies= -3781.413488
Sum of electronic and thermal Enthalpies= -3781.412544
Sum of electronic and thermal Free Energies= -3781.586928

C	-2.06486	1.66529	1.88213
C	-0.83553	1.80848	2.53908
C	0.23379	2.49728	1.94402
C	0.03027	3.09336	0.69266
C	-1.19219	2.97264	0.00906
C	-2.23832	2.26708	0.62449
C	-3.16418	0.84801	2.48038
C	-2.98868	-0.52214	2.82367
C	-4.07763	-1.21501	3.38518
C	-5.31192	-0.59534	3.60434
C	-5.4825	0.74155	3.23944
C	-4.41671	1.45078	2.68021
C	-1.77448	-3.32856	2.17678
C	-1.05614	-4.31071	2.88221
C	-1.2305	-5.67125	2.6026
C	-2.12769	-6.07195	1.60771
C	-2.85478	-5.10901	0.89645
C	-2.67782	-3.75286	1.18121
C	0.00034	-1.22246	3.58636
C	-0.22425	-1.02849	4.9625
C	0.83731	-0.76265	5.83387
C	2.14422	-0.67943	5.34032
C	2.38694	-0.87703	3.97749
C	1.3239	-1.15083	3.11306
C	-1.32684	3.62549	-1.33075
C	-1.68086	2.94218	-2.53067
C	-1.72017	3.69907	-3.72193
C	-1.42684	5.06484	-3.75751
C	-1.07201	5.71865	-2.57846
C	-1.02337	4.99861	-1.3846
C	-3.69664	0.65219	-1.87854
C	-3.86358	-0.55934	-1.18285
C	-5.04583	-0.83439	-0.48874
C	-6.09266	0.09238	-0.49116
C	-5.95557	1.29268	-1.19691
C	-4.76654	1.5689	-1.87909
C	-2.19496	0.69266	-4.57244
C	-3.41208	0.76831	-5.27452
C	-3.47208	0.49397	-6.64515
C	-2.31121	0.1327	-7.33735
C	-1.09317	0.0433	-6.6537
C	-1.03838	0.31981	-5.28414
C	1.55543	2.55629	2.63676
C	2.77611	2.17685	2.00947
C	3.95998	2.24388	2.76991
C	3.96624	2.66737	4.10173
C	2.76256	3.02121	4.71273
C	1.57398	2.96059	3.98351
C	2.91966	2.86196	-1.03891
C	2.20198	2.71004	-2.24122
C	2.12923	3.74824	-3.17361
C	2.78642	4.95808	-2.9256
C	3.51178	5.12555	-1.74107
C	3.57103	4.08756	-0.80443
C	4.46172	0.41031	0.08677
C	4.33031	-0.98845	0.19117
C	5.44025	-1.82927	0.0594
C	6.70674	-1.28325	-0.1754
C	6.85618	0.10389	-0.28885
C	5.74156	0.94	-0.16508
C	0.79715	-2.05259	-1.03684
C	1.39028	-3.3552	-1.12973
C	0.76858	-4.46584	-0.50942
C	1.36839	-5.72105	-0.54911
C	2.59821	-5.92676	-1.20118
C	3.2121	-4.82098	-1.8143
C	2.62521	-3.5565	-1.78585
C	3.21972	-7.29941	-1.25807
H	-0.68997	1.34165	3.51267
H	0.84139	3.64733	0.22244
H	-3.19574	2.1653	0.11818
H	-3.96747	-2.27408	3.63649
H	-6.13905	-1.15952	4.04288
H	-6.44584	1.23609	3.38901
H	-4.55048	2.49808	2.39779
H	-0.33796	-4.01042	3.65056
H	-0.65828	-6.41958	3.15724
H	-2.25907	-7.13363	1.38272
H	-3.55364	-5.41669	0.11429
H	-3.23935	-3.01126	0.60721
H	-1.24396	-1.06301	5.35926
H	0.64331	-0.60649	6.89848
H	2.9721	-0.44949	6.01575
H	3.40126	-0.79613	3.57992
H	1.53256	-1.27967	2.04901
H	-1.97651	3.20408	-4.66094
H	-1.46887	5.60828	-4.70493
H	-0.83139	6.78486	-2.58275
H	-0.74761	5.51107	-0.45984
H	-3.05153	-1.2903	-1.16165
H	-5.1496	-1.76741	0.07051
H	-7.0104	-0.11727	0.06387
H	-6.7704	2.02157	-1.2022
H	-4.66065	2.52889	-2.39433
H	-4.33	1.04081	-4.74505
H	-4.42733	0.55726	-7.17337
H	-2.35637	-0.08425	-8.40802
H	-0.18488	-0.24609	-7.1893
H	-0.08421	0.2378	-4.75571
H	4.90608	1.93271	2.31922
H	4.90494	2.70523	4.66037
H	2.74466	3.34361	5.75703
H	0.63325	3.24286	4.46249

H	1.6648	1.78013	-2.4445
H	1.54005	3.61962	-4.08473
H	2.72254	5.77451	-3.64973
H	4.02082	6.07204	-1.5397
H	4.11445	4.24692	0.13248
H	3.34395	-1.42927	0.35492
H	5.31036	-2.91252	0.12953
H	7.57624	-1.93794	-0.27895
H	7.84235	0.53398	-0.48367
H	5.87313	2.02071	-0.2789
H	0.87165	-6.56124	-0.05504
H	4.17256	-4.95197	-2.3211
H	4.29462	-7.2507	-1.48839
H	2.74203	-7.91475	-2.04084
H	3.09436	-7.83789	-0.30532
Mo	0.11118	-0.50221	-0.60379
O	-0.95875	-0.91087	0.89753
O	-0.8572	0.09227	-2.16072
O	1.62178	0.50931	-0.06244
Si	-1.42529	-1.49225	2.38919
Si	-2.07294	1.08563	-2.7316
Si	2.92448	1.48667	0.2481
H	-0.17876	-4.32654	0.01389
H	3.12599	-2.70713	-2.255

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.564347

5$_{calc}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 0.959946 (Hartree/Particle)
Thermal correction to Energy= 1.023915
Thermal correction to Enthalpy= 1.024860
Thermal correction to Gibbs Free Energy= 0.849371
Sum of electronic and zero-point Energies= -3553.019670
Sum of electronic and thermal Energies= -3552.955701
Sum of electronic and thermal Enthalpies= -3552.954757
Sum of electronic and thermal Free Energies= -3553.130245

C	-0.73158	4.63029	-1.80316
C	0.2806	5.18235	-0.99541
C	0.33731	6.55937	-0.75343
C	-0.61747	7.41005	-1.32112
C	-1.63116	6.87866	-2.12678
C	-1.6886	5.50096	-2.35956
C	-0.3141	2.25478	-3.81311
C	-0.00578	0.90023	-4.0564
C	0.38843	0.46817	-5.32527
C	0.47206	1.38566	-6.37972
C	0.16523	2.73214	-6.15898
C	-0.22027	3.16211	-4.8837
C	-2.55718	2.14278	-1.71167
C	-3.47377	1.88508	-2.74906
C	-4.75811	1.40165	-2.47324
C	-5.14103	1.15619	-1.15076
C	-4.24333	1.40622	-0.10661
C	-2.96733	1.90109	-0.38598
C	-0.45987	-0.67024	-0.38581
C	-1.43627	-1.69736	-0.62722
C	-2.55679	-1.46601	-1.45283
C	-3.49491	-2.47379	-1.66958
C	-3.35585	-3.74433	-1.08621
C	-2.23374	-3.97276	-0.26901
C	-1.29093	-2.97541	-0.03928
C	-4.35844	-4.83966	-1.34702
C	2.48219	-2.41318	-2.55976
C	3.34943	-2.27583	-3.66129
C	2.93547	-2.6176	-4.95314
C	1.64068	-3.10192	-5.16853
C	0.76214	-3.24101	-4.08802
C	1.18241	-2.90361	-2.79827
C	4.8826	-1.76097	-0.71736
C	5.50271	-0.55878	-0.32963
C	6.89532	-0.46928	-0.22506
C	7.69182	-1.58339	-0.50861
C	7.09203	-2.78753	-0.8965
C	5.70062	-2.87289	-0.99841
C	2.30854	-3.05674	0.47228
C	2.03123	-4.41038	0.2054
C	1.46646	-5.23698	1.18383
C	1.16667	-4.722	2.45003
C	1.44783	-3.38149	2.74097
C	2.01675	-2.56386	1.76037
C	-0.34682	2.75256	3.65171
C	-0.37528	3.67267	2.58386
C	-0.52924	5.04271	2.81659
C	-0.65484	5.5179	4.12703
C	-0.62366	4.6202	5.20015
C	-0.46971	3.24985	4.96225
C	-1.93705	0.16534	3.14693
C	-3.09552	0.88205	3.50198
C	-4.36145	0.29189	3.41291
C	-4.4907	-1.01916	2.94143
C	-3.35095	-1.7429	2.574
C	-2.08765	-1.15859	2.69149
C	0.79508	-0.0603	4.53646
C	0.1877	-0.84903	5.53144
C	0.95775	-1.61613	6.41315
C	2.35241	-1.61218	6.30794
C	2.97437	-0.83405	5.32426
C	2.20163	-0.06448	4.45058
H	1.02477	4.52182	-0.54279
H	1.12772	6.96884	-0.11855
H	-0.57465	8.48617	-1.13307
H	-2.38282	7.53894	-2.56763
H	-2.50096	5.10058	-2.97461
H	-0.06432	0.16704	-3.24535
H	0.63782	-0.58308	-5.48429
H	0.78127	1.04992	-7.3733
H	0.23343	3.45142	-6.97965
H	-0.44432	4.2206	-4.72089
H	-3.17608	2.0454	-3.78956
H	-5.4547	1.2037	-3.29234
H	-6.13708	0.76216	-0.93216
H	-4.52803	1.19941	0.92623
H	-2.27917	2.08014	0.44445
H	-2.6914	-0.48861	-1.91239
H	-4.36045	-2.26328	-2.30419
H	-2.09712	-4.95108	0.2009
H	-0.4323	-3.17587	0.5996
H	4.3654	-1.90047	-3.50953
H	3.62486	-2.50509	-5.7941
H	1.31573	-3.36834	-6.17788
H	-0.25329	-3.61309	-4.24753
H	0.48483	-3.02709	-1.96883

H	4.88342	0.31493	-0.10993
H	7.36026	0.47321	0.07682
H	8.78005	-1.51483	-0.42832
H	7.7111	-3.66073	-1.11953
H	5.24873	-3.82206	-1.30416
H	2.23489	-4.82381	-0.7865
H	1.24795	-6.28304	0.95296
H	0.71371	-5.36426	3.20989
H	1.2215	-2.96513	3.72579
H	2.21698	-1.51942	2.00902
H	-0.27242	3.32056	1.55382
H	-0.54728	5.73579	1.97126
H	-0.77402	6.58876	4.31259
H	-0.7158	4.98933	6.22522
H	-0.44064	2.5605	5.81222
H	-3.00985	1.91416	3.85335
H	-5.24978	0.86123	3.69932
H	-5.48052	-1.47549	2.85594
H	-3.44242	-2.76001	2.1856
H	-1.20632	-1.74066	2.41331
H	-0.90287	-0.8795	5.60971
H	0.46776	-2.22561	7.17716
H	2.95542	-2.21858	6.98893
H	4.06381	-0.8339	5.23405
H	2.69837	0.52786	3.67683
H	-4.49223	-5.48278	-0.46324
H	-4.02243	-5.49126	-2.17306
H	-5.34053	-4.43205	-1.63071
Mo	0.77275	0.52189	-0.03211
O	0.26541	2.10041	-0.99681
O	2.4307	-0.34512	-0.47244
O	0.62904	0.81131	1.84347
Si	-0.82382	2.77283	-2.0797
Si	3.01008	-1.8863	-0.83096
Si	-0.21827	0.91245	3.28613

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.834686

$3_{135°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.09176	1.71832	1.96392
C	-0.85901	1.89374	2.6042
C	0.19657	2.58362	1.98804
C	-0.02599	3.15226	0.72888
C	-1.25468	3.00229	0.0602
C	-2.2863	2.29173	0.69473
C	-3.1594	0.89756	2.61632
C	-2.95752	-0.47141	2.95659
C	-4.00007	-1.15869	3.60428
C	-5.21561	-0.53696	3.90817
C	-5.41616	0.79546	3.54171
C	-4.39423	1.50203	2.90095
C	-1.86385	-3.28286	2.07652
C	-1.25864	-4.28005	2.86294
C	-1.49418	-5.63697	2.61287
C	-2.34013	-6.01896	1.56671
C	-2.95423	-5.04078	0.77457
C	-2.71596	-3.68805	1.02959
C	0.093	-1.29248	3.31777
C	0.05411	-0.74616	4.61465
C	1.21856	-0.6063	5.37648
C	2.44949	-1.01675	4.8545
C	2.50624	-1.59151	3.58042
C	1.337	-1.73772	2.82913
C	-1.40055	3.65267	-1.2815
C	-1.68096	2.9646	-2.49729
C	-1.7238	3.73146	-3.68244
C	-1.50151	5.11058	-3.6976
C	-1.21873	5.77024	-2.50261
C	-1.16901	5.04076	-1.31452
C	-3.64051	0.6193	-1.93863
C	-3.84896	-0.6638	-1.40087
C	-5.05375	-0.99384	-0.77219
C	-6.07922	-0.04724	-0.67898
C	-5.90041	1.22635	-1.22978
C	-4.6913	1.55359	-1.85162
C	-2.06101	0.72765	-4.58214
C	-3.26121	0.79336	-5.31379
C	-3.28146	0.53974	-6.68947
C	-2.09699	0.20996	-7.3571
C	-0.89517	0.13162	-6.64401
C	-0.88007	0.38698	-5.26923
C	1.52019	2.67249	2.67396
C	2.73423	2.24922	2.06401
C	3.92222	2.34518	2.81498
C	3.93723	2.84477	4.12043
C	2.73957	3.24644	4.7144
C	1.54633	3.15292	3.99544
C	2.82423	2.7984	-1.00703
C	2.08153	2.60585	-2.18778
C	1.99483	3.60831	-3.15762
C	2.66221	4.82313	-2.96916
C	3.41291	5.03072	-1.80679
C	3.48669	4.02841	-0.83321
C	4.38743	0.40026	0.18204
C	4.26001	-0.99727	0.29889
C	5.37108	-1.83705	0.17047
C	6.63585	-1.29046	-0.07214
C	6.78155	0.09598	-0.19853
C	5.66525	0.93054	-0.07931
C	0.69498	-2.07031	-0.87344
C	1.32878	-3.35275	-0.98157
C	0.75009	-4.49853	-0.38505
C	1.40047	-5.72785	-0.44493
C	2.63877	-5.87271	-1.0966
C	3.20934	-4.73257	-1.68899
C	2.57283	-3.49367	-1.63793
C	3.31465	-7.21805	-1.17718
H	-0.6992	1.45725	3.58815
H	0.77119	3.71146	0.24122
H	-3.24353	2.15811	0.19397
H	-3.87149	-2.21656	3.85272
H	-6.00766	-1.09729	4.41167
H	-6.36727	1.28972	3.75651
H	-4.54688	2.54841	2.6241
H	-0.57809	-3.99653	3.67068
H	-1.00885	-6.39774	3.22995
H	-2.51795	-7.07849	1.36444
H	-3.61034	-5.33459	-0.04893
H	-3.17935	-2.932	0.39249
H	-0.8992	-0.40892	5.0329
H	1.16698	-0.16444	6.37487
H	3.36369	-0.88852	5.4395
H	3.46282	-1.91706	3.16447
H	1.40284	-2.19714	1.8384
H	-1.92588	3.23451	-4.63331
H	-1.54274	5.66023	-4.64145
H	-1.03545	6.84774	-2.48984
H	-0.94774	5.55633	-0.37687

H	-3.05251	-1.40982	-1.45438
H	-5.19333	-1.9893	-0.34292
H	-7.01571	-0.30176	-0.17604
H	-6.69957	1.96945	-1.16384
H	-4.555	2.56346	-2.25066
H	-4.19656	1.0433	-4.80376
H	-4.2239	0.59486	-7.2411
H	-2.11103	0.00938	-8.4318
H	0.03158	-0.13245	-7.16069
H	0.06154	0.31395	-4.71759
H	4.86307	1.9996	2.37852
H	4.87842	2.90601	4.67277
H	2.73034	3.63107	5.73759
H	0.60914	3.46949	4.46003
H	1.53253	1.67444	-2.34579
H	1.38541	3.44775	-4.05008
H	2.58669	5.61225	-3.72187
H	3.93033	5.98136	-1.65152
H	4.04978	4.22055	0.08582
H	3.27521	-1.43523	0.47245
H	5.24328	-2.91997	0.24938
H	7.50658	-1.94402	-0.1724
H	7.76604	0.52673	-0.40018
H	5.79453	2.01025	-0.20452
H	0.93657	-6.59683	0.03085
H	4.17521	-4.81589	-2.19551
H	4.39128	-7.12143	-1.38313
H	2.87757	-7.82827	-1.98723
H	3.19053	-7.78765	-0.24273
Mo	0.03244	-0.48825	-0.51893
O	-1.36966	-0.80094	0.74314
O	-0.77298	0.11144	-2.15911
O	1.53603	0.49112	0.10346
Si	-1.48006	-1.45307	2.29013
Si	-2.00077	1.09907	-2.73435
Si	2.85016	1.47719	0.33618
H	-0.20505	-4.40832	0.13304
H	3.04047	-2.61616	-2.08888

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.559506

$3_{140°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.09094	1.70337	1.95216
C	-0.85849	1.87668	2.59378
C	0.19687	2.56806	1.97931
C	-0.02496	3.13781	0.72025
C	-1.25283	2.98874	0.05009
C	-2.28526	2.27887	0.68401
C	-3.15829	0.87758	2.59708
C	-2.94987	-0.48893	2.9431
C	-3.99654	-1.18379	3.57658
C	-5.22147	-0.57181	3.86132
C	-5.42748	0.75838	3.48965
C	-4.40232	1.47207	2.86249
C	-1.8384	-3.28977	2.07708
C	-1.18044	-4.29914	2.80293
C	-1.41615	-5.65214	2.53212
C	-2.31546	-6.0181	1.52582
C	-2.98351	-5.02762	0.79469
C	-2.74502	-3.67913	1.07053
C	0.10839	-1.29573	3.35
C	0.06212	-0.77148	4.65538
C	1.22753	-0.61144	5.41191
C	2.46596	-0.97719	4.8745
C	2.53098	-1.52628	3.58948
C	1.36157	-1.69272	2.84262
C	-1.39677	3.63615	-1.29308
C	-1.68505	2.94529	-2.50566
C	-1.72336	3.70778	-3.69382
C	-1.49099	5.08526	-3.71468
C	-1.20229	5.74763	-2.52265
C	-1.15552	5.02239	-1.33187
C	-3.66325	0.62132	-1.92556
C	-3.86861	-0.63835	-1.33361
C	-5.07805	-0.94842	-0.70336
C	-6.11066	-0.00599	-0.66207
C	-5.93303	1.24482	-1.26317
C	-4.71944	1.55296	-1.88599
C	-2.09874	0.7052	-4.57977
C	-3.30058	0.78285	-5.30755
C	-3.32846	0.52625	-6.68256
C	-2.15018	0.18142	-7.35354
C	-0.94703	0.09055	-6.64428
C	-0.92431	0.34889	-5.27018
C	1.51923	2.66114	2.66677
C	2.73729	2.25118	2.05576
C	3.92358	2.35448	2.80863
C	3.93325	2.84821	4.11633
C	2.73167	3.2364	4.71122
C	1.5401	3.13555	3.99063
C	2.84612	2.83066	-1.00661
C	2.0916	2.66263	-2.18361
C	2.01162	3.67777	-3.14074
C	2.69743	4.88085	-2.94304
C	3.45871	5.06469	-1.78361
C	3.52566	4.04986	-0.82267
C	4.41579	0.42991	0.17637
C	4.29887	-0.96751	0.3059
C	5.41704	-1.79973	0.19101
C	6.67869	-1.24551	-0.05087
C	6.81396	0.14071	-0.19006
C	5.69056	0.96763	-0.08404
C	0.72451	-2.07074	-0.89597
C	1.33728	-3.36438	-0.99172
C	0.6964	-4.50733	-0.45625
C	1.32166	-5.75009	-0.49929
C	2.59556	-5.91177	-1.07428
C	3.22718	-4.7748	-1.60735
C	2.61643	-3.5222	-1.57196
C	3.24533	-7.27095	-1.13607
H	-0.69879	1.43573	3.57613
H	0.77282	3.69741	0.23408
H	-3.24275	2.1472	0.183
H	-3.86342	-2.24027	3.82837
H	-6.01626	-1.13799	4.3538
H	-6.3858	1.24505	3.68917
H	-4.56005	2.51623	2.58035
H	-0.45945	-4.02817	3.57917
H	-0.88924	-6.42209	3.10186
H	-2.4939	-7.07425	1.30716
H	-3.68332	-5.30824	0.0032
H	-3.25679	-2.91443	0.48229
H	-0.89741	-0.46571	5.08385
H	1.17073	-0.18796	6.41798
H	3.38025	-0.83227	5.45543
H	3.49413	-1.81521	3.16177

H	1.4341	-2.13127	1.84298
H	-1.93045	3.20859	-4.64244
H	-1.52925	5.63143	-4.66068
H	-1.0113	6.82383	-2.51434
H	-0.92871	5.54007	-0.39673
H	-3.06672	-1.38024	-1.34445
H	-5.21653	-1.9249	-0.23224
H	-7.05106	-0.24536	-0.15902
H	-6.73674	1.98544	-1.236
H	-4.58483	2.54655	-2.32474
H	-4.23139	1.04439	-4.79513
H	-4.27208	0.59099	-7.23109
H	-2.17015	-0.02121	-8.42776
H	-0.02513	-0.18559	-7.16336
H	0.01831	0.2658	-4.72171
H	4.86794	2.01924	2.37181
H	4.87346	2.91521	4.66965
H	2.71801	3.61614	5.73618
H	0.59984	3.44212	4.45567
H	1.52774	1.74107	-2.34765
H	1.39293	3.53687	-4.0301
H	2.62773	5.67967	-3.68602
H	3.99001	6.00636	-1.62073
H	4.09761	4.22351	0.09458
H	3.31668	-1.41167	0.47946
H	5.29757	-2.88279	0.28068
H	7.55504	-1.89308	-0.14029
H	7.79601	0.5773	-0.39099
H	5.81192	2.04713	-0.21836
H	0.80932	-6.61615	-0.07016
H	4.22066	-4.87146	-2.05463
H	4.32874	-7.19703	-1.31344
H	2.81639	-7.87402	-1.95565
H	3.08523	-7.83611	-0.20417
Mo	0.06096	-0.48923	-0.54136
O	-1.27651	-0.79897	0.77742
O	-0.80387	0.08584	-2.16017
O	1.56628	0.50014	0.06371
Si	-1.45385	-1.46276	2.31006
Si	-2.02379	1.0813	-2.73306
Si	2.86862	1.49433	0.32143
H	-0.28697	-4.40382	0.00346
H	3.13109	-2.64811	-1.97567

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.561291

3_{145^o}

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.08708	1.69116	1.94084
C	-0.85554	1.85988	2.58612
C	0.20048	2.55448	1.97619
C	-0.01853	3.12929	0.71866
C	-1.24429	2.98256	0.04469
C	-2.27805	2.2709	0.67438
C	-3.16127	0.86801	2.57669
C	-2.96059	-0.49874	2.92458
C	-4.01784	-1.19259	3.54199
C	-5.24525	-0.57847	3.81046
C	-5.44275	0.75293	3.43844
C	-4.40767	1.46483	2.82605
C	-1.82926	-3.30091	2.1012
C	-1.14745	-4.30759	2.80838
C	-1.37067	-5.66121	2.53012
C	-2.28057	-6.03019	1.53454
C	-2.97185	-5.04231	0.82163
C	-2.74634	-3.69324	1.10529
C	0.09566	-1.28722	3.39376
C	0.03501	-0.8238	4.72098
C	1.19975	-0.63609	5.47247
C	2.44959	-0.90566	4.90472
C	2.52951	-1.3855	3.59316
C	1.36135	-1.58467	2.85252
C	-1.38817	3.63218	-1.29696
C	-1.69144	2.94373	-2.50732
C	-1.73231	3.70637	-3.69529
C	-1.48849	5.08189	-3.71793
C	-1.1848	5.7417	-2.52814
C	-1.13527	5.01627	-1.33762
C	-3.67353	0.61843	-1.9189
C	-3.86874	-0.63639	-1.31303
C	-5.07679	-0.95017	-0.68191
C	-6.11765	-0.01639	-0.65283
C	-5.94924	1.22985	-1.26595
C	-4.73724	1.54177	-1.89003
C	-2.11809	0.70338	-4.57793
C	-3.3215	0.77986	-5.30321
C	-3.3523	0.52168	-6.67788
C	-2.17544	0.17627	-7.35103
C	-0.97075	0.08641	-6.64426
C	-0.9451	0.34646	-5.27056
C	1.52157	2.64873	2.66628
C	2.74134	2.23853	2.05862
C	3.92544	2.34265	2.81458
C	3.93166	2.83793	4.12172
C	2.72871	3.22748	4.71282
C	1.53896	3.12541	3.98931
C	2.8647	2.83989	-0.99689
C	2.10766	2.68635	-2.17429
C	2.03338	3.70963	-3.12318
C	2.72756	4.90645	-2.91666
C	3.49101	5.07606	-1.7565
C	3.55213	4.05318	-0.80374
C	4.42746	0.4277	0.1747
C	4.30715	-0.97133	0.28303
C	5.42507	-1.80391	0.16798
C	6.68992	-1.24861	-0.05362
C	6.82866	0.13914	-0.17249
C	5.70567	0.96652	-0.06592
C	0.74793	-2.06481	-0.92862
C	1.34877	-3.36419	-1.02217
C	0.69971	-4.49651	-0.47381
C	1.31068	-5.74636	-0.51367
C	2.57815	-5.92584	-1.09764
C	3.21801	-4.79935	-1.64285
C	2.62138	-3.5397	-1.61118
C	3.21241	-7.29254	-1.15535
H	-0.69789	1.41286	3.5666
H	0.78076	3.69055	0.23694
H	-3.23529	2.14338	0.17183
H	-3.8905	-2.24955	3.79457
H	-6.04807	-1.14363	4.29089
H	-6.40248	1.2417	3.62558
H	-4.55962	2.50942	2.54245
H	-0.4179	-4.03329	3.57548
H	-0.82573	-6.42909	3.08546
H	-2.44934	-7.08667	1.30994
H	-3.68018	-5.32531	0.03863
H	-3.27807	-2.9308	0.53155
H	-0.93447	-0.58495	5.16941

H	1.13336	-0.26358	6.498
H	3.36192	-0.73537	5.48181
H	3.50197	-1.59293	3.13999
H	1.4443	-1.96807	1.83164
H	-1.95037	3.20872	-4.64229
H	-1.52938	5.62846	-4.66359
H	-0.98433	6.81617	-2.52144
H	-0.89739	5.53231	-0.40435
H	-3.0606	-1.37193	-1.31496
H	-5.20803	-1.92272	-0.20079
H	-7.05695	-0.25863	-0.14913
H	-6.7591	1.964	-1.24742
H	-4.61015	2.53192	-2.33882
H	-4.25135	1.04152	-4.78913
H	-4.29713	0.5856	-7.22444
H	-2.1977	-0.02763	-8.42497
H	-0.04993	-0.19024	-7.16499
H	-0.0012	0.26424	-4.72414
H	4.87105	2.00705	2.38083
H	4.87041	2.9054	4.67748
H	2.71245	3.60902	5.73707
H	0.59735	3.43231	4.45138
H	1.5371	1.77003	-2.34454
H	1.41263	3.58014	-4.01288
H	2.66263	5.71156	-3.65326
H	4.02867	6.01287	-1.58663
H	4.12586	4.21587	0.1144
H	3.32259	-1.41687	0.43897
H	5.30275	-2.88783	0.24174
H	7.56611	-1.89638	-0.14309
H	7.81332	0.57679	-0.35771
H	5.83045	2.04752	-0.18404
H	0.79217	-6.6037	-0.07455
H	4.2068	-4.91002	-2.09726
H	4.29439	-7.23198	-1.34594
H	2.76733	-7.89808	-1.96443
H	3.0573	-7.84792	-0.2167
Mo	0.07631	-0.49121	-0.55613
O	-1.19291	-0.82135	0.81332
O	-0.81813	0.08777	-2.15786
O	1.5789	0.50231	0.04518
Si	-1.44931	-1.47377	2.33624
Si	-2.03733	1.08074	-2.73159
Si	2.8804	1.49247	0.32014
H	-0.27859	-4.3789	-0.00624
H	3.14245	-2.67409	-2.02495

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.562751

$3_{150°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.07781	1.68456	1.92538
C	-0.84651	1.84707	2.57317
C	0.21138	2.54224	1.967
C	-0.00473	3.12251	0.71122
C	-1.22969	2.98145	0.0351
C	-2.26569	2.26971	0.66122
C	-3.15818	0.86491	2.55425
C	-2.96456	-0.50186	2.90444
C	-4.03028	-1.19326	3.51041
C	-5.25872	-0.57603	3.76637
C	-5.44847	0.75626	3.39348
C	-4.40546	1.46515	2.79146
C	-1.81957	-3.3078	2.12701
C	-1.12997	-4.31193	2.83015
C	-1.34378	-5.66617	2.54742
C	-2.25188	-6.03821	1.55134
C	-2.95097	-5.05287	0.84255
C	-2.73502	-3.7032	1.13068
C	0.0803	-1.27682	3.44628
C	-0.01374	-0.86937	4.78986
C	1.13475	-0.66827	5.56277
C	2.40058	-0.86607	5.00051
C	2.5139	-1.28419	3.67036
C	1.36245	-1.49677	2.90774
C	-1.37175	3.63267	-1.30556
C	-1.69393	2.94696	-2.51266
C	-1.73404	3.70849	-3.70131
C	-1.47139	5.08048	-3.72777
C	-1.14866	5.73737	-2.54133
C	-1.09991	5.01305	-1.35014
C	-3.68875	0.62736	-1.91322
C	-3.87809	-0.62455	-1.2994
C	-5.08345	-0.93942	-0.66377
C	-6.12773	-0.00937	-0.63809
C	-5.96502	1.23409	-1.25843
C	-4.75551	1.5471	-1.88693
C	-2.14471	0.70599	-4.57727
C	-3.35155	0.78005	-5.29703
C	-3.38894	0.51763	-6.67077
C	-2.21532	0.17019	-7.34847
C	-1.0072	0.08274	-6.64722
C	-0.975	0.34718	-5.27453
C	1.53248	2.63107	2.65774
C	2.75213	2.22434	2.0475
C	3.93634	2.32401	2.80384
C	3.9428	2.81028	4.11431
C	2.7398	3.19527	4.70827
C	1.55011	3.0988	3.98396
C	2.8888	2.84791	-1.00227
C	2.16578	2.68866	-2.20033
C	2.0901	3.72016	-3.14008
C	2.75044	4.9307	-2.90435
C	3.48216	5.10527	-1.72474
C	3.54363	4.07425	-0.78072
C	4.43218	0.41339	0.1589
C	4.30162	-0.98511	0.26393
C	5.41412	-1.82508	0.14978
C	6.68326	-1.27803	-0.0679
C	6.83204	0.10895	-0.18352
C	5.71463	0.94389	-0.07756
C	0.76577	-2.05416	-0.96595
C	1.36185	-3.35592	-1.05649
C	0.72147	-4.47761	-0.47665
C	1.32657	-5.73041	-0.51251
C	2.57969	-5.92335	-1.12265
C	3.21117	-4.80728	-1.69815
C	2.61999	-3.54484	-1.67143
C	3.20743	-7.29328	-1.1756
H	-0.69127	1.39379	3.55143
H	0.7973	3.68225	0.23225
H	-3.22324	2.14792	0.15803
H	-3.90828	-2.25037	3.76481
H	-6.06791	-1.1392	4.23835
H	-6.40851	1.24785	3.57137
H	-4.55188	2.51006	2.50625
H	-0.40196	-4.03497	3.59783
H	-0.79312	-6.43207	3.09987
H	-2.41337	-7.09508	1.32329

H	-3.65814	-5.33832	0.05938
H	-3.2736	-2.94302	0.55978
H	-0.9964	-0.68357	5.23471
H	1.04277	-0.34128	6.60183
H	3.29908	-0.68546	5.5959
H	3.49841	-1.43189	3.21948
H	1.47129	-1.82613	1.87098
H	-1.96633	3.21245	-4.64582
H	-1.51249	5.6265	-4.67375
H	-0.93301	6.80891	-2.53773
H	-0.84807	5.52737	-0.41962
H	-3.06782	-1.35792	-1.30044
H	-5.20948	-1.90958	-0.17642
H	-7.06498	-0.25202	-0.13083
H	-6.77751	1.9654	-1.24205
H	-4.63298	2.53522	-2.34158
H	-4.27902	1.04281	-4.77924
H	-4.33642	0.57964	-7.21294
H	-2.24275	-0.03723	-8.42162
H	-0.08889	-0.19552	-7.17151
H	-0.0284	0.26695	-4.73245
H	4.88208	1.99195	2.36758
H	4.88164	2.87415	4.67034
H	2.72352	3.56955	5.7352
H	0.60865	3.40288	4.44819
H	1.62531	1.75913	-2.39591
H	1.49619	3.58541	-4.04724
H	2.68431	5.74195	-3.63408
H	3.99394	6.05223	-1.53266
H	4.09079	4.24017	0.15286
H	3.3136	-1.42507	0.41486
H	5.28414	-2.90827	0.22057
H	7.55509	-1.93173	-0.1569
H	7.82017	0.54004	-0.36571
H	5.84685	2.02435	-0.19275
H	0.81497	-6.57914	-0.04918
H	4.18914	-4.92839	-2.17286
H	4.28662	-7.23923	-1.38338
H	2.74779	-7.90541	-1.97151
H	3.06456	-7.8382	-0.22893
Mo	0.08488	-0.48994	-0.5727
O	-1.11897	-0.84937	0.84135
O	-0.83875	0.09242	-2.1575
O	1.58604	0.5119	0.015
Si	-1.44058	-1.47992	2.35786
Si	-2.05462	1.08653	-2.73186
Si	2.8935	1.4899	0.30415
H	-0.24527	-4.3492	0.01214
H	3.13483	-2.68737	-2.1094

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.563763

$3_{155°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.07173	1.67846	1.91158
C	-0.84023	1.83238	2.56126
C	0.22205	2.52365	1.95794
C	0.00938	3.11073	0.70435
C	-1.21548	2.97795	0.02668
C	-2.25503	2.26854	0.64943
C	-3.15918	0.86203	2.53166
C	-2.97291	-0.50569	2.8805
C	-4.04732	-1.19631	3.47198
C	-5.27719	-0.57679	3.71529
C	-5.45898	0.7573	3.34489
C	-4.40748	1.46497	2.7566
C	-1.80289	-3.31262	2.15519
C	-1.1016	-4.30904	2.85768
C	-1.30134	-5.66562	2.57572
C	-2.20679	-6.04773	1.58104
C	-2.91718	-5.07018	0.87274
C	-2.71534	-3.71814	1.16007
C	0.05327	-1.24922	3.50645
C	-0.09319	-0.92298	4.86767
C	1.02467	-0.69228	5.67634
C	2.31167	-0.77802	5.13376
C	2.47716	-1.11288	3.78583
C	1.35695	-1.35358	2.98599
C	-1.35678	3.63109	-1.31273
C	-1.69425	2.94796	-2.51725
C	-1.73731	3.70971	-3.7056
C	-1.46297	5.07942	-3.7342
C	-1.12441	5.73335	-2.55049
C	-1.07267	5.00884	-1.35956
C	-3.69339	0.62886	-1.90752
C	-3.87591	-0.62076	-1.28692
C	-5.07685	-0.93655	-0.64349
C	-6.1239	-0.00972	-0.6169
C	-5.96838	1.23113	-1.24433
C	-4.76309	1.54513	-1.88038
C	-2.1635	0.70766	-4.57863
C	-3.37424	0.7808	-5.2919
C	-3.41915	0.5165	-6.66507
C	-2.24928	0.16798	-7.34865
C	-1.03735	0.08142	-6.65388
C	-0.99764	0.34783	-5.28177
C	1.5443	2.59737	2.64805
C	2.76315	2.2012	2.02885
C	3.94812	2.28471	2.78586
C	3.95681	2.74414	4.10585
C	2.75471	3.11727	4.70883
C	1.56452	3.03777	3.98357
C	2.90203	2.85528	-1.01933
C	2.18	2.7017	-2.21881
C	2.10553	3.73771	-3.15361
C	2.76584	4.947	-2.91127
C	3.49618	5.11594	-1.72999
C	3.55669	4.08034	-0.79085
C	4.43989	0.40758	0.12325
C	4.30622	-0.99061	0.22987
C	5.41601	-1.83337	0.10983
C	6.68516	-1.28956	-0.11559
C	6.83694	0.09702	-0.23246
C	5.72233	0.93485	-0.12034
C	0.77726	-2.05148	-0.99459
C	1.3731	-3.35349	-1.08176
C	0.74524	-4.46748	-0.47397
C	1.34931	-5.72087	-0.50703
C	2.58938	-5.92174	-1.14083
C	3.20883	-4.81304	-1.743
C	2.61806	-3.5503	-1.72033
C	3.21588	-7.29239	-1.1905
H	-0.68782	1.37345	3.53732
H	0.81467	3.66773	0.22768
H	-3.21284	2.15366	0.14534
H	-3.93038	-2.25404	3.72608
H	-6.09317	-1.13927	4.17628
H	-6.41957	1.25103	3.51359
H	-4.54819	2.5109	2.47231

H	-0.37592	-4.02402	3.62468
H	-0.74197	-6.42541	3.12788
H	-2.35747	-7.10636	1.35375
H	-3.62236	-5.36351	0.09069
H	-3.26343	-2.96443	0.58919
H	-1.09409	-0.82432	5.29973
H	0.89127	-0.43029	6.72933
H	3.18499	-0.57458	5.75845
H	3.47747	-1.17163	3.34965
H	1.50791	-1.60907	1.9343
H	-1.9811	3.21551	-4.64821
H	-1.50706	5.62586	-4.67979
H	-0.89892	6.80287	-2.54886
H	-0.80921	5.5211	-0.43112
H	-3.06422	-1.35266	-1.2897
H	-5.1967	-1.90452	-0.15027
H	-7.05748	-0.25263	-0.1031
H	-6.78313	1.9599	-1.22724
H	-4.646	2.53156	-2.34017
H	-4.29889	1.044	-4.76935
H	-4.36958	0.57773	-7.20214
H	-2.2826	-0.04106	-8.42132
H	-0.12196	-0.19775	-7.18278
H	-0.0481	0.26826	-4.74475
H	4.89299	1.9602	2.3421
H	4.89633	2.79554	4.66203
H	2.73941	3.46945	5.74353
H	0.62434	3.3338	4.45541
H	1.63993	1.77277	-2.41857
H	1.51272	3.60753	-4.06218
H	2.70072	5.76172	-3.63721
H	4.00783	6.06193	-1.5329
H	4.10321	4.24146	0.14394
H	3.31792	-1.42896	0.38568
H	5.2838	-2.9162	0.18176
H	7.55478	-1.94552	-0.2095
H	7.82514	0.52545	-0.42049
H	5.85639	2.01501	-0.2363
H	0.84753	-6.56351	-0.02232
H	4.17692	-4.94022	-2.23606
H	4.29292	-7.24034	-1.40979
H	2.7481	-7.90975	-1.97763
H	3.0825	-7.83067	-0.23872
Mo	0.09173	-0.49338	-0.58698
O	-1.05155	-0.87355	0.86859
O	-0.84623	0.09522	-2.16291
O	1.59536	0.51588	-0.02231
Si	-1.43326	-1.48166	2.37731
Si	-2.06309	1.08868	-2.73374
Si	2.90475	1.48795	0.27684
H	-0.21062	-4.33253	0.03433
H	3.12343	-2.69859	-2.1801

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.56432

$3_{160°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.06779	1.66591	1.88534
C	-0.83828	1.80992	2.54171
C	0.23082	2.49816	1.94577
C	0.02677	3.09312	0.69404
C	-1.19595	2.97164	0.01092
C	-2.24186	2.26632	0.62709
C	-3.16584	0.84863	2.48596
C	-2.9886	-0.52106	2.83045
C	-4.0753	-1.2137	3.39651
C	-5.30911	-0.59418	3.61903
C	-5.48163	0.74208	3.25257
C	-4.41803	1.45107	2.68874
C	-1.77718	-3.32701	2.17337
C	-1.0604	-4.30972	2.87961
C	-1.23658	-5.67019	2.60076
C	-2.13399	-6.07021	1.6058
C	-2.85946	-5.10668	0.89368
C	-2.68072	-3.75062	1.17768
C	0.00555	-1.22328	3.57473
C	-0.21046	-1.01332	4.94989
C	0.85783	-0.74854	5.81329
C	2.16304	-0.68258	5.31264
C	2.39733	-0.89706	3.95089
C	1.32745	-1.1699	3.09463
C	-1.33027	3.6247	-1.32894
C	-1.68079	2.94169	-2.53005
C	-1.71894	3.69944	-3.72084
C	-1.42784	5.0657	-3.75491
C	-1.07658	5.71929	-2.57469
C	-1.0291	4.99842	-1.38129
C	-3.69598	0.65079	-1.8829
C	-3.86583	-0.56447	-1.19449
C	-5.04898	-0.84102	-0.50249
C	-6.09365	0.08823	-0.49937
C	-5.95378	1.29222	-1.19827
C	-4.76403	1.56966	-1.87871
C	-2.19148	0.69433	-4.57509
C	-3.40774	0.77227	-5.2784
C	-3.46653	0.49979	-6.64945
C	-2.30528	0.13813	-7.34084
C	-1.0881	0.04648	-6.65596
C	-1.03453	0.32111	-5.28597
C	1.55247	2.55778	2.63835
C	2.77297	2.17719	2.01152
C	3.95685	2.24467	2.77189
C	3.96331	2.67008	4.10309
C	2.7598	3.02535	4.71362
C	1.57117	2.96404	3.98454
C	2.9165	2.8603	-1.03671
C	2.19917	2.70854	-2.23924
C	2.12674	3.74686	-3.17155
C	2.78394	4.95662	-2.92325
C	3.50901	5.12392	-1.73851
C	3.56791	4.08584	-0.80197
C	4.45784	0.40884	0.0902
C	4.32672	-0.98992	0.19456
C	5.43706	-1.83049	0.06448
C	6.70373	-1.28418	-0.16865
C	6.85289	0.10298	-0.28225
C	5.73788	0.9388	-0.16013
C	0.79337	-2.05461	-1.031
C	1.38808	-3.35661	-1.12298
C	0.7676	-4.46805	-0.50299
C	1.36938	-5.72236	-0.54187
C	2.60003	-5.92636	-1.19289
C	3.21267	-4.8198	-1.80588
C	2.62382	-3.55624	-1.77817
C	3.22378	-7.29802	-1.249
H	-0.69227	1.34415	3.51566
H	0.83754	3.64697	0.22311
H	-3.19922	2.16325	0.12084
H	-3.96391	-2.27248	3.64857

H	-6.13451	-1.15806	4.06119
H	-6.44473	1.23633	3.40462
H	-4.5531	2.49799	2.40549
H	-0.34187	-4.01001	3.64783
H	-0.66553	-6.41899	3.15596
H	-2.26673	-7.13184	1.38135
H	-3.55839	-5.41386	0.11138
H	-3.24078	-3.00849	0.60297
H	-1.22858	-1.03406	5.35167
H	0.67055	-0.57937	6.8771
H	2.99626	-0.45319	5.98161
H	3.41055	-0.83079	3.54779
H	1.52976	-1.31339	2.03119
H	-1.97263	3.20475	-4.66071
H	-1.46884	5.60969	-4.70206
H	-0.83781	6.78592	-2.57769
H	-0.75595	5.51064	-0.45563
H	-3.05552	-1.29745	-1.17754
H	-5.15528	-1.77758	0.0504
H	-7.01206	-0.12267	0.05409
H	-6.76702	2.0229	-1.19963
H	-4.65603	2.53216	-2.38876
H	-4.32591	1.04522	-4.74957
H	-4.4211	0.56486	-7.17867
H	-2.34948	-0.07733	-8.41184
H	-0.17953	-0.24319	-7.19094
H	-0.08106	0.23737	-4.75655
H	4.9028	1.93239	2.32168
H	4.90204	2.70836	4.66166
H	2.74208	3.34937	5.75742
H	0.63054	3.24734	4.4631
H	1.66196	1.77872	-2.44283
H	1.5378	3.61834	-4.08284
H	2.72029	5.77314	-3.64731
H	4.01805	6.07037	-1.5369
H	4.111	4.2451	0.13515
H	3.34029	-1.431	0.35692
H	5.30731	-2.91375	0.13463
H	7.57356	-1.93864	-0.27081
H	7.83919	0.53333	-0.47583
H	5.86933	2.01952	-0.27394
H	0.87353	-6.56318	-0.04799
H	4.17371	-4.94943	-2.31191
H	4.29926	-7.24747	-1.47628
H	2.7493	-7.91347	-2.03364
H	3.09658	-7.83742	-0.29704
Mo	0.10736	-0.50272	-0.60309
O	-0.97447	-0.90543	0.89158
O	-0.85613	0.09036	-2.16348
O	1.6173	0.50858	-0.05931
Si	-1.42768	-1.49091	2.38633
Si	-2.07133	1.08512	-2.73368
Si	2.92062	1.4854	0.25075
H	-0.18038	-4.33014	0.01944
H	3.12365	-2.70622	-2.24714

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.564351

3_{165^a}

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.04634	1.66616	1.8685
C	-0.81683	1.80665	2.52601
C	0.25177	2.4991	1.93325
C	0.04852	3.09954	0.68363
C	-1.17372	2.9805	-0.00027
C	-2.2194	2.27356	0.61372
C	-3.15054	0.84924	2.45788
C	-2.98237	-0.52241	2.79777
C	-4.08141	-1.2155	3.33952
C	-5.31797	-0.59508	3.54218
C	-5.48	0.74426	3.1831
C	-4.40444	1.45386	2.64402
C	-1.75918	-3.3313	2.19746
C	-1.03501	-4.31399	2.89626
C	-1.20353	-5.6738	2.60958
C	-2.10086	-6.0735	1.61441
C	-2.83416	-5.11018	0.91012
C	-2.66292	-3.75474	1.20186
C	-0.02443	-1.21991	3.65616
C	-0.29419	-1.11049	5.0335
C	0.73002	-0.84454	5.94861
C	2.04426	-0.67588	5.49834
C	2.33139	-0.78568	4.13419
C	1.30609	-1.05878	3.22498
C	-1.31273	3.63075	-1.3402
C	-1.68403	2.94401	-2.53291
C	-1.73142	3.69509	-3.72739
C	-1.4298	5.05889	-3.77228
C	-1.05762	5.71582	-2.60022
C	-1.00063	5.00136	-1.40335
C	-3.70192	0.6557	-1.85851
C	-3.85904	-0.54618	-1.1439
C	-5.03977	-0.82137	-0.44741
C	-6.09503	0.09549	-0.46659
C	-5.967	1.28661	-1.18932
C	-4.77924	1.56339	-1.87356
C	-2.20604	0.67808	-4.55481
C	-3.42353	0.75038	-5.25664
C	-3.48558	0.46283	-6.62446
C	-2.32641	0.09122	-7.31403
C	-1.1081	0.00477	-6.63051
C	-1.05124	0.29467	-5.26378
C	1.57362	2.55704	2.62606
C	2.79503	2.17951	1.99856
C	3.97824	2.24417	2.76042
C	3.98324	2.66377	4.09355
C	2.77917	3.01725	4.70404
C	1.59127	2.95889	3.97349
C	2.93725	2.87296	-1.05032
C	2.2133	2.72127	-2.24892
C	2.13824	3.7586	-3.18208
C	2.79907	4.96733	-2.93838
C	3.53023	5.13464	-1.75739
C	3.59206	4.09746	-0.81999
C	4.48306	0.42	0.06826
C	4.34778	-0.97907	0.16491
C	5.455	-1.82197	0.02394
C	6.72215	-1.27794	-0.2121
C	6.87527	0.10946	-0.31714
C	5.76345	0.9479	-0.18436
C	0.8142	-2.04012	-1.061
C	1.39731	-3.34621	-1.16511
C	0.76936	-4.45456	-0.5467
C	1.35762	-5.71483	-0.59687
C	2.58161	-5.92788	-1.2576
C	3.20184	-4.82425	-1.86815
C	2.62654	-3.55468	-1.82944
C	3.19033	-7.30575	-1.32598
H	-0.67073	1.33524	3.49754

H	0.86006	3.65441	0.21519
H	-3.17765	2.1763	0.10838
H	-3.97694	-2.2755	3.5889
H	-6.15281	-1.16024	3.96452
H	-6.44435	1.24025	3.32075
H	-4.53226	2.50266	2.36453
H	-0.31771	-4.0147	3.66587
H	-0.627	-6.42239	3.15941
H	-2.22796	-7.13459	1.38424
H	-3.53376	-5.41687	0.12823
H	-3.23059	-3.01313	0.63374
H	-1.32092	-1.21422	5.3991
H	0.50053	-0.75644	7.014
H	2.84267	-0.44721	6.20896
H	3.35029	-0.63293	3.77111
H	1.54847	-1.11393	2.16176
H	-2.00052	3.19711	-4.66133
H	-1.47869	5.5984	-4.72162
H	-0.81002	6.78036	-2.6124
H	-0.71191	5.51645	-0.48403
H	-3.04016	-1.26922	-1.11016
H	-5.1352	-1.74541	0.12788
H	-7.01177	-0.11383	0.09015
H	-6.78812	2.00825	-1.20635
H	-4.68073	2.51683	-2.40232
H	-4.34034	1.03035	-4.72918
H	-4.44114	0.52372	-7.1524
H	-2.37319	-0.13623	-8.38244
H	-0.2012	-0.29286	-7.16395
H	-0.09693	0.21464	-4.73529
H	4.92465	1.93413	2.30949
H	4.92134	2.69948	4.65332
H	2.76042	3.33713	5.74907
H	0.65018	3.23997	4.45243
H	1.67315	1.79213	-2.44794
H	1.54428	3.63036	-4.09016
H	2.73349	5.78313	-3.66307
H	4.0421	6.08034	-1.55948
H	4.14066	4.25662	0.11395
H	3.36044	-1.4178	0.32999
H	5.32265	-2.90532	0.08792
H	7.5894	-1.9344	-0.32307
H	7.862	0.53794	-0.51267
H	5.89759	2.02892	-0.29218
H	0.85638	-6.55325	-0.10433
H	4.15803	-4.96112	-2.38141
H	4.26441	-7.26534	-1.56173
H	2.70302	-7.91208	-2.10987
H	3.06514	-7.84878	-0.3758
Mo	0.13087	-0.49718	-0.5995
O	-0.87497	-0.93188	0.93752
O	-0.86398	0.10189	-2.13748
O	1.64557	0.51743	-0.07675
Si	-1.40808	-1.49498	2.41123
Si	-2.08067	1.08688	-2.71765
Si	2.9465	1.4961	0.23471
H	-0.17363	-4.30961	-0.01659
H	3.13207	-2.70723	-2.29704

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.564212

$3_{170°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.02009	1.67437	1.8625
C	-0.78903	1.82073	2.51675
C	0.27461	2.51779	1.91951
C	0.06435	3.11747	0.67042
C	-1.15899	2.99261	-0.00948
C	-2.19931	2.28153	0.60841
C	-3.12589	0.85961	2.45243
C	-2.96461	-0.5106	2.80092
C	-4.07158	-1.19681	3.33626
C	-5.30797	-0.5722	3.52515
C	-5.46244	0.7661	3.1593
C	-4.37986	1.46883	2.62602
C	-1.76356	-3.32776	2.2301
C	-1.04726	-4.32945	2.90994
C	-1.2293	-5.68252	2.60041
C	-2.13221	-6.05691	1.60051
C	-2.85822	-5.07474	0.91507
C	-2.67399	-3.72623	1.23015
C	-0.04836	-1.25373	3.76107
C	-0.33134	-1.40583	5.13202
C	0.65557	-1.18789	6.09922
C	1.94381	-0.80361	5.70978
C	2.24185	-0.645	4.35268
C	1.25544	-0.87382	3.38944
C	-1.30665	3.63805	-1.35022
C	-1.68337	2.94312	-2.53598
C	-1.74123	3.68581	-3.73498
C	-1.4448	5.05047	-3.78962
C	-1.06681	5.7157	-2.62398
C	-0.99916	5.00905	-1.42299
C	-3.70244	0.66082	-1.85181
C	-3.86952	-0.54225	-1.14136
C	-5.05407	-0.8123	-0.44951
C	-6.10385	0.11092	-0.47027
C	-5.9666	1.30252	-1.19037
C	-4.77464	1.57429	-1.86948
C	-2.17256	0.64398	-4.52942
C	-3.37648	0.72671	-5.2534
C	-3.42074	0.41658	-6.61689
C	-2.25716	0.01121	-7.27964
C	-1.05262	-0.08621	-6.57369
C	-1.01334	0.22665	-5.21131
C	1.60087	2.58621	2.60358
C	2.82113	2.21574	1.96882
C	4.00925	2.29379	2.72221
C	4.02048	2.72256	4.05262
C	2.81794	3.07056	4.66942
C	1.62513	2.99669	3.94817
C	2.93709	2.89673	-1.08671
C	2.1932	2.7362	-2.27188
C	2.1073	3.7648	-3.2137
C	2.77597	4.97342	-2.99191
C	3.52568	5.14968	-1.82391
C	3.59916	4.12112	-0.87789
C	4.50902	0.46076	0.02895
C	4.37974	-0.93879	0.12787
C	5.48821	-1.77746	-0.02749
C	6.75032	-1.22878	-0.27943
C	6.89732	0.15918	-0.38555
C	5.78419	0.99361	-0.23899
C	0.83078	-2.03065	-1.05314
C	1.39765	-3.34209	-1.17558
C	0.75984	-4.4475	-0.56163
C	1.32862	-5.7157	-0.63146
C	2.54236	-5.93957	-1.30747
C	3.17308	-4.83856	-1.912

C	2.61723	-3.56105	-1.85399
C	3.12934	-7.32558	-1.39784
H	-0.63896	1.35083	3.48878
H	0.87212	3.67557	0.19927
H	-3.15916	2.18126	0.10675
H	-3.97353	-2.256	3.59157
H	-6.14816	-1.13323	3.94235
H	-6.42602	1.2663	3.28646
H	-4.50213	2.51666	2.34058
H	-0.32662	-4.05097	3.68401
H	-0.65896	-6.44564	3.13656
H	-2.26977	-7.11267	1.3525
H	-3.56306	-5.36117	0.13018
H	-3.23844	-2.97023	0.67798
H	-1.33874	-1.68663	5.45635
H	0.41666	-1.3081	7.15939
H	2.71217	-0.61755	6.46488
H	3.23637	-0.31815	4.04044
H	1.50099	-0.71928	2.33725
H	-2.01389	3.18094	-4.66429
H	-1.50151	5.58432	-4.74172
H	-0.82259	6.78089	-2.6446
H	-0.70555	5.53044	-0.50876
H	-3.05588	-1.27153	-1.10977
H	-5.15706	-1.73734	0.12285
H	-7.0237	-0.09417	0.08289
H	-6.78365	2.02873	-1.20901
H	-4.66857	2.52818	-2.3959
H	-4.29678	1.03298	-4.74679
H	-4.36577	0.48623	-7.16242
H	-2.29004	-0.23402	-8.34464
H	-0.14266	-0.4102	-7.08613
H	-0.07016	0.13792	-4.66458
H	4.95475	1.98865	2.26595
H	4.96227	2.76973	4.60524
H	2.80431	3.39781	5.71223
H	0.68506	3.27236	4.43227
H	1.64584	1.80745	-2.45206
H	1.49805	3.63035	-4.11066
H	2.70194	5.78248	-3.72333
H	4.04361	6.0955	-1.64305
H	4.16363	4.28713	0.04536
H	3.3961	-1.38038	0.30763
H	5.36108	-2.86135	0.03851
H	7.61843	-1.88212	-0.40163
H	7.88008	0.5912	-0.59295
H	5.91308	2.07507	-0.3488
H	0.82017	-6.55194	-0.14258
H	4.12192	-4.98415	-2.43639
H	4.20259	-7.29846	-1.63925
H	2.62846	-7.91362	-2.18712
H	3.001	-7.87946	-0.4544
Mo	0.1526	-0.49433	-0.56279
O	-0.78668	-0.94253	1.01353
O	-0.86182	0.11443	-2.08284
O	1.6707	0.53867	-0.08851
Si	-1.38707	-1.49756	2.46175
Si	-2.07217	1.08319	-2.69833
Si	2.96744	1.52766	0.20547
H	-0.17505	-4.2939	-0.01922
H	3.13042	-2.71609	-2.31787

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.563991

$3_{175°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-2.00801	1.67371	1.84806
C	-0.77647	1.81915	2.50185
C	0.28495	2.52215	1.90751
C	0.0728	3.12832	0.66163
C	-1.15115	3.00466	-0.01711
C	-2.18943	2.28898	0.59837
C	-3.11553	0.85938	2.43447
C	-2.95639	-0.50882	2.79106
C	-4.06828	-1.19219	3.32079
C	-5.30642	-0.5675	3.49621
C	-5.45815	0.76902	3.12305
C	-4.37129	1.46901	2.59553
C	-1.76193	-3.33322	2.26496
C	-1.04278	-4.3368	2.93896
C	-1.22263	-5.68879	2.62334
C	-2.12629	-6.06035	1.62304
C	-2.85552	-5.07637	0.94366
C	-2.6735	-3.72897	1.26491
C	-0.06408	-1.25576	3.81965
C	-0.35927	-1.42937	5.18529
C	0.61367	-1.20594	6.16543
C	1.89922	-0.79486	5.79454
C	2.20908	-0.61453	4.44268
C	1.23688	-0.84891	3.46655
C	-1.3079	3.65321	-1.35453
C	-1.70207	2.95811	-2.53406
C	-1.77575	3.69865	-3.73321
C	-1.47773	5.06287	-3.79279
C	-1.08122	5.7283	-2.63317
C	-0.99796	5.02318	-1.43218
C	-3.71488	0.66665	-1.84379
C	-3.87544	-0.53191	-1.1239
C	-5.06375	-0.80971	-0.44189
C	-6.1234	0.10164	-0.48072
C	-5.99162	1.28932	-1.20817
C	-4.79618	1.56859	-1.87833
C	-2.15783	0.63502	-4.50707
C	-3.35177	0.70917	-5.2484
C	-3.37741	0.38324	-6.60866
C	-2.2049	-0.03	-7.25055
C	-1.01019	-0.11911	-6.5271
C	-0.98933	0.20996	-5.1681
C	1.6109	2.58988	2.59266
C	2.83125	2.21619	1.96001
C	4.01827	2.29224	2.71556
C	4.02829	2.72324	4.04533
C	2.8256	3.07487	4.65973
C	1.63378	3.00189	3.93679
C	2.94473	2.90109	-1.09496
C	2.17418	2.75243	-2.26452
C	2.08677	3.78166	-3.20556
C	2.78015	4.97894	-2.99845
C	3.55554	5.14355	-1.84554
C	3.63075	4.11454	-0.90016
C	4.52144	0.46569	0.01693
C	4.39111	-0.93461	0.10342
C	5.49965	-1.77249	-0.05569
C	6.76284	-1.22238	-0.29899
C	6.91089	0.16634	-0.39271
C	5.79774	1.0001	-0.24246
C	0.82969	-2.0221	-1.07039
C	1.38771	-3.33556	-1.20924
C	0.74952	-4.44062	-0.59471

C	1.30912	-5.71205	-0.67891
C	2.51389	-5.93941	-1.36968
C	3.14529	-4.83865	-1.97401
C	2.59833	-3.55799	-1.90228
C	3.09082	-7.32853	-1.47583
H	-0.62491	1.34668	3.47231
H	0.87933	3.69019	0.19273
H	-3.15034	2.19226	0.09794
H	-3.97231	-2.2497	3.58339
H	-6.14971	-1.12705	3.9091
H	-6.42271	1.26982	3.23981
H	-4.49156	2.51555	2.30471
H	-0.32166	-4.06062	3.71345
H	-0.65023	-6.45332	3.15529
H	-2.26228	-7.11521	1.37038
H	-3.56143	-5.36046	0.15886
H	-3.24155	-2.97174	0.71778
H	-1.36468	-1.73259	5.49535
H	0.36597	-1.3434	7.22149
H	2.65621	-0.60552	6.56026
H	3.20108	-0.26743	4.14435
H	1.48815	-0.67745	2.41828
H	-2.06143	3.19286	-4.65828
H	-1.54694	5.59643	-4.74423
H	-0.83482	6.79289	-2.65873
H	-0.6906	5.54487	-0.52265
H	-3.05435	-1.25216	-1.0768
H	-5.16148	-1.73089	0.13755
H	-7.0466	-0.10923	0.06468
H	-6.81611	2.00661	-1.24015
H	-4.69544	2.51925	-2.41163
H	-4.2791	1.02097	-4.7581
H	-4.31483	0.44662	-7.16791
H	-2.22322	-0.28774	-8.31294
H	-0.09334	-0.44905	-7.02321
H	-0.05365	0.12809	-4.60755
H	4.96394	1.98473	2.26129
H	4.96933	2.76911	4.59935
H	2.81094	3.40351	5.70208
H	0.69329	3.27925	4.41912
H	1.60593	1.83377	-2.43049
H	1.45643	3.65717	-4.08932
H	2.70522	5.78866	-3.72906
H	4.09264	6.08073	-1.67596
H	4.21634	4.27202	0.01139
H	3.40663	-1.37701	0.27658
H	5.37189	-2.85686	0.00091
H	7.631	-1.87512	-0.42404
H	7.8945	0.59963	-0.59327
H	5.92781	2.08233	-0.34275
H	0.80076	-6.54814	-0.18965
H	4.08746	-4.98714	-2.50951
H	4.16371	-7.30638	-1.71939
H	2.58429	-7.90461	-2.27034
H	2.96056	-7.89143	-0.53805
Mo	0.15863	-0.49535	-0.5426
O	-0.71398	-0.98315	1.06055
O	-0.87036	0.15159	-2.03493
O	1.68356	0.54108	-0.1028
Si	-1.37546	-1.50397	2.49347
Si	-2.08113	1.09583	-2.68059
Si	2.97861	1.5305	0.19537
H	-0.1782	-4.28436	-0.04037
H	3.11175	-2.7134	-2.3667

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3786.563659

5$_{135°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.37848	4.84468	-1.54863
C	0.67491	5.40596	-0.80245
C	0.78366	6.79113	-0.63889
C	-0.16051	7.64154	-1.22466
C	-1.21367	7.10155	-1.97174
C	-1.32122	5.7159	-2.1271
C	-0.01561	2.39328	-3.43884
C	0.07037	1.014	-3.71914
C	0.49859	0.55611	-4.96754
C	0.83919	1.47392	-5.96813
C	0.75177	2.84614	-5.71388
C	0.33165	3.29968	-4.45792
C	-2.31153	2.46692	-1.38155
C	-3.20443	2.21657	-2.4414
C	-4.54481	1.89626	-2.19647
C	-5.01428	1.81931	-0.8816
C	-4.14271	2.07429	0.18373
C	-2.80562	2.39654	-0.06448
C	-0.48336	-0.40017	-0.2483
C	-1.49199	-1.39717	-0.47097
C	-2.56833	-1.1869	-1.35664
C	-3.50125	-2.19815	-1.58272
C	-3.3965	-3.44618	-0.94578
C	-2.31993	-3.64819	-0.06358
C	-1.38688	-2.64755	0.18075
C	-4.42247	-4.52882	-1.16523
C	2.07824	-2.43024	-2.7999
C	2.8779	-2.45831	-3.95917
C	2.34124	-2.82041	-5.19969
C	0.98799	-3.15784	-5.30592
C	0.17308	-3.12385	-4.16827
C	0.71498	-2.76632	-2.93043
C	4.68398	-1.96883	-1.19364
C	5.41649	-0.80301	-0.9036
C	6.81554	-0.80553	-0.9373
C	7.50599	-1.9774	-1.26267
C	6.79363	-3.14729	-1.55281
C	5.39642	-3.1406	-1.51628
C	2.1762	-3.15681	0.20651
C	1.65968	-4.43174	-0.08769
C	1.16154	-5.26004	0.92474
C	1.17331	-4.82725	2.25457
C	1.6988	-3.56864	2.57017
C	2.19594	-2.74751	1.55567
C	-0.94393	2.37248	3.27837
C	-0.31964	3.44042	2.60231
C	-0.95015	4.68113	2.46876
C	-2.21994	4.88192	3.02013
C	-2.85096	3.84069	3.70946
C	-2.2182	2.59936	3.83475
C	-1.43385	-0.66373	3.23488
C	-2.62228	-0.4681	2.50448
C	-3.60262	-1.45936	2.43456
C	-3.40869	-2.67881	3.09058
C	-2.23254	-2.89923	3.81504
C	-1.25845	-1.8985	3.88867
C	0.96272	0.38354	4.83828
C	0.43594	0.49541	6.13934

C	1.2239	0.22201	7.26107
C	2.55797	-0.17113	7.0997
C	3.09915	-0.28493	5.81505
C	2.30692	-0.00759	4.69519
H	1.4092	4.74526	-0.3342
H	1.60604	7.20838	-0.05129
H	-0.07772	8.72425	-1.09727
H	-1.95617	7.76186	-2.42798
H	-2.16085	5.30947	-2.70002
H	-0.18709	0.27666	-2.95251
H	0.57221	-0.51651	-5.1531
H	1.17602	1.11694	-6.9452
H	1.01831	3.56632	-6.49225
H	0.27917	4.37567	-4.26847
H	-2.84654	2.25653	-3.47431
H	-5.2208	1.69928	-3.03282
H	-6.05896	1.56341	-0.68594
H	-4.50573	2.02391	1.21358
H	-2.14056	2.59198	0.77949
H	-2.66815	-0.22676	-1.86068
H	-4.33055	-2.01224	-2.27124
H	-2.21561	-4.60675	0.45205
H	-0.57035	-2.81817	0.88157
H	3.93894	-2.20219	-3.894
H	2.98157	-2.83906	-6.08555
H	0.56747	-3.44142	-6.27438
H	-0.88779	-3.37679	-4.24176
H	0.06318	-2.75713	-2.05585
H	4.88023	0.11456	-0.64758
H	7.36836	0.1099	-0.70922
H	8.599	-1.981	-1.28933
H	7.32949	-4.0662	-1.80563
H	4.85566	-4.06535	-1.74257
H	1.62288	-4.77902	-1.12365
H	0.7526	-6.24207	0.67251
H	0.77173	-5.46729	3.04452
H	1.71512	-3.2208	3.60597
H	2.58465	-1.76081	1.82091
H	0.66015	3.29373	2.14224
H	-0.45859	5.48293	1.91257
H	-2.72065	5.84692	2.90593
H	-3.8445	3.9919	4.14004
H	-2.73832	1.78994	4.35481
H	-2.78191	0.46817	1.96955
H	-4.50822	-1.28627	1.84776
H	-4.16965	-3.46136	3.02959
H	-2.07337	-3.85303	4.3252
H	-0.35034	-2.08123	4.46887
H	-0.60617	0.79827	6.28422
H	0.79804	0.31445	8.26383
H	3.17484	-0.38736	7.97607
H	4.14089	-0.59013	5.68438
H	2.73494	-0.09448	3.69302
H	-5.12953	-4.57419	-0.31806
H	-3.95042	-5.5212	-1.24202
H	-5.01165	-4.35458	-2.07802
Mo	0.91468	0.59008	0.10626
O	0.53897	2.34779	-0.59042
O	2.37522	-0.4168	-0.63997
O	0.94403	0.65389	2.01917
Si	-0.5345	2.97691	-1.7262
Si	2.80434	-1.97177	-1.12181
Si	-0.11612	0.6781	3.32742

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

HF = -3557.835154

$5_{140°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.75765	4.64667	-1.80799
C	0.22703	5.24736	-1.00074
C	0.24084	6.63089	-0.79141
C	-0.72994	7.43975	-1.39188
C	-1.71619	6.86008	-2.19841
C	-1.73062	5.47616	-2.39863
C	-0.28213	2.24437	-3.7633
C	-0.00186	0.88426	-4.00916
C	0.40102	0.4482	-5.27385
C	0.52013	1.36744	-6.3233
C	0.23964	2.71933	-6.10119
C	-0.15367	3.15297	-4.82948
C	-2.51824	2.12685	-1.65759
C	-3.43595	1.89334	-2.70034
C	-4.72509	1.41746	-2.43468
C	-5.11178	1.15272	-1.11711
C	-4.21401	1.37996	-0.06796
C	-2.93422	1.87101	-0.3369
C	-0.47874	-0.61128	-0.41081
C	-1.43991	-1.65126	-0.66008
C	-2.54019	-1.45104	-1.52007
C	-3.45326	-2.47848	-1.75112
C	-3.30905	-3.7391	-1.14791
C	-2.20805	-3.9365	-0.29493
C	-1.29031	-2.91934	-0.05136
C	-4.2826	-4.85601	-1.42643
C	2.45909	-2.42876	-2.56918
C	3.33053	-2.30361	-3.66891
C	2.91877	-2.65158	-4.9598
C	1.62207	-3.13018	-5.17621
C	0.73909	-3.25634	-4.09773
C	1.15694	-2.91232	-2.80895
C	4.86076	-1.77516	-0.72843
C	5.48133	-0.57083	-0.34813
C	6.87402	-0.48085	-0.24518
C	7.67018	-1.59665	-0.52293
C	7.06993	-2.803	-0.90323
C	5.67842	-2.88883	-1.00348
C	2.2853	-3.06622	0.46525
C	1.98215	-4.41398	0.19692
C	1.40928	-5.23273	1.17715
C	1.12758	-4.71584	2.44669
C	1.4359	-3.38172	2.7396
C	2.01297	-2.57196	1.75726
C	-0.3282	2.75634	3.65967
C	-0.35514	3.67608	2.59137
C	-0.50506	5.04661	2.82406
C	-0.62766	5.52269	4.13444
C	-0.59742	4.62536	5.20788
C	-0.44776	3.2545	4.97025
C	-1.93357	0.17741	3.16535
C	-3.08542	0.89136	3.5465
C	-4.3535	0.30419	3.46818
C	-4.49186	-1.00037	2.98136
C	-3.35891	-1.72054	2.58663
C	-2.09319	-1.13955	2.69364
C	0.80188	-0.06235	4.54425
C	0.19327	-0.84921	5.53992
C	0.96191	-1.62143	6.4184
C	2.35626	-1.62455	6.30913
C	2.97941	-0.84829	5.3247

C	2.20814	-0.0736	4.45427
H	0.98371	4.61978	-0.5228
H	1.01062	7.0782	-0.15662
H	-0.72086	8.52082	-1.22925
H	-2.47992	7.48764	-2.66557
H	-2.52124	5.038	-3.01623
H	-0.08992	0.14877	-3.20334
H	0.62898	-0.60772	-5.43354
H	0.83565	1.02859	-7.31383
H	0.33422	3.44011	-6.91793
H	-0.35799	4.21521	-4.66612
H	-3.13529	2.06614	-3.73795
H	-5.42186	1.23917	-3.25811
H	-6.11105	0.76265	-0.90632
H	-4.50185	1.16057	0.96138
H	-2.25079	2.03796	0.49933
H	-2.6787	-0.48307	-1.99756
H	-4.30323	-2.292	-2.41371
H	-2.0664	-4.90642	0.19053
H	-0.445	-3.09858	0.61105
H	4.34819	-1.93323	-3.51646
H	3.61157	-2.54856	-5.79917
H	1.29891	-3.40158	-6.18479
H	-0.27815	-3.62309	-4.25796
H	0.45546	-3.02537	-1.98134
H	4.86233	0.3042	-0.13297
H	7.33926	0.46336	0.05083
H	8.75848	-1.52771	-0.44397
H	7.68874	-3.67754	-1.1216
H	5.22619	-3.83978	-1.30317
H	2.17135	-4.82817	-0.79746
H	1.17004	-6.274	0.94512
H	0.66783	-5.35173	3.20784
H	1.2238	-2.96409	3.72705
H	2.23382	-1.53185	2.00721
H	-0.25454	3.32405	1.56114
H	-0.52316	5.73945	1.97848
H	-0.74392	6.59392	4.31972
H	-0.68719	4.99509	6.23293
H	-0.41973	2.5654	5.82046
H	-2.99275	1.9186	3.91019
H	-5.23663	0.87092	3.77504
H	-5.48359	-1.45411	2.90481
H	-3.4576	-2.73261	2.18678
H	-1.21655	-1.71898	2.39666
H	-0.89722	-0.87421	5.6212
H	0.47101	-2.2294	7.183
H	2.9581	-2.23498	6.98755
H	4.06857	-0.85363	5.23136
H	2.70569	0.51716	3.67984
H	-4.4197	-5.50121	-0.54476
H	-3.91669	-5.50054	-2.24531
H	-5.26749	-4.46981	-1.72984
Mo	0.77898	0.54575	-0.02661
O	0.33057	2.18242	-0.93743
O	2.41127	-0.35878	-0.48157
O	0.63247	0.80337	1.85193
Si	-0.79502	2.77904	-2.03457
Si	2.98814	-1.90021	-0.84117
Si	-0.21013	0.91524	3.29666

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.834154

$5_{145°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.82574	4.63515	-1.80118
C	0.15902	5.20748	-0.9738
C	0.18268	6.58528	-0.73055
C	-0.77804	7.41644	-1.31677
C	-1.76443	6.86484	-2.14254
C	-1.78906	5.48638	-2.3765
C	-0.35335	2.25774	-3.80144
C	-0.02945	0.90525	-4.03637
C	0.38432	0.472	-5.29855
C	0.47113	1.38641	-6.35549
C	0.14804	2.73051	-6.14354
C	-0.25625	3.16174	-4.87441
C	-2.60457	2.1188	-1.70914
C	-3.5126	1.84651	-2.75033
C	-4.79532	1.35584	-2.47941
C	-5.18527	1.1176	-1.15768
C	-4.29568	1.38095	-0.1098
C	-3.02124	1.88267	-0.38435
C	-0.50751	-0.64236	-0.37747
C	-1.44361	-1.7032	-0.62999
C	-2.58641	-1.5048	-1.43303
C	-3.47772	-2.55149	-1.66368
C	-3.26873	-3.82837	-1.116
C	-2.12483	-4.02308	-0.32037
C	-1.22812	-2.98728	-0.0773
C	-4.22018	-4.96467	-1.39255
C	2.5752	-2.39513	-2.57161
C	3.46568	-2.28353	-3.65662
C	3.0699	-2.62945	-4.95338
C	1.77069	-3.09136	-5.18925
C	0.86905	-3.20498	-4.12447
C	1.27047	-2.86311	-2.83012
C	4.91251	-1.605	-0.68437
C	5.44268	-0.36236	-0.29083
C	6.82354	-0.18013	-0.15643
C	7.69806	-1.24043	-0.41553
C	7.18821	-2.48384	-0.80798
C	5.80801	-2.66228	-0.93916
C	2.38875	-3.05731	0.45434
C	2.11652	-4.40827	0.17109
C	1.55187	-5.24773	1.13885
C	1.24738	-4.74827	2.41009
C	1.52375	-3.41023	2.71738
C	2.09217	-2.57988	1.7475
C	-0.42369	2.71765	3.6743
C	-0.46866	3.64732	2.6152
C	-0.66197	5.0103	2.8598
C	-0.81125	5.4689	4.17366
C	-0.7643	4.56167	5.23822
C	-0.57096	3.19843	4.98846
C	-1.94003	0.09275	3.1387
C	-3.12066	0.78322	3.47208
C	-4.37059	0.16241	3.36751
C	-4.46152	-1.154	2.90227
C	-3.29924	-1.85262	2.55798
C	-2.05214	-1.23748	2.69054
C	0.79683	-0.0759	4.52698
C	0.21112	-0.87482	5.5269
C	1.00111	-1.63222	6.39929
C	2.39445	-1.6084	6.2796
C	2.99497	-0.82038	5.29055
C	2.20229	-0.06053	4.42621

H	0.90766	4.56211	-0.50691
H	0.9519	7.0106	-0.08022
H	-0.76121	8.4931	-1.12765
H	-2.52057	7.50983	-2.59814
H	-2.58064	5.06971	-3.00764
H	-0.09144	0.17474	-3.22311
H	0.64644	-0.57741	-5.45063
H	0.79546	1.05022	-7.34408
H	0.21842	3.44723	-6.96626
H	-0.49235	4.21862	-4.71835
H	-3.20964	2.00214	-3.79
H	-5.48508	1.14699	-3.30157
H	-6.18015	0.71874	-0.94258
H	-4.58559	1.17886	0.92258
H	-2.33952	2.0722	0.44909
H	-2.77372	-0.52381	-1.86546
H	-4.36128	-2.36796	-2.28171
H	-1.93369	-5.00546	0.12121
H	-0.35142	-3.16126	0.54504
H	4.48431	-1.9226	-3.48854
H	3.77687	-2.53684	-5.7821
H	1.45981	-3.36026	-6.20237
H	-0.14987	-3.55963	-4.30063
H	0.55409	-2.96415	-2.01294
H	4.76167	0.46867	-0.08889
H	7.21828	0.79244	0.14992
H	8.7773	-1.09933	-0.31211
H	7.8686	-3.31521	-1.01117
H	5.42701	-3.64187	-1.24583
H	2.32278	-4.80864	-0.82565
H	1.33689	-6.29173	0.89555
H	0.7941	-5.40061	3.16115
H	1.29316	-3.00549	3.7062
H	2.28649	-1.53671	2.00678
H	-0.34759	3.30855	1.58266
H	-0.6922	5.71095	2.02096
H	-0.96138	6.53417	4.36869
H	-0.87516	4.91794	6.26598
H	-0.5304	2.50177	5.83197
H	-3.06521	1.8192	3.81803
H	-5.27645	0.71198	3.63725
H	-5.43873	-1.63431	2.80418
H	-3.36046	-2.87403	2.17495
H	-1.15335	-1.80044	2.42833
H	-0.87806	-0.92118	5.61655
H	0.5278	-2.24973	7.16735
H	3.01303	-2.20716	6.95335
H	4.08328	-0.80494	5.18866
H	2.68213	0.53968	3.64795
H	-4.3166	-5.63096	-0.52109
H	-3.85949	-5.58298	-2.23363
H	-5.22264	-4.5988	-1.66146
Mo	0.73349	0.54226	-0.03066
O	0.22039	2.12797	-0.98498
O	2.36123	-0.36291	-0.48239
O	0.60971	0.82778	1.84713
Si	-0.87936	2.77528	-2.07226
Si	3.05616	-1.85174	-0.83502
Si	-0.24291	0.88554	3.28952

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.83427

$5_{150°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.74078	4.60268	-1.79074
C	0.27462	5.12227	-0.96587
C	0.34631	6.49204	-0.68931
C	-0.59673	7.36758	-1.23867
C	-1.61392	6.86834	-2.06032
C	-1.68629	5.4977	-2.32792
C	-0.32394	2.27512	-3.85939
C	0.00273	0.92798	-4.11915
C	0.40316	0.51728	-5.39319
C	0.47629	1.44936	-6.43556
C	0.15291	2.78912	-6.19772
C	-0.23983	3.19765	-4.91763
C	-2.58854	2.12201	-1.78094
C	-3.48717	1.836	-2.82618
C	-4.76611	1.33286	-2.5601
C	-5.16171	1.09778	-1.23949
C	-4.28139	1.37517	-0.18739
C	-3.01005	1.88687	-0.4572
C	-0.44076	-0.71135	-0.34511
C	-1.42263	-1.73422	-0.58159
C	-2.53516	-1.50034	-1.41798
C	-3.48131	-2.5012	-1.63094
C	-3.35799	-3.76722	-1.03398
C	-2.24352	-3.99826	-0.20735
C	-1.29271	-3.00756	0.01917
C	-4.36955	-4.85514	-1.29138
C	2.47884	-2.40137	-2.54821
C	3.34007	-2.25551	-3.65333
C	2.91764	-2.58338	-4.94604
C	1.62012	-3.06174	-5.1586
C	0.74781	-3.21007	-4.07428
C	1.17679	-2.88728	-2.78363
C	4.88849	-1.77016	-0.71101
C	5.51698	-0.57273	-0.32208
C	6.91044	-0.49181	-0.2217
C	7.69938	-1.60987	-0.51081
C	7.09118	-2.80934	-0.90012
C	5.69898	-2.88608	-0.99781
C	2.31398	-3.05826	0.48155
C	2.04069	-4.41217	0.21213
C	1.48545	-5.24433	1.19138
C	1.19048	-4.73456	2.4608
C	1.4662	-3.39327	2.75372
C	2.0261	-2.5705	1.77228
C	-0.34414	2.77461	3.66697
C	-0.40099	3.70299	2.60744
C	-0.5454	5.07137	2.85504
C	-0.63304	5.53646	4.17227
C	-0.57393	4.63032	5.23703
C	-0.42961	3.26156	4.98419
C	-1.93993	0.19517	3.13402
C	-3.09957	0.93091	3.44384
C	-4.36811	0.34741	3.34948
C	-4.49867	-0.97733	2.9185
C	-3.35781	-1.72076	2.59684
C	-2.09241	-1.14184	2.7187
C	0.79366	-0.04626	4.52079
C	0.18742	-0.83607	5.51569
C	0.95819	-1.60696	6.39346
C	2.35257	-1.60578	6.28451
C	2.97349	-0.82668	5.30097
C	2.19999	-0.05332	4.43128
H	1.00971	4.44208	-0.52773
H	1.13898	6.87631	-0.04168
H	-0.54208	8.43809	-1.02367

H	-2.35654	7.54813	-2.4866
H	-2.50108	5.12207	-2.95532
H	-0.04628	0.18453	-3.31686
H	0.66542	-0.52883	-5.56543
H	0.79044	1.13049	-7.43313
H	0.21356	3.51974	-7.00891
H	-0.47688	4.25123	-4.74142
H	-3.17937	1.99038	-3.86462
H	-5.4489	1.11267	-3.38516
H	-6.15377	0.68985	-1.02839
H	-4.57509	1.17493	0.84421
H	-2.33276	2.08229	0.37873
H	-2.65751	-0.52639	-1.88877
H	-4.34066	-2.28865	-2.27321
H	-2.11949	-4.97327	0.27282
H	-0.44027	-3.20939	0.66571
H	4.35775	-1.88383	-3.50382
H	3.60227	-2.4642	-5.78997
H	1.28841	-3.317	-6.16864
H	-0.26939	-3.57832	-4.23151
H	0.48434	-3.01801	-1.95098
H	4.90356	0.30405	-0.09806
H	7.38197	0.44705	0.08127
H	8.78825	-1.54803	-0.43375
H	7.70432	-3.6856	-1.1275
H	5.24039	-3.83169	-1.30466
H	2.24102	-4.82202	-0.78196
H	1.27056	-6.29072	0.95863
H	0.74516	-5.38126	3.22143
H	1.24305	-2.98046	3.74075
H	2.22421	-1.52616	2.02268
H	-0.32756	3.35763	1.57238
H	-0.58482	5.77129	2.01614
H	-0.74429	6.60612	4.3694
H	-0.63636	4.99158	6.26713
H	-0.37781	2.56529	5.82737
H	-3.01281	1.97271	3.76494
H	-5.25713	0.93203	3.60084
H	-5.49017	-1.42927	2.82931
H	-3.45001	-2.74934	2.24019
H	-1.21097	-1.73943	2.47544
H	-0.90296	-0.86413	5.59728
H	0.46893	-2.21708	7.1574
H	2.95612	-2.21507	6.96243
H	4.06266	-0.82865	5.20773
H	2.69594	0.5402	3.65794
H	-4.50407	-5.49845	-0.40791
H	-4.04226	-5.50781	-2.1201
H	-5.34995	-4.44002	-1.57023
Mo	0.77169	0.51124	-0.03127
O	0.2096	2.03045	-1.04874
O	2.44408	-0.34096	-0.45591
O	0.62599	0.85946	1.835
Si	-0.85052	2.75576	-2.12091
Si	3.01486	-1.88434	-0.81887
Si	-0.21998	0.93873	3.28021

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.834502

5$_{155°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.84864	4.69458	-1.7504
C	0.12698	5.29802	-0.93433
C	0.09077	6.67044	-0.66433
C	-0.9225	7.46516	-1.21128
C	-1.90111	6.88228	-2.02472
C	-1.86528	5.50894	-2.28595
C	-0.2457	2.39535	-3.80319
C	0.1484	1.06751	-4.06888
C	0.58047	0.68548	-5.34145
C	0.61864	1.62734	-6.37692
C	0.2287	2.94811	-6.13335
C	-0.19587	3.32815	-4.85457
C	-2.50003	2.08127	-1.73882
C	-3.37372	1.76692	-2.79751
C	-4.61951	1.17716	-2.55427
C	-5.00564	0.88055	-1.24337
C	-4.15131	1.1872	-0.17817
C	-2.91472	1.78836	-0.42484
C	-0.21495	-0.59628	-0.40493
C	-1.11242	-1.68306	-0.6877
C	-2.21098	-1.51799	-1.5585
C	-3.06525	-2.58509	-1.82817
C	-2.86244	-3.85163	-1.25377
C	-1.76505	-4.01256	-0.38926
C	-0.90487	-2.95502	-0.10696
C	-3.77348	-5.00822	-1.57831
C	2.83696	-2.11481	-2.5521
C	3.69297	-1.86742	-3.64346
C	3.3159	-2.2036	-4.94782
C	2.06999	-2.79394	-5.18622
C	1.20352	-3.0444	-4.11622
C	1.58688	-2.71088	-2.81382
C	5.17549	-1.35267	-0.67541
C	5.72059	-0.13042	-0.24056
C	7.10448	0.03608	-0.11634
C	7.96735	-1.01991	-0.42671
C	7.44269	-2.24307	-0.86116
C	6.0597	-2.40535	-0.9829
C	2.66728	-2.80002	0.4767
C	2.48511	-4.16843	0.20376
C	1.96384	-5.03368	1.17292
C	1.6143	-4.54361	2.43631
C	1.8015	-3.18815	2.73346
C	2.3262	-2.33137	1.76174
C	-0.41837	2.79501	3.65117
C	-0.50335	3.7195	2.59014
C	-0.76905	5.07089	2.83112
C	-0.95181	5.52264	4.14316
C	-0.86588	4.62051	5.20961
C	-0.60005	3.26891	4.96352
C	-1.79008	0.09613	3.09849
C	-3.00662	0.71964	3.43506
C	-4.22107	0.0329	3.32435
C	-4.24005	-1.28332	2.85027
C	-3.04129	-1.91555	2.50223
C	-1.82946	-1.23454	2.64025
C	0.92851	0.07402	4.53151
C	0.36767	-0.75003	5.52537
C	1.1807	-1.45785	6.41798
C	2.57274	-1.35822	6.32508
C	3.14861	-0.54442	5.34229
C	2.33268	0.16561	4.45746
H	0.91629	4.681	-0.49702
H	0.85389	7.1199	-0.02317
H	-0.95263	8.53759	-1.00095
H	-2.69815	7.49852	-2.44931
H	-2.65065	5.06654	-2.90713
H	0.12717	0.31631	-3.27252

H	0.89419	-0.34555	-5.5181
H	0.95718	1.33102	-7.37346
H	0.26164	3.68662	-6.93899
H	-0.48599	4.36754	-4.674
H	-3.07032	1.96624	-3.82949
H	-5.28235	0.93665	-3.38984
H	-5.96988	0.40299	-1.05014
H	-4.43777	0.94221	0.8458
H	-2.26105	2.01174	0.4226
H	-2.39408	-0.54578	-2.0126
H	-3.91555	-2.42644	-2.49761
H	-1.58049	-4.98562	0.075
H	-0.06245	-3.10483	0.56628
H	4.67129	-1.40897	-3.47347
H	3.99541	-2.00375	-5.78054
H	1.77364	-3.05635	-6.2054
H	0.2258	-3.49998	-4.29378
H	0.89866	-2.91981	-1.99384
H	5.04907	0.69782	0.00077
H	7.51066	0.99326	0.22199
H	9.04888	-0.89113	-0.33126
H	8.11387	-3.0709	-1.10545
H	5.66734	-3.36834	-1.32566
H	2.72951	-4.56491	-0.78588
H	1.81899	-6.09135	0.93714
H	1.19613	-5.21702	3.18912
H	1.53666	-2.79075	3.71653
H	2.45244	-1.27656	2.01463
H	-0.35578	3.38585	1.55932
H	-0.82871	5.76796	1.99107
H	-1.15846	6.57895	4.33526
H	-1.00276	4.97186	6.23594
H	-0.52925	2.57631	5.80836
H	-3.00749	1.75455	3.7887
H	-5.1556	0.53075	3.5966
H	-5.18967	-1.8154	2.74843
H	-3.0468	-2.93667	2.11366
H	-0.90069	-1.74598	2.37807
H	-0.71891	-0.85548	5.59456
H	0.72698	-2.09587	7.18109
H	3.20978	-1.91793	7.01501
H	4.23624	-0.46959	5.26166
H	2.79421	0.7869	3.68465
H	-3.8167	-5.73424	-0.75201
H	-3.41508	-5.55103	-2.47095
H	-4.79776	-4.668	-1.7952
Mo	0.9268	0.67773	-0.03003
O	0.311	2.22206	-0.98709
O	2.64671	-0.07897	-0.44336
O	0.73852	0.95736	1.84292
Si	-0.8114	2.84163	-2.06723
Si	3.31385	-1.58184	-0.81034
Si	-0.13833	0.97479	3.27161

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.834718

$5_{160°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.76938	4.50069	-1.72629
C	0.24135	4.96539	-0.86385
C	0.29941	6.31034	-0.48269
C	-0.65444	7.2153	-0.96167
C	-1.66829	6.7703	-1.81781
C	-1.72601	5.42384	-2.19117
C	-0.20896	2.34062	-3.9422
C	0.22197	1.0363	-4.26032
C	0.68222	0.72406	-5.54262
C	0.71669	1.71352	-6.53237
C	0.29424	3.01334	-6.2345
C	-0.16183	3.32298	-4.9481
C	-2.61099	2.03778	-2.02859
C	-3.36328	1.57692	-3.12483
C	-4.64411	1.03994	-2.94586
C	-5.18994	0.95022	-1.66166
C	-4.45532	1.4014	-0.55861
C	-3.1808	1.94204	-0.74225
C	-0.42756	-0.80413	-0.20111
C	-1.41844	-1.8295	-0.37771
C	-2.55746	-1.60405	-1.18002
C	-3.52187	-2.59846	-1.33093
C	-3.38917	-3.84964	-0.70464
C	-2.24719	-4.07204	0.08587
C	-1.27784	-3.0869	0.25157
C	-4.42141	-4.93198	-0.89534
C	2.40759	-2.39303	-2.5342
C	3.22712	-2.23024	-3.66816
C	2.75115	-2.52262	-4.95086
C	1.44005	-2.97931	-5.12431
C	0.60938	-3.14608	-4.01043
C	1.09251	-2.86142	-2.72999
C	4.88288	-1.78247	-0.78157
C	5.52223	-0.58067	-0.4252
C	6.91833	-0.49327	-0.3852
C	7.69904	-1.60926	-0.7031
C	7.07998	-2.81321	-1.06024
C	5.68522	-2.89633	-1.09767
C	2.35956	-3.094	0.49118
C	2.0787	-4.44411	0.21093
C	1.57744	-5.29723	1.20124
C	1.34296	-4.81189	2.49251
C	1.62427	-3.47377	2.79502
C	2.1322	-2.63067	1.8028
C	-0.33684	2.83058	3.73969
C	-0.44756	3.80139	2.72354
C	-0.56921	5.15894	3.03447
C	-0.57814	5.57003	4.37249
C	-0.46439	4.62081	5.39435
C	-0.34477	3.26287	5.07823
C	-1.96766	0.30578	3.06762
C	-3.11272	1.12079	3.16069
C	-4.3938	0.58302	2.99818
C	-4.55069	-0.77931	2.72029
C	-3.42498	-1.60348	2.61925
C	-2.14879	-1.06537	2.80312
C	0.75789	-0.02724	4.47664
C	0.14474	-0.81227	5.47106
C	0.90782	-1.60167	6.33917
C	2.30145	-1.62293	6.22217
C	2.9293	-0.84922	5.23876
C	2.1633	-0.05864	4.37793
H	0.98434	4.26176	-0.47911
H	1.08851	6.65168	0.19254
H	-0.61083	8.26646	-0.66438
H	-2.41957	7.47287	-2.18832
H	-2.53731	5.08727	-2.84462
H	0.20573	0.24951	-3.49928
H	1.0179	-0.29186	-5.76164
H	1.07722	1.47131	-7.53579
H	0.32489	3.78933	-7.00417

H	-0.4795	4.34632	-4.72577
H	-2.93879	1.62372	-4.13188
H	-5.21184	0.68292	-3.80934
H	-6.1844	0.5198	-1.51699
H	-4.86491	1.3126	0.44903
H	-2.61641	2.27167	0.13563
H	-2.68384	-0.64073	-1.67174
H	-4.40201	-2.39255	-1.94674
H	-2.11709	-5.03551	0.58735
H	-0.40632	-3.278	0.87577
H	4.25341	-1.87106	-3.55008
H	3.40376	-2.38963	-5.8178
H	1.06557	-3.20402	-6.1266
H	-0.41723	-3.49996	-4.13666
H	0.43138	-3.00543	-1.87417
H	4.91491	0.29437	-0.17887
H	7.39828	0.449	-0.107
H	8.78994	-1.54236	-0.67345
H	7.68673	-3.68791	-1.30973
H	5.21798	-3.84533	-1.38016
H	2.23237	-4.83497	-0.79902
H	1.35719	-6.34068	0.96055
H	0.93957	-5.47475	3.26259
H	1.44621	-3.07926	3.79849
H	2.33816	-1.5899	2.06204
H	-0.43303	3.49625	1.67321
H	-0.65227	5.89289	2.22865
H	-0.67074	6.63123	4.61896
H	-0.46541	4.93994	6.44015
H	-0.25126	2.53168	5.8874
H	-3.00358	2.18926	3.36646
H	-5.27123	1.22996	3.08219
H	-5.5505	-1.19845	2.5791
H	-3.53671	-2.66398	2.38211
H	-1.2805	-1.72457	2.72681
H	-0.94523	-0.82002	5.5617
H	0.413	-2.20756	7.10288
H	2.8988	-2.24567	6.89328
H	4.01765	-0.86893	5.1385
H	2.66391	0.53175	3.60524
H	-4.52135	-5.55811	0.0049
H	-4.13886	-5.60247	-1.7263
H	-5.40972	-4.51202	-1.1367
Mo	0.75596	0.4691	-0.00594
O	0.12135	1.86117	-1.14255
O	2.44489	-0.36213	-0.42463
O	0.61169	0.99972	1.81953
Si	-0.85402	2.68785	-2.21324
Si	3.00672	-1.90077	-0.81813
Si	-0.23839	1.01353	3.26786

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.833552

5_{165^a}

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.23111	4.59064	-1.32814
C	1.03484	4.88913	-0.78924
C	1.35147	6.1849	-0.37116
C	0.40309	7.20857	-0.48675
C	-0.86111	6.9295	-1.017
C	-1.17432	5.62974	-1.42976
C	-0.17008	2.52741	-3.67636
C	0.22067	1.2364	-4.08358
C	0.54295	0.97108	-5.41815
C	0.47662	1.99489	-6.36999
C	0.08969	3.2829	-5.98384
C	-0.22765	3.54511	-4.64682
C	-2.44962	2.44057	-1.5836
C	-3.29642	1.98767	-2.61237
C	-4.61026	1.58666	-2.34148
C	-5.09877	1.63117	-1.0318
C	-4.27457	2.08982	0.00304
C	-2.96466	2.49164	-0.27142
C	-0.34714	-0.83115	-0.06877
C	-1.43506	-1.74018	-0.29249
C	-2.57985	-1.31638	-1.00246
C	-3.63243	-2.19875	-1.23124
C	-3.58696	-3.52577	-0.76881
C	-2.44162	-3.94148	-0.06861
C	-1.38348	-3.07037	0.17521
C	-4.74659	-4.46627	-0.97829
C	2.26651	-2.39275	-2.74021
C	3.07863	-2.27287	-3.88433
C	2.54707	-2.43944	-5.16794
C	1.18731	-2.72482	-5.33079
C	0.3619	-2.84165	-4.20631
C	0.89906	-2.6822	-2.92588
C	4.8352	-2.11694	-1.03387
C	5.5731	-0.97526	-0.67034
C	6.97244	-0.99108	-0.6777
C	7.65762	-2.1518	-1.05082
C	6.93975	-3.29738	-1.41499
C	5.54224	-3.27773	-1.40432
C	2.26864	-3.37476	0.19505
C	1.86565	-4.65594	-0.22543
C	1.34461	-5.58457	0.68295
C	1.21306	-5.24499	2.03338
C	1.61492	-3.97805	2.47316
C	2.14013	-3.05745	1.56255
C	-1.06844	2.52421	3.08831
C	-0.45292	3.56928	2.37092
C	-1.09501	4.79703	2.1853
C	-2.37107	5.00402	2.71948
C	-2.99765	3.98279	3.44227
C	-2.35065	2.75561	3.62382
C	-1.4462	-0.53936	3.17954
C	-2.64752	-0.41796	2.45425
C	-3.56221	-1.47103	2.38847
C	-3.28615	-2.67635	3.04026
C	-2.09544	-2.82222	3.76011
C	-1.18851	-1.76096	3.8317
C	0.84775	0.70822	4.80204
C	0.3658	1.1382	6.05274
C	1.12258	0.96195	7.21514
C	2.37955	0.34979	7.14521
C	2.87657	-0.08044	5.9103
C	2.1164	0.10006	4.74958
H	1.77638	4.09228	-0.68265
H	2.33705	6.39748	0.05144
H	0.64783	8.22181	-0.15729
H	-1.60723	7.72418	-1.10067
H	-2.17396	5.42127	-1.82312
H	0.28031	0.42431	-3.35274
H	0.84924	-0.03624	-5.70791
H	0.73058	1.78917	-7.41341
H	0.04127	4.08585	-6.72441
H	-0.518	4.55952	-4.35566
H	-2.92128	1.93139	-3.63822
H	-5.25077	1.23158	-3.15326

H	-6.12139	1.31009	-0.81658
H	-4.65028	2.13307	1.02867
H	-2.33648	2.83986	0.55203
H	-2.63742	-0.28895	-1.36164
H	-4.51155	-1.84575	-1.77811
H	-2.38124	-4.96805	0.30426
H	-0.51241	-3.4077	0.73414
H	4.14348	-2.04911	-3.77369
H	3.19519	-2.34369	-6.04313
H	0.76989	-2.85311	-6.3331
H	-0.70281	-3.05921	-4.32495
H	0.24029	-2.78571	-2.06199
H	5.04084	-0.06619	-0.3779
H	7.52969	-0.09473	-0.39193
H	8.75085	-2.1656	-1.05745
H	7.47152	-4.20737	-1.70586
H	4.99743	-4.18381	-1.68896
H	1.93886	-4.93022	-1.28168
H	1.02895	-6.57108	0.33324
H	0.794	-5.96393	2.74224
H	1.50975	-3.7027	3.52549
H	2.44025	-2.07085	1.92578
H	0.53257	3.41383	1.92512
H	-0.60777	5.58176	1.60372
H	-2.88069	5.95852	2.56373
H	-3.99709	4.13886	3.85727
H	-2.86361	1.96111	4.17329
H	-2.86767	0.50519	1.91402
H	-4.47751	-1.35912	1.80271
H	-3.99347	-3.50727	2.97666
H	-1.8713	-3.76628	4.26389
H	-0.26557	-1.88633	4.4053
H	-0.61353	1.62246	6.12368
H	0.73327	1.30412	8.17784
H	2.97252	0.21122	8.05324
H	3.85978	-0.55512	5.85085
H	2.51465	-0.23055	3.78612
H	-4.40417	-5.4978	-1.15601
H	-5.3733	-4.15837	-1.82901
H	-5.39526	-4.49114	-0.0845
Mo	0.92323	0.35583	0.10109
O	0.28317	1.80553	-0.95236
O	2.51817	-0.56826	-0.46336
O	0.89548	0.7962	1.96511
Si	-0.63327	2.84091	-1.88296
Si	2.95513	-2.09751	-1.01168
Si	-0.19492	0.86367	3.24557

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.835148

$5_{170°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.46513	4.53526	-1.4477
C	0.72958	4.87425	-0.78414
C	0.94968	6.17277	-0.31622
C	-0.02448	7.15956	-0.5068
C	-1.21935	6.84125	-1.16128
C	-1.43716	5.53843	-1.62318
C	-0.10951	2.49302	-3.80798
C	0.31045	1.20234	-4.18831
C	0.76289	0.94726	-5.48649
C	0.80144	1.98167	-6.42852
C	0.38865	3.26923	-6.06856
C	-0.06088	3.52097	-4.76782
C	-2.56325	2.31472	-1.91923
C	-3.27412	1.71553	-2.97537
C	-4.58116	1.24875	-2.79147
C	-5.19861	1.37249	-1.54262
C	-4.51063	1.9749	-0.48222
C	-3.20805	2.44348	-0.67197
C	-0.38784	-0.82759	-0.02031
C	-1.45619	-1.76557	-0.21806
C	-2.58779	-1.39689	-0.97897
C	-3.60751	-2.3144	-1.21461
C	-3.5436	-3.62379	-0.7054
C	-2.41435	-3.98411	0.04851
C	-1.3882	-3.07622	0.29862
C	-4.67208	-4.59938	-0.9243
C	2.24655	-2.43336	-2.63335
C	3.04602	-2.31966	-3.78703
C	2.50582	-2.52005	-5.06215
C	1.14983	-2.83248	-5.20706
C	0.33825	-2.94876	-4.07257
C	0.88449	-2.75705	-2.80033
C	4.81232	-2.02916	-0.9459
C	5.52898	-0.86862	-0.59998
C	6.92837	-0.8605	-0.60105
C	7.63498	-2.01573	-0.95056
C	6.93846	-3.17956	-1.29782
C	5.54075	-3.18373	-1.29345
C	2.27083	-3.2543	0.3624
C	1.89425	-4.56781	0.02617
C	1.39934	-5.44838	0.99528
C	1.26854	-5.02719	2.32268
C	1.64468	-3.72629	2.6791
C	2.14323	-2.85365	1.70832
C	-0.82035	2.69691	3.39992
C	-0.84018	3.52143	2.2581
C	-1.40537	4.80073	2.29496
C	-1.95747	5.28199	3.48652
C	-1.93833	4.48224	4.63574
C	-1.37603	3.20242	4.59043
C	-1.58435	-0.25629	3.0834
C	-2.73989	0.13514	2.38087
C	-3.79259	-0.75753	2.16731
C	-3.71506	-2.05958	2.67081
C	-2.58026	-2.46512	3.38046
C	-1.52369	-1.57254	3.57964
C	0.95825	0.40999	4.68849
C	0.43562	0.11999	5.9642
C	1.26781	-0.30149	7.00587
C	2.64221	-0.4494	6.78681
C	3.17886	-0.17306	5.52476
C	2.34323	0.2541	4.48712
H	1.49046	4.10637	-0.61827
H	1.8793	6.41514	0.20523
H	0.1446	8.17459	-0.13787
H	-1.98639	7.60698	-1.3044
H	-2.38403	5.29809	-2.11621
H	0.29115	0.38229	-3.46402
H	1.08871	-0.06016	-5.75467
H	1.1573	1.7846	-7.44341
H	0.42224	4.08012	-6.80123
H	-0.37161	4.53494	-4.4969
H	-2.79576	1.59651	-3.95181
H	-5.11547	0.78038	-3.62235
H	-6.2155	0.99975	-1.39409
H	-4.98944	2.07527	0.4955
H	-2.68335	2.90727	0.16846

H	-2.65716	-0.38516	-1.37789
H	-4.47512	-2.00343	-1.80375
H	-2.33961	-4.99612	0.45698
H	-0.52564	-3.37198	0.89332
H	4.10657	-2.0702	-3.69097
H	3.14373	-2.42718	-5.94516
H	0.72522	-2.98382	-6.20312
H	-0.72283	-3.19026	-4.17652
H	0.23624	-2.85762	-1.92827
H	4.97994	0.03661	-0.32723
H	7.46892	0.05035	-0.32936
H	8.72831	-2.01086	-0.9524
H	7.48703	-4.08508	-1.57092
H	5.01257	-4.10334	-1.56575
H	1.96805	-4.90682	-1.01119
H	1.10384	-6.46177	0.71094
H	0.87182	-5.70995	3.07867
H	1.54676	-3.38774	3.71395
H	2.42398	-1.84089	2.00949
H	-0.40714	3.16521	1.32173
H	-1.40562	5.41657	1.3924
H	-2.3986	6.28177	3.52209
H	-2.36305	4.85799	5.57064
H	-1.37024	2.59438	5.50044
H	-2.8129	1.14781	1.97602
H	-4.66635	-0.44072	1.59285
H	-4.5321	-2.76386	2.49525
H	-2.51035	-3.4868	3.76297
H	-0.63568	-1.90929	4.12107
H	-0.63974	0.20619	6.14824
H	0.84305	-0.52203	7.98886
H	3.29347	-0.78382	7.59876
H	4.25116	-0.29206	5.34756
H	2.76843	0.46443	3.50198
H	-4.30727	-5.6369	-0.97676
H	-5.22676	-4.37986	-1.84946
H	-5.39574	-4.55178	-0.09093
Mo	0.8434	0.40829	0.05836
O	0.1117	1.76355	-1.06497
O	2.46521	-0.49176	-0.46861
O	0.82319	0.95775	1.89066
Si	-0.74341	2.78225	-2.06475
Si	2.93231	-2.04292	-0.92339
Si	-0.14668	0.94205	3.26515

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.832422

5$_{175°}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-0.46135	4.50641	-1.43929
C	0.74241	4.81329	-0.77652
C	0.99318	6.10278	-0.29934
C	0.04117	7.11278	-0.47999
C	-1.16222	6.82674	-1.13368
C	-1.41085	5.53265	-1.60464
C	-0.13798	2.47308	-3.81147
C	0.27977	1.18081	-4.18855
C	0.73757	0.9231	-5.48438
C	0.78355	1.95644	-6.42717
C	0.37298	3.24567	-6.07036
C	-0.08176	3.50007	-4.77203
C	-2.60715	2.33105	-1.93274
C	-3.31334	1.70607	-2.97686
C	-4.61893	1.23827	-2.78542
C	-5.23982	1.38738	-1.541
C	-4.55695	2.01668	-0.49293
C	-3.2556	2.48576	-0.69027
C	-0.38083	-0.86054	0.00434
C	-1.4534	-1.7921	-0.19869
C	-2.58916	-1.40316	-0.94392
C	-3.61519	-2.31119	-1.18822
C	-3.55445	-3.62962	-0.7023
C	-2.42163	-4.00948	0.03663
C	-1.38822	-3.11175	0.29433
C	-4.69028	-4.59463	-0.93001
C	2.26157	-2.42414	-2.63486
C	3.06236	-2.31683	-3.78816
C	2.52483	-2.529	-5.06253
C	1.17018	-2.84714	-5.20707
C	0.3571	-2.95682	-4.07294
C	0.90065	-2.75317	-2.80141
C	4.82314	-1.99247	-0.94646
C	5.52874	-0.82464	-0.60229
C	6.92798	-0.80363	-0.6017
C	7.64558	-1.95308	-0.94789
C	6.96017	-3.12402	-1.29338
C	5.56254	-3.14107	-1.29055
C	2.2924	-3.24041	0.36004
C	1.92852	-4.55695	0.02152
C	1.44364	-5.44463	0.98928
C	1.30917	-5.02742	2.31754
C	1.6724	-3.72346	2.67628
C	2.16231	-2.8443	1.70703
C	-0.81569	2.70598	3.41043
C	-0.85771	3.52638	2.26625
C	-1.41595	4.80834	2.31107
C	-1.93985	5.29595	3.51281
C	-1.89864	4.50013	4.66415
C	-1.34239	3.21789	4.6112
C	-1.59959	-0.23892	3.07162
C	-2.75171	0.16485	2.37015
C	-3.80996	-0.71958	2.15019
C	-3.7414	-2.02557	2.645
C	-2.60961	-2.44344	3.35207
C	-1.54758	-1.55888	3.55854
C	0.95016	0.39704	4.67848
C	0.42838	0.09933	5.95276
C	1.25987	-0.33838	6.98833
C	2.6325	-0.49512	6.76439
C	3.16824	-0.21116	5.50362
C	2.3334	0.2323	4.47221
H	1.48697	4.02766	-0.61916
H	1.92946	6.3201	0.22124
H	0.23417	8.12088	-0.10386
H	-1.91193	7.6108	-1.26908
H	-2.36405	5.31758	-2.09709
H	0.25463	0.36222	-3.46287
H	1.06187	-0.08548	-5.74999
H	1.14357	1.75737	-7.4402
H	0.41246	4.05572	-6.80368
H	-0.39036	4.51541	-4.50372
H	-2.83192	1.56626	-3.94909
H	-5.14951	0.74925	-3.60677
H	-6.25549	1.0137	-1.38645
H	-5.03843	2.13706	0.48124
H	-2.73391	2.96897	0.14125
H	-2.65712	-0.38319	-1.32306

H	-4.48574	-1.98535	-1.76486
H	-2.34972	-5.02907	0.42634
H	-0.52171	-3.42255	0.87591
H	4.12197	-2.06327	-3.69245
H	3.16384	-2.44101	-5.94524
H	0.74768	-3.00805	-6.20253
H	-0.70298	-3.20279	-4.17675
H	0.25125	-2.84916	-1.92957
H	4.97103	0.07608	-0.33217
H	7.45982	0.11273	-0.33133
H	8.73882	-1.93818	-0.94846
H	7.51739	-4.02505	-1.56382
H	5.04305	-4.06606	-1.56131
H	2.00482	-4.89317	-1.01658
H	1.15869	-6.46052	0.70309
H	0.92004	-5.71577	3.07241
H	1.5717	-3.38762	3.7118
H	2.43491	-1.83017	2.01086
H	-0.44667	3.16506	1.32201
H	-1.43209	5.42146	1.40677
H	-2.37566	6.29782	3.5547
H	-2.30091	4.88105	5.60686
H	-1.31797	2.61316	5.52309
H	-2.81752	1.18021	1.97031
H	-4.68108	-0.39334	1.57699
H	-4.56273	-2.72338	2.46377
H	-2.5463	-3.4684	3.72683
H	-0.66167	-1.90537	4.09736
H	-0.64587	0.19191	6.14016
H	0.83583	-0.56477	7.97031
H	3.28307	-0.84234	7.57151
H	4.2391	-0.33699	5.32253
H	2.75787	0.44855	3.48805
H	-4.33396	-5.63473	-0.98852
H	-5.24103	-4.36448	-1.85498
H	-5.41567	-4.54625	-0.09819
Mo	0.82656	0.399	0.05718
O	0.03054	1.70779	-1.07683
O	2.46226	-0.47423	-0.47633
O	0.81172	0.96883	1.88403
Si	-0.77843	2.76557	-2.0714
Si	2.94326	-2.02275	-0.92562
Si	-0.15364	0.94814	3.26178

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.831075

5$_{\text{constrained}}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-3.18334	0.79604	2.3393
C	-2.98951	-0.53576	2.75433
C	-4.02727	-1.17306	3.45875
C	-5.21917	-0.49868	3.74736
C	-5.39261	0.82412	3.32779
C	-4.37279	1.47127	2.62092
C	-1.62653	-3.24804	2.08744
C	-0.83677	-4.21397	2.73716
C	-0.99082	-5.57694	2.45842
C	-1.93946	-5.99665	1.52063
C	-2.73602	-5.05024	0.86375
H	2.83614	-0.21302	6.14355
H	3.38993	-0.91177	3.81124
H	1.58458	-1.44421	2.21489
C	-2.57995	-3.69086	1.14763
C	-0.0305	-1.05496	3.61583
C	-0.32479	-0.657	4.93243
C	0.69899	-0.36557	5.84031
C	2.03594	-0.45908	5.44079
C	2.34798	-0.85348	4.13552
C	1.32273	-1.15064	3.23521
C	-1.32782	3.08751	-1.17537
C	-1.62476	2.69378	-2.49695
C	-1.35589	3.6062	-3.53293
C	-0.80448	4.86346	-3.26011
C	-0.49978	5.22598	-1.94514
C	-0.76313	4.33477	-0.89878
C	-3.78847	0.62248	-1.78633
C	-4.02988	-0.64897	-1.22949
C	-5.15714	-0.88751	-0.43865
C	-6.06862	0.1439	-0.19081
C	-5.84968	1.4116	-0.73854
C	-4.71701	1.648	-1.52477
C	-2.42683	0.57365	-4.62467
C	-3.46213	1.16436	-5.37484
C	-3.58661	0.91832	-6.7455
C	-2.67672	0.07073	-7.38859
C	-1.64599	-0.52883	-6.65719
C	-1.52294	-0.2782	-5.28624
C	1.264	2.241	2.2581
C	2.58644	2.13535	1.78544
C	3.63503	2.4578	2.66634
C	3.37215	2.88279	3.97307
C	2.05196	2.97797	4.42481
C	0.99684	2.65421	3.56541
C	3.0269	2.97662	-1.1742
C	2.46327	2.87271	-2.4599
C	2.5431	3.93275	-3.36689
C	3.19207	5.11769	-3.00385
C	3.75224	5.24191	-1.72786
C	3.66504	4.18054	-0.82046
C	4.43078	0.43803	-0.02566
C	4.28372	-0.95201	0.15261
C	5.39441	-1.80139	0.1392
C	6.67692	-1.27208	-0.04422
C	6.84222	0.10591	-0.22411
C	5.72682	0.95076	-0.22101
C	0.77312	-2.07568	-1.05888
C	1.4049	-3.35819	-1.17615
C	0.79845	-4.51114	-0.62438
C	1.43598	-5.7462	-0.69846
C	2.68923	-5.88952	-1.32157
C	3.28773	-4.74152	-1.86907
C	2.66428	-3.49635	-1.80269
C	3.35193	-7.24056	-1.41801
H	-3.91047	-2.21317	3.77838
H	-6.01678	-1.00916	4.29389
H	-6.32708	1.34887	3.54377
H	-4.51159	2.49873	2.27562
H	-0.08233	-3.89842	3.46337
H	-0.36392	-6.31234	2.9694
H	-2.057	-7.06038	1.29766
H	-3.47594	-5.37325	0.12677
H	-3.20453	-2.96233	0.62303
H	-1.36715	-0.56011	5.25146
H	0.4527	-0.05113	6.85811
H	-1.56938	3.32877	-4.56944
H	-0.59515	5.55617	-4.07949
H	-0.04579	6.19764	-1.73539
H	-0.51929	4.60763	0.13134

H	-3.31537	-1.45881	-1.40311
H	-5.32123	-1.8755	-0.00068
H	-6.9407	-0.03745	0.44202
H	-6.55498	2.22289	-0.53913
H	-4.54607	2.65221	-1.92495
H	-4.1861	1.82391	-4.88537
H	-4.39578	1.3851	-7.3136
H	-2.77372	-0.12393	-8.46007
H	-0.93635	-1.19432	-7.1562
H	-0.71788	-0.75057	-4.7165
H	4.67436	2.36016	2.33678
H	4.19971	3.12552	4.64524
H	1.8452	3.29105	5.45153
H	-0.03572	2.70485	3.92017
H	1.93572	1.95956	-2.74943
H	2.08478	3.83906	-4.35425
H	3.25155	5.94897	-3.71156
H	4.2506	6.17038	-1.43608
H	4.08824	4.30058	0.18197
H	3.28688	-1.38063	0.28526
H	5.25448	-2.87864	0.26235
H	7.54715	-1.9339	-0.05414
H	7.84187	0.5219	-0.37633
H	5.87028	2.02357	-0.38476
H	0.95021	-6.62052	-0.25528
H	4.2656	-4.82344	-2.35236
H	4.431	-7.15191	-1.61453
H	2.91461	-7.83492	-2.23962
H	3.2157	-7.82264	-0.49282
C	-1.64881	-5.19231	2.47115
C	-2.52892	-5.52318	1.43565
C	-3.19398	-4.5091	0.73501
C	-2.97254	-3.17002	1.06854
C	-0.43984	-0.73766	3.76814
C	-0.88503	-0.34855	5.04491
C	0.02191	-0.15024	6.09169
C	1.39146	-0.33408	5.87407
C	1.85201	-0.71589	4.60971
C	0.94364	-0.91488	3.56743
C	-2.46501	2.99099	-3.99443
C	-1.65631	1.86666	-4.24811
C	-0.56106	2.01894	-5.122
C	-0.28344	3.25087	-5.72203
C	-1.10001	4.35684	-5.45748
C	-2.19057	4.2261	-4.59128
C	-3.72388	0.13717	-2.69921
C	-3.93263	0.04699	-1.31011
C	-5.22296	-0.03067	-0.77468
C	-6.3319	-0.02062	-1.62674
C	-6.14562	0.06929	-3.0117
C	-4.85343	0.14664	-3.54047
C	-1.61351	-1.2102	-4.56857
C	-1.88889	-1.16057	-5.9482
C	-1.61982	-2.25624	-6.77584
C	-1.06178	-3.42077	-6.23634
C	-0.77552	-3.48651	-4.86796
C	-1.05164	-2.39164	-4.04363
C	1.61234	2.51842	2.5243
C	2.87192	2.34361	1.91653
C	4.01884	2.4379	2.72562
C	3.91276	2.70873	4.09525
C	2.65347	2.87824	4.67899
C	1.50117	2.78025	3.89126
C	2.77023	3.52571	-0.9544
C	1.92974	3.54476	-2.08399
C	1.77992	4.70478	-2.85103
Mo	0.09099	-0.50037	-0.71484
O	-0.84164	-0.7292	0.91525
O	-1.06865	-0.10942	-2.19011
O	1.58228	0.63457	-0.40602
Si	-1.37554	-1.40348	2.35268
Si	-2.22769	0.93154	-2.79447
Si	2.90725	1.53895	0.02962
H	-0.16772	-4.42074	-0.12727
H	3.15387	-2.61362	-2.21894
H	-1.5331	2.40559	-0.34332
H	-2.39859	1.30166	1.77022
H	0.43153	1.97166	1.60325

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.820722

5$_{178^o}$

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)

C	-3.09252	1.41181	1.96297
C	-3.14195	0.08845	2.44199
C	-4.34518	-0.36956	3.01115
C	-5.46084	0.47001	3.10827
C	-5.3917	1.78188	2.62788
C	-4.20554	2.2519	2.05228
C	-2.08246	-2.81732	2.10424
C	-1.42859	-3.8499	2.80062
C	2.47655	5.86735	-2.5032
C	3.3168	5.86799	-1.38414
C	3.4561	4.70805	-0.61499
C	4.53421	1.02391	-0.34625
C	4.50278	-0.38534	-0.34443
C	5.64806	-1.13102	-0.64038
C	6.84974	-0.47824	-0.9385
C	6.89899	0.92022	-0.94661
C	5.74857	1.66291	-0.65801
C	0.94423	-1.73951	-0.93952
C	1.36789	-3.09757	-1.11026
C	0.56383	-4.14766	-0.60267
C	0.9534	-5.4733	-0.76718
C	2.1441	-5.81014	-1.43831
C	2.9405	-4.76398	-1.93472
C	2.56744	-3.42934	-1.77737
C	2.53336	-7.25389	-1.633
H	-4.41763	-1.39886	3.37516
H	-6.38799	0.09695	3.55131
H	-6.26446	2.43661	2.6952
H	-4.15127	3.27345	1.66722
H	-0.72419	-3.60357	3.60056
H	-1.12685	-5.98147	3.01887
H	-2.69646	-6.57096	1.1723
H	-3.88103	-4.76288	-0.07654
H	-3.49013	-2.38957	0.50172
H	-1.95268	-0.18857	5.22527
H	-0.33995	0.15595	7.07698
H	2.10244	-0.16712	6.68745
H	2.92308	-0.83831	4.43051
H	1.31668	-1.19237	2.57734
H	0.0817	1.16143	-5.34283
H	0.57135	3.34983	-6.39622
H	-0.88494	5.32077	-5.92632
H	-2.83015	5.08783	-4.38257
H	-3.07938	0.03923	-0.62977
H	-5.35501	-0.09123	0.30795

H	-7.34207	-0.08084	-1.2128
H	-7.01026	0.07744	-3.68096
H	-4.72816	0.21168	-4.62617
H	-2.30924	-0.25111	-6.3888
H	-1.83959	-2.19959	-7.84547
H	-0.84598	-4.27501	-6.88383
H	-0.33107	-4.38927	-4.43994
H	-0.81422	-2.45246	-2.97898
H	5.00932	2.28627	2.2855
H	4.81486	2.77678	4.70943
H	2.56761	3.07323	5.75116
H	0.51425	2.88749	4.3482
H	1.37576	2.64547	-2.3688
H	1.11392	4.69677	-3.71673
H	2.35991	6.7753	-3.10111
H	3.85685	6.77674	-1.10473
H	4.09831	4.7324	0.27145
H	3.5669	-0.9049	-0.12146
H	5.60009	-2.22352	-0.6407
H	7.74697	-1.05899	-1.16902
H	7.83451	1.43328	-1.18552
H	5.79883	2.75593	-0.68741
H	0.31803	-6.26663	-0.36253
H	3.87327	-4.99994	-2.45498
H	3.59024	-7.35602	-1.92107
H	1.92582	-7.72105	-2.42788
H	2.36738	-7.84176	-0.71609
Mo	0.20313	-0.19216	-0.60764
O	-0.77729	-0.59694	0.96044
O	-0.96131	0.05726	-2.0908
O	1.66145	0.98279	-0.25702
Si	-1.6216	-1.00808	2.33543
Si	-1.97795	0.21855	-3.39993
Si	2.96018	1.96312	0.07471
H	-0.36205	-3.90772	-0.07518
H	3.20168	-2.63018	-2.16723
H	-3.32492	2.89985	-3.3243
H	-2.1738	1.78622	1.50178
H	0.70271	2.42884	1.9234

B3LYP-D3/def2TZVP-SDD(Mo)-CPCM(benzene)//B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
HF = -3557.814798

[Mo]L$_3$-A

B3LYP/LANL2DZ
Zero-point correction= 0.855096 (Hartree/Particle)
Thermal correction to Energy= 0.912957
Thermal correction to Enthalpy= 0.913901
Thermal correction to Gibbs Free Energy= 0.744990
Sum of electronic and zero-point Energies= -2427.480289
Sum of electronic and thermal Energies= -2427.422428
Sum of electronic and thermal Enthalpies= -2427.421484
Sum of electronic and thermal Free Energies= -2427.590395

C	48.09321	10.24019	-56.77211
C	49.07297	10.88279	-55.9753
C	48.89136	12.20519	-55.52927
C	47.72446	12.91378	-55.87833
C	46.73917	12.28968	-56.66688
C	46.92348	10.96445	-57.10739
C	49.40686	8.48637	-59.0011
C	50.28326	7.41547	-59.30335
C	51.01906	7.39703	-60.50335
C	50.88841	8.45174	-61.42749
C	50.02321	9.52571	-61.1422
C	49.29147	9.54089	-59.9393
C	46.75174	7.57751	-57.64672
C	46.44943	6.90139	-58.8537
C	45.23205	6.21136	-59.01567
C	44.29386	6.18103	-57.9665
C	44.5785	6.84442	-56.75638
C	45.79417	7.53504	-56.60149
C	48.25285	5.2769	-55.03283
C	51.34254	3.22694	-57.58851
C	52.32919	2.82896	-58.52258
C	51.98578	2.51271	-59.85198
C	50.6449	2.59455	-60.27267
C	49.65003	2.99398	-59.3582
C	49.99693	3.30298	-58.03028
C	53.6548	3.81135	-55.57151
C	54.2833	5.07623	-55.67193
C	55.67822	5.2046	-55.53236
C	56.47152	4.0656	-55.29239
C	55.86219	2.80022	-55.18657
C	54.46613	2.67712	-55.32409
C	51.06578	2.37858	-54.60067
C	50.45598	1.18173	-55.04623
C	49.93595	0.24635	-54.12936
C	50.01541	0.49559	-52.74639
C	50.61806	1.68319	-52.28425
C	51.13964	2.61135	-53.20343
C	49.05782	8.71354	-51.01986
C	48.78908	9.71587	-51.98321
C	48.63477	11.06308	-51.60438
C	48.74518	11.43183	-50.24995
C	49.01776	10.44841	-49.27905
C	49.17276	9.10271	-49.66304
C	47.55909	6.00791	-51.38554
C	46.36476	6.70873	-51.08914
C	45.12936	6.03753	-51.00536
C	45.06646	4.64789	-51.2227
C	46.24364	3.93432	-51.5234
C	47.47578	4.60871	-51.6028
C	50.54691	5.99434	-50.54761
C	50.24086	5.30391	-49.34968
C	51.24907	4.66128	-48.60464
C	52.5845	4.69481	-49.05
C	52.90571	5.3732	-50.24256
C	51.89588	6.01906	-50.97998
H	49.97653	10.34356	-55.69798
H	49.65773	12.68065	-54.92077
H	47.58425	13.93785	-55.53861
H	45.83303	12.82842	-56.93526
H	46.14512	10.49275	-57.70475
H	50.4063	6.59633	-58.59828
H	51.68774	6.56504	-60.71152
H	51.45741	8.44013	-62.35479
H	49.9227	10.34794	-61.8474
H	48.64103	10.38788	-59.72808
H	47.16376	6.91584	-59.67434
H	45.01784	5.704	-59.95389
H	43.35284	5.64895	-58.08967
H	43.86054	6.82321	-55.93967
H	45.994	8.04342	-55.65978
H	53.37197	2.7731	-58.21729

H	52.76007	2.20826	-60.55283
H	50.37844	2.35353	-61.29958
H	48.61243	3.06593	-59.67612
H	49.2148	3.61337	-57.33949
H	53.67567	5.96134	-55.84693
H	56.14183	6.18561	-55.60975
H	57.54979	4.16309	-55.18481
H	56.46768	1.91724	-54.99392
H	54.01	1.69354	-55.2218
H	50.38226	0.97504	-56.11196
H	49.47258	-0.66807	-54.49355
H	49.61549	-0.22586	-52.0368
H	50.68726	1.88459	-51.21763
H	51.60368	3.51997	-52.82408
H	48.7148	9.44904	-53.03503
H	48.42808	11.81396	-52.36332
H	48.62624	12.4722	-49.95455
H	49.11334	10.72724	-48.2319
H	49.399	8.35952	-48.9001
H	46.39673	7.78282	-50.91796
H	44.22503	6.59495	-50.77098
H	44.11337	4.127	-51.1577
H	46.20344	2.86105	-51.69548
H	48.37323	4.039	-51.83687
H	49.21113	5.25293	-48.99977
H	50.99314	4.13692	-47.68642
H	53.36434	4.19694	-48.4777
H	53.93395	5.39862	-50.59603
H	52.15492	6.53719	-51.90097
Mo	49.6676	6.30533	-54.9631
O	49.34267	7.69904	-56.21833
O	51.14526	5.19392	-55.42197
O	49.74922	6.91681	-53.16432
Si	48.39229	8.48641	-57.40728
Si	51.78846	3.64922	-55.79941
Si	49.21717	6.90338	-51.53481
H	47.35598	4.65728	-55.05046

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3287.30568

[Mo]L$_3$-TS-A

B3LYP/LANL2DZ
Imaginary frequency = -194.49 cm^{-1}
Zero-point correction= 0.884385 (Hartree/Particle)
Thermal correction to Energy= 0.944370
Thermal correction to Enthalpy= 0.945315
Thermal correction to Gibbs Free Energy= 0.775746
Sum of electronic and zero-point Energies= -2504.748744
Sum of electronic and thermal Energies= -2504.688759
Sum of electronic and thermal Enthalpies= -2504.687815
Sum of electronic and thermal Free Energies= -2504.857384

O	-0.60872	-0.2708	-0.99358
O	1.89371	0.45169	-0.01287
O	-1.42101	0.28982	1.58971
Si	-1.21918	-0.53184	-2.56021
Si	3.56726	0.61386	-0.24201
Si	-2.45172	-0.13122	2.86051
Mo	0.05398	0.80541	0.44262
C	4.48106	0.19874	1.3691
C	5.08166	-1.07094	1.55375
C	4.54586	1.1235	2.44233
C	5.72411	-1.40593	2.76169
H	5.05392	-1.80294	0.7494
C	5.18561	0.79496	3.65161
H	4.09657	2.10893	2.33575
C	5.77749	-0.47325	3.81471
H	6.1793	-2.38707	2.87815
H	5.22295	1.52242	4.45966
H	6.27408	-0.72946	4.74824
C	3.96446	2.38324	-0.78543
C	3.07599	3.06516	-1.65528
C	5.156	3.04414	-0.39864
C	3.36585	4.36272	-2.11622
H	2.15699	2.58175	-1.97816
C	5.45138	4.34195	-0.86
H	5.86072	2.54904	0.26665
C	4.5552	5.00551	-1.7195
H	2.67061	4.86432	-2.78595
H	6.37386	4.82941	-0.55158
H	4.78181	6.00759	-2.0778
C	4.02607	-0.63857	-1.58188
C	3.11035	-1.64992	-1.95823
C	5.28834	-0.6038	-2.2235
C	3.44184	-2.59818	-2.94598
H	2.13372	-1.68934	-1.48265
C	5.62637	-1.55132	-3.20841
H	6.01141	0.16885	-1.96525
C	4.70239	-2.55159	-3.57172
H	2.71756	-3.36063	-3.22267
H	6.60055	-1.50724	-3.69095
H	4.96121	-3.28218	-4.33534
C	-1.51317	-0.09407	4.50995
C	-1.62518	0.99242	5.4106
C	-0.6224	-1.14544	4.84526
C	-0.87623	1.03064	6.603
H	-2.30215	1.81387	5.18435
C	0.13349	-1.11075	6.03172
H	-0.52455	-2.00304	4.18125
C	0.00787	-0.0198	6.91506
H	-0.98177	1.8741	7.28195
H	0.81019	-1.92905	6.26785
H	0.58826	0.00843	7.83487
C	-3.85786	1.13707	2.88695
C	-4.99786	0.97516	3.71135
C	-3.78395	2.29003	2.06829
C	-6.03037	1.93206	3.71994
H	-5.09194	0.0964	4.34764
C	-4.81506	3.2496	2.07154
H	-2.9175	2.43022	1.42565
C	-5.94093	3.07353	2.89867
H	-6.89871	1.78714	4.35904
H	-4.74078	4.12667	1.43192
H	-6.73902	3.81295	2.9021
C	-3.0566	-1.89396	2.53942
C	-3.60658	-2.68995	3.57386
C	-2.99487	-2.43985	1.23437
C	-4.08787	-3.98705	3.31283
H	-3.64762	-2.30867	4.5934
C	-3.4712	-3.73772	0.96959
H	-2.56789	-1.84951	0.42794
C	-4.02299	-4.51297	2.00768
H	-4.50616	-4.58316	4.12116
H	-3.41652	-4.13618	-0.04111
H	-4.39441	-5.51512	1.80365

C	-0.51413	0.7403	-3.77408
C	0.83979	0.67183	-4.19059
C	-1.30673	1.80938	-4.25942
C	1.38168	1.63534	-5.06097
H	1.47799	-0.13537	-3.83766
C	-0.7699	2.77492	-5.13338
H	-2.35014	1.88625	-3.96099
C	0.57677	2.68998	-5.53579
H	2.42371	1.5634	-5.36362
H	-1.39888	3.58425	-5.49819
H	0.99362	3.43331	-6.2124
C	-3.10375	-0.36195	-2.48476
C	-3.91523	-0.8327	-3.54674
C	-3.73917	0.26542	-1.38677
C	-5.31372	-0.6776	-3.51554
H	-3.46138	-1.33296	-4.40111
C	-5.13849	0.42168	-1.3496
H	-3.14456	0.62099	-0.5499
C	-5.9289	-0.04733	-2.41558
H	-5.91856	-1.04915	-4.34004
H	-5.60261	0.89927	-0.48986
H	-7.01027	0.06932	-2.38765
C	-0.70166	-2.27942	-3.06552
C	-0.47946	-3.27065	-2.07859
C	-0.57726	-2.65148	-4.42588
C	-0.14616	-4.59009	-2.43772
H	-0.55549	-3.00458	-1.02637
C	-0.2483	-3.97143	-4.79117
H	-0.72181	-1.9082	-5.20834
C	-0.03387	-4.94527	-3.79682
H	0.02353	-5.33515	-1.66343
H	-0.15657	-4.23564	-5.84247
H	0.21967	-5.96577	-4.0763
C	-0.20862	2.521	0.04895
H	-0.35087	3.55924	-0.24754
C	0.77323	2.47781	2.09189
H	0.74078	3.54966	2.11106
C	1.00782	1.30669	2.4904
H	1.36058	0.56396	3.18059

B3LYP-D3/defTZVP-SDD(Mo)-
CPCM(benzene)//B3LYP/LANL2DZ
HF = -3364.67008

[Mo]L$_3$-MCBD-A

B3LYP/LANL2DZ
Zero-point correction= 0.887142
(Hartree/Particle)
Thermal correction to Energy= 0.946733
Thermal correction to Enthalpy= 0.947677
Thermal correction to Gibbs Free Energy=
0.777577
Sum of electronic and zero-point Energies= -
2504.764443
Sum of electronic and thermal Energies= -
2504.704852
Sum of electronic and thermal Enthalpies= -
2504.703908
Sum of electronic and thermal Free Energies= -
2504.874008

O	-0.77945	-1.05403	-1.63139
O	1.63615	0.01306	-1.21202
O	-1.85398	0.01504	0.56849
C	0.51587	1.47251	0.90857
C	0.76857	-0.98424	1.35782
C	0.94967	0.48178	1.76322
Si	-1.52665	-1.18484	-3.17163
Si	3.32369	0.09744	-1.31748
Si	-2.95922	-0.15404	1.84184
Mo	-0.01802	-0.19452	-0.14251
H	1.11614	-1.80905	1.96537
H	1.40188	0.64375	2.73725
H	0.5499	2.54544	1.02058
C	4.13368	-0.72641	0.19289
C	4.41154	-2.11617	0.18772
C	4.42943	0.00165	1.37236
C	4.96299	-2.75545	1.31455
H	4.20937	-2.70268	-0.70657
C	4.98446	-0.62987	2.50165
H	4.23407	1.07193	1.40872
C	5.25141	-2.01279	2.47619
H	5.17219	-3.8226	1.28362
H	5.21149	-0.0472	3.39217
H	5.68379	-2.50313	3.34595
C	3.82275	1.92352	-1.39255
C	2.87093	2.90377	-1.7659
C	5.14825	2.34919	-1.1305
C	3.22896	4.26083	-1.87498
H	1.84495	2.6016	-1.96465
C	5.51303	3.70487	-1.2412
H	5.90241	1.62451	-0.82694
C	4.55308	4.665	-1.61523
H	2.48054	4.9967	-2.16164
H	6.53713	4.00907	-1.03546
H	4.83244	5.71305	-1.70052
C	3.84173	-0.82852	-2.88449
C	2.99259	-1.81589	-3.43879
C	5.08659	-0.58655	-3.51549
C	3.37233	-2.54153	-4.58447
H	2.02496	-2.00911	-2.98261
C	5.47288	-1.31082	-4.65897
H	5.7569	0.17866	-3.12761
C	4.61586	-2.29241	-5.19515
H	2.6965	-3.2875	-4.99504
H	6.43206	-1.10745	-5.13064
H	4.91184	-2.8501	-6.0814
C	-2.13794	0.31333	3.49313
C	-2.181	1.64343	3.9792
C	-1.40766	-0.64168	4.24441
C	-1.51955	2.00911	5.16715
H	-2.74326	2.39875	3.43343
C	-0.74296	-0.28332	5.43284
H	-1.36864	-1.67631	3.90871
C	-0.79533	1.0458	5.89681
H	-1.5728	3.03574	5.52333
H	-0.1951	-1.03619	5.99584
H	-0.28703	1.32488	6.81748
C	-4.3767	1.05467	1.49476
C	-5.65189	0.90361	2.09162
C	-4.16907	2.16495	0.64085
C	-6.68402	1.83011	1.84777
H	-5.8529	0.05245	2.73971
C	-5.19752	3.09381	0.39087
H	-3.20137	2.29098	0.15928
C	-6.45824	2.93001	0.99687
H	-7.65699	1.69274	2.31477
H	-5.01724	3.93588	-0.27387
H	-7.25505	3.64561	0.80527
C	-3.54274	-1.9512	1.94345
C	-4.1843	-2.45684	3.10154
C	-3.3718	-2.82266	0.84084
C	-4.64504	-3.78605	3.15554

H	-4.31471	-1.8195	3.97524
C	-3.8278	-4.15339	0.89133
H	-2.88229	-2.45778	-0.05817
C	-4.46811	-4.63819	2.04797
H	-5.1348	-4.15419	4.05464
H	-3.69048	-4.80368	0.03025
H	-4.82332	-5.66592	2.08712
C	-1.15317	0.36349	-4.18798
C	0.13766	0.94996	-4.16979
C	-2.14374	0.94539	-5.01662
C	0.42644	2.08206	-4.95423
H	0.91143	0.53282	-3.5303
C	-1.85544	2.07534	-5.80671
H	-3.14774	0.52609	-5.03852
C	-0.56832	2.64519	-5.7777
H	1.42317	2.51664	-4.92549
H	-2.63047	2.50805	-6.43567
H	-0.34371	3.51821	-6.3871
C	-3.3907	-1.3821	-2.94076
C	-4.12281	-2.3481	-3.6733
C	-4.10152	-0.52752	-2.06197
C	-5.52104	-2.45343	-3.53735
H	-3.60456	-3.02705	-4.34771
C	-5.49658	-0.63399	-1.91773
H	-3.56488	0.20947	-1.47089
C	-6.21052	-1.59566	-2.6593
H	-6.06519	-3.20207	-4.1093
H	-6.01607	0.02374	-1.22525
H	-7.28957	-1.67991	-2.54842
C	-0.80923	-2.74139	-3.96928
C	-0.47834	-3.86893	-3.17827
C	-0.65126	-2.83972	-5.37249
C	-0.00638	-5.05604	-3.76865
H	-0.57872	-3.81476	-2.09595
C	-0.18615	-4.02818	-5.96942
H	-0.87726	-1.98365	-6.00562
C	0.1356	-5.14042	-5.16822
H	0.2475	-5.90866	-3.14267
H	-0.07305	-4.08224	-7.04996
H	0.49508	-6.05921	-5.62676

B3LYP-D3/defTZVP-SDD(Mo)-
CPCM(benzene)//B3LYP/LANL2DZ
HF = -3364.690761

[Mo]SiP-A

B3LYP/LANL2DZ
Zero-point correction= 0.894138
(Hartree/Particle)
Thermal correction to Energy= 0.953313
Thermal correction to Enthalpy= 0.954257
Thermal correction to Gibbs Free Energy=
0.790917
Sum of electronic and zero-point Energies= -
2656.040134
Sum of electronic and thermal Energies= -
2655.980959
Sum of electronic and thermal Enthalpies= -
2655.980015
Sum of electronic and thermal Free Energies= -
2656.143355

C	-1.60571	1.1125	1.91033
C	-0.29474	1.2871	2.40149
C	0.66031	2.03818	1.68324
C	0.27463	2.64593	0.46913
C	-1.03288	2.49307	-0.03917
C	-1.96656	1.73061	0.69489
C	-2.62357	0.33748	2.69549
C	-2.4921	-1.04462	3.02586
C	-3.49895	-1.63444	3.83369
C	-4.60936	-0.90828	4.29654
C	-4.74779	0.4436	3.93674
C	-3.76205	1.05127	3.14291
C	-1.82181	-3.91482	2.07802
C	-1.06772	-5.09361	2.29793
C	-1.56791	-6.35785	1.93166
C	-2.83575	-6.46738	1.32998
C	-3.59776	-5.30594	1.09591
C	-3.09344	-4.04542	1.46425
C	0.28886	-2.34977	3.74216
C	0.07327	-3.02284	4.97006
C	1.09001	-3.10768	5.9395
C	2.34652	-2.51824	5.6972
C	2.57737	-1.84494	4.48258
C	1.55608	-1.7623	3.51696
C	-1.42688	3.18443	-1.3115
C	-1.89152	2.50154	-2.47538
C	-2.26951	3.28039	-3.59962
C	-2.1938	4.68399	-3.59721
C	-1.70972	5.34613	-2.45569
C	-1.32894	4.5969	-1.33065
C	-3.70802	-0.0556	-2.2062
C	-3.85382	-1.38749	-1.74695
C	-5.12131	-1.9099	-1.42802
C	-6.27125	-1.10865	-1.56638
C	-6.14457	0.21857	-2.01904
C	-4.87394	0.73774	-2.335
C	-1.61828	0.18072	-4.49114
C	-2.50084	-0.59727	-5.27763
C	-2.18028	-0.94235	-6.60576
C	-0.9638	-0.5168	-7.17045
C	-0.07174	0.25776	-6.40184
C	-0.39848	0.60302	-5.07847
C	2.03903	2.22244	2.24716
C	3.23656	1.83199	1.57298
C	4.47597	2.08317	2.21715
C	4.55385	2.69491	3.4806
C	3.36918	3.05594	4.14542
C	2.13018	2.81545	3.5302
C	3.41357	2.1582	-1.54815
C	3.17286	1.71031	-2.87097
C	3.2624	2.59327	-3.9624
C	3.60427	3.94404	-3.75209
C	3.85127	4.40491	-2.44546
C	3.75457	3.51803	-1.35482
C	4.85688	-0.18675	-0.14415
C	4.79212	-1.49466	0.39633
C	5.91775	-2.33903	0.39016
C	7.13582	-1.88776	-0.15524
C	7.21731	-0.59276	-0.70152
C	6.08617	0.24672	-0.69652
C	0.84601	-2.49935	-1.44021
H	-0.01144	0.82591	3.34401
H	0.99555	3.23564	-0.09049
H	-2.97719	1.60782	0.3139
H	-3.42905	-2.68917	4.09267
H	-5.35869	-1.39486	4.91643
H	-5.60649	1.0195	4.27417
H	-3.85485	2.10202	2.87876
H	-0.08337	-5.02832	2.75683
H	-0.97092	-7.249	2.11232
H	-3.22428	-7.44308	1.0459

H	-4.57846	-5.38359	0.63103
H	-3.69845	-3.15988	1.27839
H	-0.89	-3.48666	5.17801
H	0.90333	-3.62887	6.87594
H	3.13364	-2.58219	6.44545
H	3.54206	-1.38208	4.28764
H	1.74569	-1.2359	2.58503
H	-2.60421	2.78136	-4.50684
H	-2.49395	5.24734	-4.47759
H	-1.63205	6.43089	-2.43861
H	-0.96728	5.10662	-0.44075
H	-2.97509	-2.01835	-1.62793
H	-5.20951	-2.93635	-1.07858
H	-7.2516	-1.5108	-1.32014
H	-7.02689	0.84637	-2.12267
H	-4.79506	1.77001	-2.67162
H	-3.44384	-0.93872	-4.85584
H	-2.87445	-1.54049	-7.19208
H	-0.71291	-0.78404	-8.19484
H	0.87041	0.58983	-6.8329
H	0.29979	1.2083	-4.50234
H	5.40029	1.77008	1.73636
H	5.52285	2.87209	3.94122
H	3.40716	3.51958	5.1285
H	1.2126	3.10481	4.03673
H	2.9091	0.6692	-3.05046
H	3.07274	2.23038	-4.9704
H	3.67434	4.62778	-4.59528
H	4.11408	5.44662	-2.27488
H	3.9407	3.89312	-0.34983
H	3.8549	-1.86432	0.80761
H	5.84385	-3.34221	0.80426
H	8.007	-2.53947	-0.1611
H	8.15146	-0.24077	-1.13392
H	6.16137	1.23733	-1.14208
Mo	0.38215	-1.03933	-0.59056
O	-0.38991	-1.57902	1.04896
O	-0.85941	-0.13984	-1.69626
O	1.97236	-0.04971	-0.29784
Si	-1.09135	-2.20785	2.45301
Si	-2.00512	0.61241	-2.68757
Si	3.33117	0.93501	-0.10796
H	1.12919	-3.4089	-1.97065

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3516.041367

[Mo]SiP-TS-A

B3LYP/LANL2DZ
Imaginary frequency = -162.03 cm^{-1}
Zero-point correction= 0.923945 (Hartree/Particle)
Thermal correction to Energy= 0.984959
Thermal correction to Enthalpy= 0.985904
Thermal correction to Gibbs Free Energy= 0.823172
Sum of electronic and zero-point Energies= -2733.310218
Sum of electronic and thermal Energies= -2733.249203
Sum of electronic and thermal Enthalpies= -2733.248259
Sum of electronic and thermal Free Energies= -2733.410990

O	-0.59386	1.03071	-1.00017
O	1.9285	0.74376	0.2185
O	-1.47153	0.23184	1.53381
H	0.41728	-1.49369	-3.12237
H	-2.37364	-2.47548	0.00566
H	1.86915	-2.65186	0.76628
C	-2.43922	-0.19938	-2.97227
C	-2.25851	-1.54375	-2.53153
C	0.22063	-1.81299	-2.1028
C	2.69976	-1.97126	-1.79975
C	-1.10849	-1.92588	-1.65165
C	1.30821	-2.06752	-1.24183
C	3.69706	-1.05523	-1.35004
C	-1.34968	-2.35792	-0.33396
C	1.04234	-2.45481	0.08896
C	-0.28486	-2.60357	0.55702
C	-0.55666	-3.06914	1.95665
C	0.04838	2.75492	1.31588
C	-1.47469	-2.42354	2.84676
C	1.01832	0.25527	2.79179
C	0.91578	1.45896	3.11385
Si	-1.26468	1.24029	-2.53394
Si	3.51951	0.2115	0.06692
Si	-2.40388	-0.78026	2.50889
Mo	0.09926	1.06749	0.7706
H	1.26127	-0.78529	2.88174
H	0.93363	2.37097	3.67381
H	-0.01728	3.80165	1.61098
C	-2.24941	2.8625	-2.50498
C	-2.36309	3.68639	-3.65059
C	-2.9027	3.27861	-1.31804
C	-3.11218	4.87901	-3.61862
H	-1.84868	3.41102	-4.56955
C	-3.6491	4.47123	-1.27933
H	-2.81296	2.68075	-0.41342
C	-3.76023	5.27289	-2.43232
H	-3.18338	5.49806	-4.51049
H	-4.13906	4.77251	-0.35583
H	-4.33774	6.19462	-2.40459
C	0.12006	1.35609	-3.81763
C	-0.1024	1.02032	-5.17523
C	1.40153	1.8279	-3.44671
C	0.92034	1.16039	-6.1337
H	-1.06972	0.63078	-5.48893
C	2.42885	1.96355	-4.39841
H	1.6008	2.0722	-2.40715
C	2.18865	1.6345	-5.74674
H	0.7303	0.89474	-7.17154
H	3.40957	2.31515	-4.08653
H	2.98199	1.73726	-6.48414
C	4.5655	1.76502	-0.24174
C	5.97163	1.77776	-0.06845
C	3.93592	2.9692	-0.64003
C	6.72508	2.94292	-0.30609
H	6.48603	0.88153	0.27564
C	4.68328	4.13858	-0.87713
H	2.85373	2.99452	-0.73913
C	6.08222	4.1269	-0.71732
H	7.80387	2.92832	-0.16598
H	4.17643	5.05211	-1.18075
H	6.66224	5.02888	-0.90096
C	4.1822	-0.60002	1.65881
C	4.4713	-1.98449	1.73091
C	4.44208	0.18853	2.80849
C	4.98646	-2.56465	2.90711
H	4.31654	-2.61508	0.85767
C	4.95556	-0.38321	3.98619

H	4.25013	1.25936	2.78182
C	5.22645	-1.76527	4.04025
H	5.20374	-3.63022	2.93477
H	5.14733	0.24391	4.85417
H	5.62592	-2.20963	4.94942
C	-4.05599	-1.06325	1.62957
C	-4.39649	-0.32137	0.47473
C	-4.99883	-1.99483	2.12963
C	-5.6386	-0.50119	-0.16326
H	-3.67958	0.38699	0.0686
C	-6.24284	-2.17804	1.49687
H	-4.76662	-2.58728	3.01374
C	-6.56605	-1.42845	0.34827
H	-5.87308	0.07196	-1.05704
H	-6.95251	-2.90002	1.89538
H	-7.52578	-1.5703	-0.14425
C	-2.76387	0.08174	4.16772
C	-1.80229	0.1581	5.20701
C	-3.99786	0.74956	4.36525
C	-2.06255	0.86377	6.39562
H	-0.84154	-0.33925	5.09434
C	-4.26479	1.46004	5.55187
H	-4.76131	0.71265	3.59144
C	-3.29726	1.51921	6.57204
H	-1.30844	0.90095	7.17911
H	-5.22193	1.9616	5.67763
H	-3.50186	2.06512	7.49071
C	-1.70761	-3.03111	4.10801
C	-1.05654	-4.21117	4.50878
H	-1.26751	-4.64531	5.48321
C	-0.12511	-4.81192	3.64502
H	0.39701	-5.71935	3.93969
C	0.11422	-4.24152	2.38475
H	0.8052	-4.72614	1.69937
H	-2.40065	-2.56494	4.8043
C	-3.56561	0.09101	-3.78184
C	-3.20005	-2.53262	-2.89376
C	-4.30365	-2.22362	-3.70699
H	-5.01229	-3.00199	-3.98082
H	-3.74377	1.11466	-4.10523
C	-4.48628	-0.90445	-4.15776
H	-5.33833	-0.64913	-4.78379
H	-3.05559	-3.5509	-2.54007
C	2.99651	-2.84436	-2.87648
C	4.95689	-1.07502	-2.00355
C	5.24503	-1.95686	-3.05856
H	6.2234	-1.93714	-3.533
C	4.25312	-2.84882	-3.50094
H	4.45178	-3.53518	-4.32087
H	2.22567	-3.5335	-3.2132
H	5.72703	-0.36953	-1.70231

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3593.408562

[Mo]SiP-MCBD-A

B3LYP/LANL2DZ
Zero-point correction= 0.926876 (Hartree/Particle)
Thermal correction to Energy= 0.987986
Thermal correction to Enthalpy= 0.988930
Thermal correction to Gibbs Free Energy= 0.824013
Sum of electronic and zero-point Energies= -2733.334944
Sum of electronic and thermal Energies= -2733.273834
Sum of electronic and thermal Enthalpies= -2733.272890
Sum of electronic and thermal Free Energies= -2733.437807

C	-1.72289	1.17199	1.96545
C	-0.42408	1.3129	2.49486
C	0.54204	2.10942	1.84592
C	0.18674	2.78559	0.6618
C	-1.10292	2.64979	0.10725
C	-2.05468	1.85815	0.77912
C	-2.75595	0.33234	2.65413
C	-2.60363	-1.06981	2.87263
C	-3.6419	-1.75754	3.55188
C	-4.80011	-1.10086	4.00425
C	-4.95198	0.27567	3.76244
C	-3.93791	0.97697	3.08994
C	-1.70253	-3.90783	1.97955
C	-1.57092	-4.88278	2.99822
C	-2.0119	-6.20577	2.80118
C	-2.591	-6.5801	1.57373
C	-2.722	-5.62554	0.54622
C	-2.28441	-4.30379	0.75046
C	0.28232	-2.12924	3.5087
C	0.10722	-1.66985	4.8359
C	1.15845	-1.73101	5.77162
C	2.40996	-2.25128	5.39206
C	2.60204	-2.71452	4.07541
C	1.54615	-2.65898	3.14778
C	-1.44949	3.35534	-1.16964
C	-1.83312	2.66253	-2.35744
C	-2.16517	3.43406	-3.49998
C	-2.11903	4.84001	-3.49123
C	-1.71485	5.5111	-2.32402
C	-1.3813	4.76824	-1.17919
C	-3.58605	0.07588	-2.00606
C	-3.68489	-0.88868	-0.9759
C	-4.93495	-1.40185	-0.57938
C	-6.11294	-0.95675	-1.20805
C	-6.03468	0.01042	-2.22971
C	-4.78247	0.51999	-2.6222
C	-1.59633	0.32871	-4.36298
C	-2.51304	-0.4389	-5.121
C	-2.24758	-0.78046	-6.46261
C	-1.05048	-0.36396	-7.07365
C	-0.12033	0.39394	-6.33417
C	-0.39407	0.7341	-4.99762
C	1.907	2.27183	2.44335
C	3.11037	1.91307	1.76625
C	4.34537	2.17871	2.41308
C	4.40919	2.76224	3.69009
C	3.21726	3.07768	4.36507
C	1.9836	2.83078	3.74159
C	3.27031	2.34548	-1.35583
C	2.18668	2.48647	-2.2543
C	2.21811	3.45413	-3.27691
C	3.33869	4.29324	-3.4228
C	4.42721	4.16366	-2.53799
C	4.38975	3.19986	-1.51332
C	4.7552	-0.02648	0.00068
C	5.0744	-0.86728	1.09754
C	6.15489	-1.76572	1.03474
C	6.94012	-1.84527	-0.13261
C	6.63407	-1.02457	-1.23419
C	5.54988	-0.12812	-1.16669

H	-0.15497	0.79636	3.41165
H	0.91923	3.41198	0.16054
H	-3.05332	1.75294	0.36474
H	-3.55976	-2.83085	3.70905
H	-5.57535	-1.65976	4.52319
H	-5.84713	0.79789	4.09263
H	-4.04719	2.04356	2.90863
H	-1.1065	-4.61746	3.94639
H	-1.8983	-6.9386	3.59715
H	-2.92923	-7.60227	1.41752
H	-3.15977	-5.90799	-0.4087
H	-2.38079	-3.58569	-0.06069
H	-0.85308	-1.25953	5.14381
H	1.00206	-1.37159	6.7863
H	3.22467	-2.29509	6.1116
H	3.56472	-3.12403	3.77645
H	1.70874	-3.03248	2.13832
H	-2.44409	2.92971	-4.42269
H	-2.38404	5.39908	-4.3858
H	-1.66252	6.59734	-2.30236
H	-1.0794	5.28323	-0.27009
H	-2.78268	-1.21708	-0.46677
H	-4.98772	-2.13392	0.22338
H	-7.07957	-1.35036	-0.90078
H	-6.94118	0.3677	-2.71387
H	-4.74702	1.27598	-3.40572
H	-3.43833	-0.78191	-4.6644
H	-2.96968	-1.37068	-7.02281
H	-0.84203	-0.62854	-8.10816
H	0.81218	0.71371	-6.79418
H	0.34285	1.31225	-4.44397
H	5.27782	1.90837	1.92241
H	5.37423	2.95432	4.15305
H	3.24642	3.51757	5.35937
H	1.05945	3.09467	4.25013
H	1.31144	1.85065	-2.14481
H	1.36542	3.56325	-3.94323
H	3.36167	5.04263	-4.21103
H	5.29534	4.81088	-2.64178
H	5.23854	3.12227	-0.83502
H	4.4799	-0.81853	2.00838
H	6.38483	-2.39822	1.88956
H	7.77722	-2.53839	-0.18251
H	7.23191	-1.08297	-2.14101
H	5.32364	0.49269	-2.03084
Mo	0.54385	-1.14991	-0.69445
O	-0.62728	-1.5383	0.7456
O	-0.66928	0.12369	-1.56692
O	1.88352	0.05965	-0.19709
Si	-1.14016	-2.11934	2.25904
Si	-1.8986	0.75996	-2.53425
Si	3.22087	1.08582	0.05393
H	-0.3802	-2.01433	-3.433
C	0.22336	-2.20511	-2.55147
C	1.0597	-3.24837	-2.2262
H	1.28746	-4.16258	-2.78266
C	1.57842	-2.8175	-0.93246
H	2.39224	-3.27411	-0.36644

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3593.426794

[Mo]L_3

B3LYP/LANL2DZ

Zero-point correction= 0.883827 (Hartree/Particle)
Thermal correction to Energy= 0.943520
Thermal correction to Enthalpy= 0.944464
Thermal correction to Gibbs Free Energy= 0.772681
Sum of electronic and zero-point Energies= -2466.773269
Sum of electronic and thermal Energies= -2466.713576
Sum of electronic and thermal Enthalpies= -2466.712632
Sum of electronic and thermal Free Energies= -2466.884415

C	-0.69813	4.63645	-1.79676
C	0.33996	5.15308	-0.98317
C	0.35755	6.50839	-0.60362
C	-0.6642	7.3763	-1.03733
C	-1.70499	6.87933	-1.845
C	-1.72019	5.52146	-2.21862
C	0.24165	2.59026	-3.97419
C	0.91475	1.37598	-4.25517
C	1.57295	1.17786	-5.4838
C	1.56702	2.19447	-6.45835
C	0.90505	3.40944	-6.19518
C	0.25013	3.60331	-4.96377
C	-2.4351	2.14882	-2.44791
C	-2.85639	1.35638	-3.54325
C	-4.15895	0.82264	-3.59714
C	-5.06651	1.07153	-2.54971
C	-4.666	1.85935	-1.45189
C	-3.36462	2.39112	-1.4048
C	-0.96555	-0.47955	-0.11839
C	-2.20004	-1.29795	-0.24613
C	2.11345	-2.54325	-2.63116
C	3.07415	-2.75185	-3.65017
C	2.68258	-3.06615	-4.9668
C	1.31677	-3.17273	-5.2904
C	0.34563	-2.96365	-4.29101
C	0.74248	-2.65526	-2.97714
C	4.49786	-1.87903	-0.73692
C	5.06424	-0.58213	-0.77661
C	6.45843	-0.3982	-0.70786
C	7.31307	-1.5125	-0.60028
C	6.766	-2.80979	-0.55602
C	5.37091	-2.98845	-0.62286
C	2.03217	-3.43786	0.35069
C	1.57934	-4.70718	-0.0822
C	1.17571	-5.68964	0.84395
C	1.21874	-5.41731	2.22411
C	1.66604	-4.15847	2.67359
C	2.06978	-3.18195	1.74507
C	-0.53985	2.81434	3.91084
C	-0.44849	3.82756	2.92721
C	-0.76408	5.16589	3.23241
C	-1.17325	5.51497	4.53321
C	-1.26411	4.51977	5.52666
C	-0.95139	3.18337	5.21534
C	-1.68098	-0.06017	3.61604
C	-2.97665	0.51072	3.65795
C	-4.12767	-0.29903	3.70965
C	-4.003	-1.70172	3.71605
C	-2.7225	-2.28844	3.67142
C	-1.57638	-1.4742	3.62175
C	1.24744	0.29794	4.55824
C	0.97997	-0.27361	5.82613

C	2.02183	-0.77106	6.63242
C	3.35397	-0.71051	6.17961
C	3.63712	-0.15088	4.91827
C	2.59287	0.35117	4.11888
H	1.1319	4.48909	-0.64291
H	1.1648	6.88507	0.02093
H	-0.65045	8.42502	-0.74786
H	-2.50037	7.54203	-2.17903
H	-2.54086	5.15171	-2.83138
H	0.94125	0.58242	-3.51163
H	2.08489	0.23724	-5.67253
H	2.07673	2.04476	-7.40789
H	0.90333	4.20253	-6.93985
H	-0.24049	4.55599	-4.77212
H	-2.16822	1.158	-4.36232
H	-4.46298	0.22084	-4.4509
H	-6.07355	0.66163	-2.58958
H	-5.36219	2.05796	-0.64018
H	-3.07494	3.00119	-0.55076
H	4.13371	-2.66543	-3.4195
H	3.43895	-3.22585	-5.73224
H	1.01223	-3.41371	-6.30664
H	-0.71198	-3.03906	-4.53356
H	-0.023	-2.49404	-2.22035
H	4.40897	0.28295	-0.85009
H	6.87366	0.6068	-0.73761
H	8.39068	-1.37229	-0.54682
H	7.41948	-3.67475	-0.46506
H	4.96494	-3.99767	-0.56964
H	1.53712	-4.9342	-1.14564
H	0.83217	-6.65918	0.48952
H	0.91095	-6.17576	2.94099
H	1.70895	-3.94076	3.73854
H	2.41455	-2.21734	2.11352
H	-0.12623	3.57135	1.92099
H	-0.69301	5.92483	2.45667
H	-1.41672	6.54822	4.77177
H	-1.57504	4.78265	6.53548
H	-1.02602	2.43092	5.99954
H	-3.09036	1.59287	3.65452
H	-5.11271	0.16113	3.74557
H	-4.8907	-2.3295	3.7571
H	-2.61717	-3.37095	3.67299
H	-0.59663	-1.94634	3.58424
H	-0.04523	-0.34509	6.18655
H	1.79524	-1.2044	7.60425
H	4.16016	-1.09645	6.79987
H	4.66278	-0.10564	4.55908
H	2.82059	0.78009	3.14539
Mo	0.47074	0.51346	0.05483
O	0.21298	1.9803	-1.14209
O	1.94726	-0.60898	-0.41537
O	0.48342	1.04346	1.88998
Si	-0.67107	2.82654	-2.33614
Si	2.62788	-2.11227	-0.86043
Si	-0.13149	1.01838	3.48265
H	-2.85715	-0.89233	-1.02866
H	-2.75788	-1.30544	0.70075
H	-1.95941	-2.34148	-0.50055

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3326.652717

[Mo]L_3-TS

B3LYP/LANL2DZ

Imaginary frequency = -143.85 cm^{-1}
Zero-point correction= 0.970828 (Hartree/Particle)
Thermal correction to Energy= 1.035662
Thermal correction to Enthalpy= 1.036606
Thermal correction to Gibbs Free Energy= 0.857047
Sum of electronic and zero-point Energies= -2622.618924
Sum of electronic and thermal Energies= -2622.554089
Sum of electronic and thermal Enthalpies= -2622.553145
Sum of electronic and thermal Free Energies= -2622.732705

O	-0.63186	-0.45642	-1.09882
O	1.918	0.10305	-0.24529
O	-1.40918	-0.40017	1.5395
Si	-1.13335	-0.79332	-2.67824
Si	3.51625	0.53446	-0.58299
Si	-2.60846	-0.39048	2.72921
Mo	0.10863	0.30909	0.49516
C	4.62062	0.23122	0.93528
C	5.36881	-0.96605	1.05357
C	4.68929	1.1586	2.00517
C	6.15387	-1.22919	2.19323
H	5.34751	-1.6959	0.24685
C	5.47286	0.90425	3.14572
H	4.13188	2.09172	1.94792
C	6.20812	-0.29363	3.24381
H	6.72127	-2.15517	2.25752
H	5.51299	1.63524	3.95077
H	6.8167	-0.49229	4.12356
C	3.61449	2.36044	-1.08921
C	2.56342	2.93313	-1.84898
C	4.7381	3.17141	-0.79454
C	2.62954	4.26716	-2.29203
H	1.69269	2.33292	-2.10236
C	4.81001	4.50725	-1.23655
H	5.56551	2.76381	-0.21684
C	3.7539	5.05947	-1.98626
H	1.81389	4.67924	-2.88222
H	5.68445	5.10991	-0.99964
H	3.80827	6.0899	-2.33164
C	4.08975	-0.58618	-1.9967
C	3.35435	-1.74889	-2.32687
C	5.26262	-0.30318	-2.73838
C	3.77356	-2.60401	-3.36495
H	2.44474	-1.97678	-1.7778
C	5.68948	-1.15593	-3.77424
H	5.84471	0.59071	-2.51834
C	4.94468	-2.3102	-4.08957
H	3.18433	-3.48612	-3.60457
H	6.59318	-0.92036	-4.33269
H	5.27138	-2.96848	-4.8921
C	-1.85516	-0.59452	4.46378
C	-1.29731	0.5034	5.16554
C	-1.80075	-1.86754	5.08295
C	-0.70873	0.33959	6.43292
H	-1.32864	1.49798	4.72421
C	-1.21159	-2.04018	6.35082
H	-2.23068	-2.73066	4.57889
C	-0.66277	-0.93585	7.02985
H	-0.29314	1.19984	6.95381
H	-1.18603	-3.02802	6.80582
H	-0.21097	-1.06536	8.01112

C	-3.59121	1.23178	2.65905
C	-4.21356	1.78303	3.80643
C	-3.77556	1.89748	1.42108
C	-4.98951	2.9559	3.72405
H	-4.09175	1.30064	4.77455
C	-4.54784	3.07068	1.33328
H	-3.31674	1.49691	0.52027
C	-5.15837	3.60394	2.48557
H	-5.4591	3.35875	4.61903
H	-4.6807	3.55922	0.37021
H	-5.7595	4.50834	2.41827
C	-3.73497	-1.87346	2.38207
C	-5.04055	-1.95135	2.926
C	-3.27441	-2.95705	1.59646
C	-5.85784	-3.07472	2.69641
H	-5.43125	-1.12941	3.5241
C	-4.08801	-4.08174	1.36084
H	-2.28234	-2.90701	1.15343
C	-5.3816	-4.14465	1.91323
H	-6.8587	-3.11295	3.12141
H	-3.7182	-4.89729	0.74346
H	-6.01324	-5.01141	1.73019
C	-0.46858	0.48971	-3.90461
C	0.83463	0.37144	-4.44981
C	-1.23435	1.62946	-4.257
C	1.34997	1.34802	-5.32227
H	1.45691	-0.48241	-4.19231
C	-0.72414	2.6093	-5.13005
H	-2.23887	1.75003	-3.85588
C	0.57075	2.46941	-5.66674
H	2.35515	1.23646	-5.72165
H	-1.33403	3.47134	-5.39271
H	0.96762	3.22389	-6.34293
C	-3.0258	-0.76365	-2.66925
C	-3.78297	-0.74098	-3.86627
C	-3.72009	-0.82662	-1.43797
C	-5.18971	-0.77544	-3.83389
H	-3.28004	-0.69524	-4.83141
C	-5.12722	-0.86169	-1.40033
H	-3.15535	-0.85462	-0.50999
C	-5.86545	-0.83589	-2.59865
H	-5.75383	-0.75765	-4.76419
H	-5.63768	-0.91807	-0.44166
H	-6.95283	-0.8655	-2.57189
C	-0.48816	-2.51994	-3.12266
C	-0.1355	-3.43429	-2.10152
C	-0.4037	-2.95741	-4.46649
C	0.28989	-4.74037	-2.40933
H	-0.18889	-3.11761	-1.06187
C	0.01786	-4.26339	-4.78133
H	-0.6603	-2.27771	-5.27761
C	0.36544	-5.15982	-3.75213
H	0.55844	-5.42595	-1.60828
H	0.07485	-4.5783	-5.82114
H	0.68941	-6.1703	-3.99279
C	-0.11987	2.0807	0.56791
C	-0.42015	3.52206	0.40732
C	0.94272	1.49605	2.36739
C	1.12221	2.81676	3.03622
C	1.14883	0.23005	2.41144
H	0.48981	4.13628	0.36423
H	-1.08035	3.90258	1.19916
H	-0.94642	3.64788	-0.54996
H	1.71461	3.50756	2.42421
H	1.65035	2.659	3.98528
H	0.16223	3.29979	3.25486
C	1.7123	-0.93329	3.14336
H	0.918	-1.65404	3.3736
H	2.46645	-1.43834	2.52737
H	2.1843	-0.62523	4.08497

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3482.706355

[Mo]L_3-MCBD

B3LYP/LANL2DZ
Zero-point correction= 0.972362 (Hartree/Particle)
Thermal correction to Energy= 1.037104
Thermal correction to Enthalpy= 1.038048
Thermal correction to Gibbs Free Energy= 0.859662
Sum of electronic and zero-point Energies= -2622.629311
Sum of electronic and thermal Energies= -2622.564568
Sum of electronic and thermal Enthalpies= -2622.563624
Sum of electronic and thermal Free Energies= -2622.742010

O	-0.65118	0.29334	-1.10375
O	1.93741	0.17607	-0.49539
O	-1.53993	-0.45445	1.29426
Si	-1.1689	-0.35844	-2.60113
Si	3.46989	0.77593	-0.84172
Si	-2.73705	-0.45261	2.47818
Mo	0.24563	0.09771	0.5526
C	4.52749	0.92319	0.73807
C	5.23838	-0.19718	1.23679
C	4.5994	2.13016	1.47756
C	5.99154	-0.11808	2.42375
H	5.21719	-1.13577	0.68565
C	5.35385	2.21904	2.66371
H	4.07763	3.01458	1.11618
C	6.05205	1.09267	3.14158
H	6.53406	-0.99092	2.78099
H	5.40527	3.16176	3.20491
H	6.64047	1.15957	4.05438
C	3.32346	2.49986	-1.61814
C	2.06823	2.97314	-2.07053
C	4.45207	3.34106	-1.7825
C	1.94389	4.24362	-2.66493
H	1.18805	2.34453	-1.96393
C	4.33384	4.61039	-2.37954
H	5.43134	3.01504	-1.43404
C	3.07611	5.06525	-2.82256
H	0.97006	4.58211	-3.01177
H	5.21405	5.23939	-2.49606
H	2.9813	6.04604	-3.2843
C	4.29292	-0.49009	-1.98991
C	3.61546	-1.69059	-2.31137
C	5.5831	-0.28656	-2.5376
C	4.20332	-2.65549	-3.15263
H	2.62445	-1.86405	-1.89823
C	6.1757	-1.24609	-3.38038
H	6.13701	0.6232	-2.31001
C	5.48569	-2.43513	-3.69053
H	3.66046	-3.56894	-3.38593
H	7.16737	-1.06807	-3.79129
H	5.94236	-3.17783	-4.34156
C	-1.96969	-0.43956	4.22334

C	-1.97828	0.72173	5.03426
C	-1.35146	-1.60333	4.74778
C	-1.39518	0.72417	6.31771
H	-2.45975	1.62806	4.67197
C	-0.76724	-1.60963	6.02784
H	-1.33838	-2.51863	4.15795
C	-0.78695	-0.4429	6.81825
H	-1.4261	1.62646	6.92513
H	-0.30787	-2.51882	6.41023
H	-0.3429	-0.44661	7.81153
C	-3.81374	1.10323	2.29392
C	-5.15116	1.12844	2.75955
C	-3.29202	2.28563	1.71504
C	-5.93823	2.29185	2.65574
H	-5.59108	0.23167	3.19219
C	-4.0738	3.45142	1.60459
H	-2.2751	2.28891	1.32857
C	-5.39978	3.45882	2.07904
H	-6.9644	2.28574	3.01719
H	-3.65415	4.34412	1.1456
H	-6.00708	4.35745	1.99383
C	-3.78957	-2.01669	2.29727
C	-4.44348	-2.6106	3.40506
C	-3.97541	-2.60541	1.02231
C	-5.25323	-3.75228	3.24704
H	-4.3143	-2.19104	4.40144
C	-4.78082	-3.74769	0.85871
H	-3.49029	-2.16864	0.15331
C	-5.42338	-4.32442	1.97172
H	-5.74429	-4.19228	4.11261
H	-4.90742	-4.18048	-0.1311
H	-6.04734	-5.20707	1.84693
C	-0.33884	0.54857	-4.03634
C	0.99864	0.26226	-4.40842
C	-1.02193	1.56907	-4.74357
C	1.62666	0.95862	-5.45622
H	1.56087	-0.50255	-3.87926
C	-0.3973	2.26903	-5.79341
H	-2.04763	1.81715	-4.47921
C	0.92893	1.96336	-6.15372
H	2.65619	0.72491	-5.71632
H	-0.94253	3.04598	-6.32521
H	1.41461	2.50513	-6.96263
C	-3.04115	-0.11011	-2.66081
C	-3.79129	-0.44809	-3.81459
C	-3.73158	0.39528	-1.53513
C	-5.18803	-0.27935	-3.84359
H	-3.29076	-0.84692	-4.69621
C	-5.12896	0.56919	-1.56057
H	-3.17214	0.64952	-0.64047
C	-5.86016	0.23261	-2.71516
H	-5.74756	-0.54539	-4.73801
H	-5.63678	0.96017	-0.68198
H	-6.94013	0.36358	-2.73637
C	-0.72341	-2.20274	-2.62396
C	-0.81151	-2.97156	-1.43591
C	-0.36159	-2.8675	-3.82061
C	-0.5386	-4.35175	-1.4423
H	-1.10778	-2.50017	-0.50017
C	-0.08881	-4.2494	-3.83182
H	-0.2858	-2.30889	-4.75122
C	-0.17541	-4.99576	-2.64144
H	-0.6187	-4.92205	-0.51927
H	0.18752	-4.73822	-4.76372
H	0.03249	-6.06367	-2.64823
C	0.67121	1.38655	1.84068
C	0.70344	2.76554	2.40371
C	1.26467	0.1378	2.53799
C	1.93739	0.36192	3.87596
C	1.15165	-1.08789	1.88282
H	1.72178	3.05874	2.69809
H	0.06199	2.8484	3.29474
H	0.34623	3.48694	1.66108
H	2.79523	1.03576	3.75844
H	2.29316	-0.58308	4.29499
H	1.2341	0.81358	4.58589
C	1.6102	-2.45759	2.22218
H	0.75991	-3.15394	2.23977
H	2.30851	-2.82429	1.45649
H	2.11352	-2.50773	3.19764

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3482.721135

[Mo]SiP

B3LYP/LANL2DZ
Zero-point correction= 0.922753 (Hartree/Particle)
Thermal correction to Energy= 0.983853
Thermal correction to Enthalpy= 0.984797
Thermal correction to Gibbs Free Energy= 0.816858
Sum of electronic and zero-point Energies= -2695.332843
Sum of electronic and thermal Energies= -2695.271743
Sum of electronic and thermal Enthalpies= -2695.270799
Sum of electronic and thermal Free Energies= -2695.438738

C	-1.9119	1.80181	2.06983
C	-0.61849	2.01697	2.59042
C	0.35068	2.74103	1.86342
C	-0.00298	3.27841	0.60693
C	-1.29283	3.08462	0.06805
C	-2.24131	2.35171	0.81325
C	-2.94559	1.0554	2.86167
C	-2.80309	-0.30267	3.27678
C	-3.83163	-0.8657	4.07596
C	-4.97218	-0.13637	4.45297
C	-5.11889	1.19021	4.01176
C	-4.11306	1.77105	3.22295
C	-2.04118	-3.21329	2.5502
C	-1.28932	-4.35512	2.92074
C	-1.74581	-5.65513	2.62941
C	-2.96662	-5.83863	1.95309
C	-3.72664	-4.71536	1.57144
C	-3.2665	-3.41907	1.86659
C	-0.01923	-1.49354	4.16408
C	-0.27957	-2.03423	5.44755
C	0.71124	-2.04112	6.44713
C	1.98643	-1.50487	6.17989
C	2.2618	-0.96268	4.9103
C	1.26622	-0.95791	3.91459
C	-1.65556	3.70571	-1.24903
C	-2.08128	2.95929	-2.38852
C	-2.43331	3.67567	-3.56156
C	-2.36945	5.07826	-3.62968
C	-1.92373	5.80294	-2.51073
C	-1.56872	5.11625	-1.33831
C	-3.87727	0.39682	-2.03693

C	-4.01991	-0.9197	-1.53396
C	-5.28807	-1.44317	-1.22005
C	-6.44249	-0.65821	-1.40714
C	-6.31933	0.65348	-1.90374
C	-5.04762	1.1736	-2.21458
C	-1.73685	0.54692	-4.27891
C	-2.60993	-0.24452	-5.0626
C	-2.25528	-0.64842	-6.3655
C	-1.0134	-0.26913	-6.9075
C	-0.13021	0.51829	-6.14149
C	-0.49122	0.9221	-4.84373
C	1.70666	2.97622	2.46211
C	2.93261	2.57731	1.84673
C	4.14498	2.88189	2.51868
C	4.16997	3.55289	3.75389
C	2.95757	3.92206	4.36177
C	1.74441	3.62986	3.71827
C	3.21468	2.75513	-1.27756
C	3.01847	2.24394	-2.58455
C	3.13679	3.07464	-3.71367
C	3.462	4.43681	-3.55725
C	3.66287	4.96115	-2.26677
C	3.53858	4.12581	-1.13877
C	4.65393	0.51836	0.2913
C	4.60604	-0.75547	0.90964
C	5.75197	-1.56835	0.98877
C	6.97455	-1.11919	0.45137
C	7.04015	0.14185	-0.17112
C	5.88867	0.94969	-0.25025
C	0.68543	-1.93228	-0.99824
C	1.10539	-3.20347	-1.64333
H	-0.35932	1.60793	3.5634
H	0.72891	3.84661	0.03923
H	-3.23881	2.19809	0.4096
H	-3.75466	-1.90344	4.39476
H	-5.73775	-0.60182	5.06929
H	-6.00012	1.7676	4.28201
H	-4.21389	2.8031	2.89544
H	-0.34173	-4.23233	3.44122
H	-1.15217	-6.51673	2.92714
H	-3.3216	-6.84187	1.72674
H	-4.6716	-4.85028	1.04917
H	-3.86979	-2.5635	1.56792
H	-1.2583	-2.45378	5.67655
H	0.48997	-2.46008	7.42642
H	2.75322	-1.50784	6.95165
H	3.24081	-0.54009	4.69615
H	1.48895	-0.5322	2.93948
H	-2.73688	3.12702	-4.45094
H	-2.64892	5.59267	-4.54613
H	-1.85563	6.88788	-2.54747
H	-1.23642	5.67452	-0.46622
H	-3.13676	-1.53577	-1.37578
H	-5.37404	-2.45741	-0.83578
H	-7.42354	-1.06081	-1.16438
H	-7.2052	1.26883	-2.04503
H	-4.9713	2.19431	-2.5853
H	-3.5723	-0.55108	-4.65797
H	-2.9433	-1.25544	-6.95005
H	-0.73648	-0.58105	-7.91239
H	0.83128	0.81557	-6.55496
H	0.2011	1.53593	-4.26943
H	5.09017	2.56401	2.08377
H	5.11976	3.76962	4.23712
H	2.95433	4.43193	5.32247
H	0.80557	3.92496	4.18061
H	2.76589	1.19368	-2.72155
H	2.98087	2.66326	-4.70878
H	3.55382	5.08051	-4.42938
H	3.91148	6.0123	-2.13764
H	3.68893	4.55013	-0.14741
H	3.66625	-1.12267	1.31752
H	5.69135	-2.545	1.46422
H	7.86167	-1.74622	0.5117
H	7.97807	0.49202	-0.59687
H	5.953	1.91356	-0.75241
Mo	0.1802	-0.43251	-0.2428
O	-0.62687	-0.92139	1.40561
O	-1.04082	0.36733	-1.45787
O	1.77478	0.57475	0.02613
Si	-1.35894	-1.46551	2.8242
Si	-2.16789	1.05971	-2.5051
Si	3.09819	1.59984	0.21642
H	0.6749	-3.29184	-2.65223
H	0.7723	-4.07102	-1.05401
H	2.20075	-3.25458	-1.7358

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3555.385737

[Mo]SiP-TS

B3LYP/LANL2DZ
Imaginary frequency = -109.99 cm^{-1}
Zero-point correction= 1.010705 (Hartree/Particle)
Thermal correction to Energy= 1.076493
Thermal correction to Enthalpy= 1.077438
Thermal correction to Gibbs Free Energy= 0.905500
Sum of electronic and zero-point Energies= -2851.173523
Sum of electronic and thermal Energies= -2851.107735
Sum of electronic and thermal Enthalpies= -2851.106791
Sum of electronic and thermal Free Energies= -2851.278728

C	-1.86317	1.10805	1.80783
C	-0.60535	1.3674	2.3828
C	0.36168	2.14063	1.70582
C	0.03699	2.67306	0.43997
C	-1.2357	2.45347	-0.14283
C	-2.18084	1.68524	0.56561
C	-2.83242	0.16205	2.44627
C	-2.53067	-1.22783	2.53589
C	-3.49882	-2.08606	3.11161
C	-4.72686	-1.59729	3.59461
C	-5.01739	-0.22549	3.49078
C	-4.07539	0.64268	2.91179
C	-1.18489	-3.78844	1.42561
C	-0.9974	-4.86193	2.32976
C	-1.24917	-6.19405	1.94537
C	-1.6922	-6.48006	0.64004
C	-1.87449	-5.42659	-0.27773
C	-1.62451	-4.098	0.1139
C	0.37167	-1.92465	3.35014
C	-0.00219	-2.23459	4.68098
C	0.9483	-2.23395	5.72006
C	2.2931	-1.91661	5.44537
C	2.67773	-1.5914	4.13061
C	1.72373	-1.59768	3.09583

C	-1.60621	3.07287	-1.45675
C	-2.17882	2.33934	-2.54559
C	-2.53638	3.06524	-3.71127
C	-2.33473	4.45265	-3.82917
C	-1.74438	5.15609	-2.76576
C	-1.38757	4.46501	-1.5963
C	-4.07991	-0.03024	-1.79189
C	-4.26118	-1.29817	-1.19228
C	-5.49563	-1.6661	-0.6259
C	-6.58265	-0.77188	-0.66098
C	-6.42358	0.49387	-1.2573
C	-5.18233	0.85949	-1.81345
C	-2.57151	-0.07203	-4.45445
C	-3.8266	-0.23038	-5.09084
C	-3.91803	-0.59911	-6.4476
C	-2.7484	-0.82063	-7.19868
C	-1.49031	-0.67622	-6.58141
C	-1.40626	-0.30633	-5.22605
C	1.65996	2.42662	2.40974
C	2.9528	2.0108	1.97026
C	4.06702	2.34756	2.78412
C	3.93861	3.06411	3.98513
C	2.66073	3.46093	4.41471
C	1.54236	3.13631	3.63262
C	3.951	2.33201	-0.91836
C	3.73814	3.72041	-0.74214
C	4.17696	4.65588	-1.7001
C	4.84501	4.21738	-2.8588
C	5.07589	2.83994	-3.04861
C	4.63429	1.91278	-2.08765
C	4.85975	-0.12233	0.6307
C	6.19479	0.35068	0.6835
C	7.27681	-0.5313	0.86439
C	7.04531	-1.91505	0.99027
C	5.72771	-2.40673	0.92364
C	4.65017	-1.51827	0.74419
H	-0.35697	0.93715	3.34887
H	0.77007	3.27498	-0.09148
H	-3.16322	1.51179	0.14041
H	-3.30585	-3.156	3.16265
H	-5.45016	-2.28094	4.03368
H	-5.96692	0.16429	3.85099
H	-4.29655	1.70414	2.82498
H	-0.63285	-4.66515	3.33582
H	-1.09523	-7.00123	2.65847
H	-1.88729	-7.50765	0.34041
H	-2.21067	-5.63776	-1.29094
H	-1.75116	-3.29873	-0.61257
H	-1.04186	-2.45516	4.91911
H	0.64034	-2.47199	6.73618
H	3.02815	-1.91102	6.24751
H	3.70923	-1.32674	3.9103
H	2.01983	-1.32173	2.08849
H	-2.95842	2.53292	-4.56033
H	-2.62482	4.96895	-4.74132
H	-1.57263	6.22764	-2.83915
H	-0.95754	5.01167	-0.76044
H	-3.42948	-1.99622	-1.15392
H	-5.6045	-2.64	-0.15426
H	-7.53744	-1.05395	-0.22232
H	-7.25603	1.19403	-1.28343
H	-5.07244	1.8506	-2.25148
H	-4.74302	-0.08375	-4.52309
H	-4.89511	-0.71755	-6.91136
H	-2.81564	-1.10744	-8.24614
H	-0.58106	-0.8518	-7.1533
H	-0.42846	-0.21456	-4.75976
H	5.06167	2.02278	2.48909
H	4.82026	3.29744	4.57757
H	2.53455	4.01191	5.34391
H	0.55156	3.44243	3.95972
H	3.24301	4.08055	0.15746
H	4.0035	5.71776	-1.53925
H	5.18822	4.9373	-3.59884
H	5.60252	2.49346	-3.93546
H	4.832	0.85392	-2.24458
H	6.39947	1.41288	0.55827
H	8.29232	-0.14258	0.90078
H	7.87955	-2.59923	1.13062
H	5.53883	-3.4746	1.01208
H	3.64031	-1.91345	0.67367
Mo	0.57886	-0.70464	-1.07079
O	-0.27377	-1.15324	0.59621
O	-1.14751	-0.40236	-1.94557
O	2.10123	0.10576	-0.15158
Si	-0.88537	-1.97885	1.93396
Si	-2.44161	0.43519	-2.62232
Si	3.38338	1.05172	0.37357
C	2.56162	-1.55034	-4.08526
C	1.80365	-0.65053	-3.17604
C	1.37936	0.4955	-2.83141
C	1.52583	-3.67616	-1.97918
C	1.15654	-2.27588	-1.67362
H	2.61384	-3.83254	-2.01465
H	1.08455	-4.03172	-2.92194
H	1.12275	-4.30562	-1.17192
H	3.39174	-2.04627	-3.56886
H	2.98025	-0.94664	-4.90201
H	1.92229	-2.32366	-4.52663
C	1.27974	1.94295	-3.16558
H	0.29176	2.17376	-3.57804
H	1.42322	2.57123	-2.28403
H	2.04011	2.21869	-3.90695

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3711.440283

[Mo]SiP-MCBD

B3LYP/LANL2DZ
Zero-point correction= 1.012285 (Hartree/Particle)
Thermal correction to Energy= 1.078178
Thermal correction to Enthalpy= 1.079122
Thermal correction to Gibbs Free Energy= 0.905441
Sum of electronic and zero-point Energies= -2851.191493
Sum of electronic and thermal Energies= -2851.125601
Sum of electronic and thermal Enthalpies= -2851.124657
Sum of electronic and thermal Free Energies= -2851.298337

C	-1.68516	1.13669	1.9668
C	-0.38902	1.27209	2.50443
C	0.58901	2.05186	1.85251
C	0.2457	2.72044	0.66135
C	-1.04128	2.59325	0.10248
C	-2.00321	1.81337	0.77184
C	-2.73345	0.30521	2.64273
C	-2.6022	-1.10206	2.83268

C	-3.65431	-1.78994	3.48874
C	-4.80734	-1.12657	3.9449
C	-4.9375	0.25739	3.733
C	-3.90844	0.95884	3.08358
C	-1.68086	-3.91934	1.86407
C	-1.62954	-4.91376	2.8718
C	-2.06561	-6.2295	2.6222
C	-2.56181	-6.57872	1.35176
C	-2.61466	-5.60519	0.3351
C	-2.18053	-4.29119	0.5919
C	0.21221	-2.20486	3.55479
C	0.03063	-1.59183	4.81834
C	1.01238	-1.6861	5.82365
C	2.2032	-2.3967	5.58224
C	2.39962	-3.01982	4.33409
C	1.41084	-2.92791	3.33781
C	-1.3788	3.31342	-1.16556
C	-1.74952	2.63383	-2.36275
C	-2.08095	3.42542	-3.49312
C	-2.04308	4.83115	-3.46168
C	-1.64723	5.48714	-2.28327
C	-1.31634	4.72663	-1.14998
C	-3.52635	0.08006	-2.02965
C	-3.61396	-0.91653	-1.02922
C	-4.86186	-1.41072	-0.60291
C	-6.04969	-0.91168	-1.16953
C	-5.98283	0.09287	-2.15553
C	-4.73256	0.58324	-2.57787
C	-1.61019	0.43162	-4.45244
C	-2.62735	-0.11521	-5.26938
C	-2.42432	-0.33238	-6.64745
C	-1.18999	-0.00707	-7.23972
C	-0.1609	0.53466	-6.44329
C	-0.37352	0.75062	-5.06975
C	1.95216	2.22944	2.4449
C	3.15835	1.94855	1.73518
C	4.38987	2.27535	2.36098
C	4.44969	2.83055	3.65074
C	3.25791	3.0539	4.3619
C	2.02671	2.75576	3.75697
C	3.26077	2.39313	-1.40162
C	2.17594	2.4678	-2.30606
C	2.15945	3.42854	-3.33568
C	3.23309	4.32647	-3.48226
C	4.32372	4.26182	-2.59272
C	4.33414	3.30437	-1.56161
C	4.87864	0.11711	-0.07682
C	5.37008	-0.60256	1.0415
C	6.51105	-1.41919	0.93976
C	7.1849	-1.54087	-0.29131
C	6.70809	-0.84159	-1.41632
C	5.56694	-0.02406	-1.30729
H	-0.12968	0.7614	3.42675
H	0.98253	3.34364	0.16312
H	-2.99986	1.71315	0.35212
H	-3.58627	-2.86705	3.62627
H	-5.59521	-1.68513	4.44505
H	-5.82796	0.78475	4.06777
H	-4.00168	2.03035	2.9228
H	-1.23328	-4.66866	3.85551
H	-2.01498	-6.9756	3.41239
H	-2.8989	-7.59446	1.15584
H	-2.99317	-5.86577	-0.65101
H	-2.22039	-3.55709	-0.209
H	-0.88645	-1.04398	5.02621
H	0.84797	-1.20796	6.78684
H	2.96449	-2.46814	6.35611
H	3.3128	-3.57918	4.14166
H	1.56988	-3.43031	2.38796
H	-2.35485	2.93751	-4.42517
H	-2.30846	5.40178	-4.34892
H	-1.60017	6.57317	-2.24422
H	-1.02172	5.22661	-0.23013
H	-2.70057	-1.27483	-0.5614
H	-4.90508	-2.16789	0.17682
H	-7.01482	-1.29009	-0.83915
H	-6.89682	0.49503	-2.58786
H	-4.70588	1.37401	-3.32648
H	-3.58332	-0.39068	-4.83096
H	-3.2239	-0.75679	-7.25115
H	-1.0297	-0.17552	-8.30258
H	0.79973	0.78528	-6.88849
H	0.43948	1.16	-4.47367
H	5.32529	2.07963	1.84205
H	5.41241	3.07191	4.09502
H	3.28474	3.46803	5.36727
H	1.1007	2.96022	4.28882
H	1.3369	1.78499	-2.19704
H	1.30481	3.48663	-4.00545
H	3.21835	5.07116	-4.27513
H	5.15659	4.9536	-2.69835
H	5.18531	3.27374	-0.88255
H	4.86476	-0.52408	2.00222
H	6.87123	-1.95686	1.81419
H	8.06825	-2.17082	-0.37206
H	7.22036	-0.93025	-2.37179
H	5.21559	0.51039	-2.18741
Mo	0.65156	-1.19509	-0.6842
O	-0.61681	-1.49022	0.72777
O	-0.59057	-0.01771	-1.71426
O	1.98756	0.04778	-0.23874
Si	-1.13067	-2.13657	2.21461
Si	-1.83133	0.72887	-2.58137
Si	3.27892	1.13729	0.01258
C	-0.58736	-2.65522	-3.50611
C	0.31486	-2.58327	-2.31586
C	1.13712	-3.55663	-1.78146
C	1.3557	-4.99617	-2.18251
C	1.75099	-2.84884	-0.65524
H	-0.59649	-3.66525	-3.94303
H	-0.27914	-1.95037	-4.28709
H	-1.62006	-2.38832	-3.2461
H	0.85775	-5.23848	-3.12726
H	0.96648	-5.67399	-1.40862
H	2.42783	-5.21186	-2.29159
C	2.99685	-3.30038	0.05627
H	3.84241	-3.37018	-0.64846
H	3.29622	-2.6257	0.86162
H	2.85516	-4.309	0.48083

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3711.444432

[Mo]SiP-MTd

B3LYP/LANL2DZ
Zero-point correction= 1.012191 (Hartree/Particle)
Thermal correction to Energy= 1.078188
Thermal correction to Enthalpy= 1.079132
Thermal correction to Gibbs Free Energy= 0.906679

Sum of electronic and zero-point Energies= -2851.193081
Sum of electronic and thermal Energies= -2851.127083
Sum of electronic and thermal Enthalpies= -2851.126139
Sum of electronic and thermal Free Energies= -2851.298592

C	-1.19579	-2.69128	-1.46726
C	-2.2118	-2.38405	-0.5405
C	-2.98453	-1.21262	-0.67302
C	-2.75186	-0.36161	-1.77141
C	-1.74134	-0.64866	-2.71119
C	-0.98095	-1.82503	-2.55825
C	-0.37061	-3.93275	-1.32104
C	0.43957	-4.19974	-0.17674
C	1.14247	-5.43152	-0.13343
C	1.07023	-6.37158	-1.17674
C	0.29391	-6.0843	-2.31269
C	-0.41409	-4.87329	-2.37737
C	-4.05434	-0.89967	0.32734
C	-4.07175	0.30076	1.09935
C	-5.16293	0.50698	1.98244
C	-6.20071	-0.43158	2.12173
C	-6.15647	-1.62508	1.3805
C	-5.08899	-1.85016	0.49633
C	-1.5082	0.27422	-3.86771
C	-0.25602	0.9129	-4.11561
C	-0.14508	1.73004	-5.27041
C	-1.22277	1.9331	-6.15059
C	-2.46063	1.32535	-5.87851
C	-2.59383	0.50743	-4.74493
C	2.37095	-3.40539	2.07838
C	3.53893	-3.34939	1.27566
C	4.8155	-3.57294	1.82148
C	4.95339	-3.86464	3.19362
C	3.8074	-3.92667	4.00808
C	2.53226	-3.69606	3.45382
C	-0.68036	-3.29494	2.61413
C	-0.87279	-4.5702	3.20146
C	-1.8813	-4.78508	4.15951
C	-2.72467	-3.72418	4.54385
C	-2.55391	-2.45392	3.96223
C	-1.53854	-2.24273	3.00974
C	-2.73968	2.51571	2.76146
C	-2.58143	1.74902	3.94424
C	-2.53058	2.35713	5.21124
C	-2.64269	3.75752	5.32528
C	-2.80274	4.53719	4.1647
C	-2.84734	3.91997	2.89848
C	-3.08007	2.94192	-0.28982
C	-4.2927	3.67531	-0.29591
C	-4.56597	4.62047	-1.3025
C	-3.62912	4.84537	-2.33029
C	-2.42371	4.11905	-2.34402
C	-2.15283	3.17928	-1.33098
C	2.31067	2.36579	-3.25501
C	1.71148	3.63376	-3.04289
C	2.45074	4.82374	-3.16561
C	3.81659	4.77224	-3.51015
C	4.4309	3.52463	-3.72569
C	3.68387	2.33663	-3.59555
C	2.35338	-0.72259	-3.48487
C	2.85557	-0.86236	-4.80264
C	3.6373	-1.97401	-5.16889
C	3.92702	-2.97411	-4.22005
C	3.42797	-2.8553	-2.9094
C	2.65146	-1.73801	-2.5467
C	2.34129	1.70225	0.86724
C	2.13089	0.76507	2.00202
C	1.28966	1.98502	1.88025
C	2.93113	0.0479	3.03933
H	-2.39299	-3.05004	0.29816
H	-3.34844	0.53852	-1.8881
H	-0.20665	-2.0623	-3.2821
H	1.77638	-5.65646	0.72129
H	1.6206	-7.30699	-1.10563
H	0.23495	-6.79403	-3.13485
H	-1.02937	-4.65354	-3.24662
H	-5.19604	1.40756	2.59146
H	-7.02277	-0.23659	2.80666
H	-6.94372	-2.36851	1.48392
H	-5.05888	-2.76437	-0.09172
H	0.79396	2.23755	-5.47939
H	-1.09789	2.56473	-7.02715
H	-3.30936	1.48037	-6.54085
H	-3.54441	0.02139	-4.53853
H	3.45493	-3.12785	0.21344
H	5.69492	-3.5211	1.18319
H	5.93888	-4.04047	3.61959
H	3.90359	-4.15004	5.06845
H	1.66096	-3.73797	4.10315
H	-0.24381	-5.40887	2.90569
H	-2.01286	-5.77284	4.59606
H	-3.51132	-3.88892	5.27703
H	-3.22091	-1.63898	4.23463
H	-1.42789	-1.26332	2.55098
H	-2.49599	0.66595	3.87994
H	-2.40538	1.745	6.10176
H	-2.60556	4.23177	6.30367
H	-2.88866	5.61893	4.24221
H	-2.96047	4.5421	2.01383
H	-5.03853	3.50551	0.47957
H	-5.50418	5.17103	-1.28889
H	-3.84103	5.56876	-3.1147
H	-1.70886	4.26986	-3.14996
H	-1.22845	2.60812	-1.36144
H	0.6579	3.69686	-2.77759
H	1.96639	5.7828	-2.99504
H	4.39133	5.69072	-3.60816
H	5.48489	3.4743	-3.99048
H	4.18037	1.38254	-3.75582
H	2.6303	-0.10878	-5.55619
H	4.01098	-2.06236	-6.18678
H	4.52432	-3.83861	-4.50181
H	3.62764	-3.63762	-2.18043
H	2.25438	-1.66418	-1.53729
Mo	0.6376	0.49182	0.52438
O	0.64167	-1.41768	0.79553
O	-1.2131	0.96449	0.79479
O	0.84011	0.64765	-1.38716
Si	0.67224	-3.02389	1.31305
Si	-2.72767	1.65984	1.06263
Si	1.2953	0.7763	-3.00699
C	3.46711	2.40401	0.18118
C	0.82779	3.12708	2.72526
H	0.32155	3.89009	2.12111
H	1.68328	3.60888	3.22483
H	0.1259	2.79798	3.49889
H	3.1003	3.17042	-0.50996
H	4.07991	1.70182	-0.3976
H	4.12423	2.89528	0.91632

H	3.55671	-0.73309	2.59409
H	2.28127	-0.43145	3.78195
H	3.59097	0.74962	3.57366

B3LYP-D3/defTZVP-SDD(Mo)-CPCM(benzene)//B3LYP/LANL2DZ
HF = -3711.463559

[W]-A

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Zero-point correction= 0.588432 (Hartree/Particle)
Thermal correction to Energy= 0.631637
Thermal correction to Enthalpy= 0.632582
Thermal correction to Gibbs Free Energy= 0.511741
Sum of electronic and zero-point Energies= -2401.637346
Sum of electronic and thermal Energies= -2401.594140
Sum of electronic and thermal Enthalpies= -2401.593196
Sum of electronic and thermal Free Energies= -2401.714037

C	-1.92213	1.82654	2.07886
C	-0.63605	2.02757	2.60272
C	0.33561	2.75071	1.89514
C	-0.0097	3.30142	0.65143
C	-1.286	3.11584	0.10001
C	-2.23627	2.38769	0.8321
C	-2.95958	1.07286	2.84565
C	-2.78787	-0.26748	3.28574
C	-3.831	-0.84934	4.03611
C	-5.00622	-0.15964	4.34436
C	-5.17402	1.14756	3.88284
C	-4.15816	1.75052	3.1397
C	-1.93799	-3.16764	2.647
C	0.03606	-1.35029	4.16242
C	-1.62993	3.72801	-1.21872
C	-2.08946	2.97635	-2.33378
C	-2.41769	3.68391	-3.50917
C	-2.29736	5.07251	-3.60552
C	-1.81809	5.79611	-2.5116
C	-1.48723	5.12386	-1.33416
C	-3.89179	0.42613	-1.93258
C	-1.78738	0.52306	-4.18428
C	1.69116	2.96336	2.4855
C	2.89742	2.59837	1.82791
C	4.11289	2.89111	2.48131
C	4.16044	3.5089	3.7336
C	2.96764	3.83689	4.38108
C	1.74923	3.56234	3.75837
C	3.11626	2.76626	-1.31487
C	4.55879	0.53605	0.23933
C	0.68327	-1.88634	-0.98802
C	1.13078	-3.13261	-1.64231
H	-0.38344	1.60755	3.5772
H	0.72973	3.88348	0.10011
H	-3.23808	2.25091	0.42252
H	-3.73508	-1.88246	4.38249
H	-5.79003	-0.64562	4.9311
H	-6.09026	1.70094	4.1047
H	-4.28033	2.7797	2.7923
H	-2.76636	3.13578	-4.3891
H	-2.5653	5.5834	-4.53397
H	-1.70695	6.88199	-2.57024
H	-1.12749	5.68955	-0.4708
H	5.05952	2.61549	2.0081
H	5.12379	3.72073	4.20467
H	2.98299	4.31113	5.36586
H	0.81473	3.83507	4.25536
W	0.14802	-0.3967	-0.21393
O	-0.67073	-0.89407	1.41626
O	-1.06937	0.43003	-1.40057
O	1.69215	0.66777	0.03329
Si	-1.32333	-1.4041	2.86554
Si	-2.20421	1.08094	-2.43764
Si	3.03827	1.64184	0.18985
H	0.66118	-3.25803	-2.63504
H	0.8722	-4.02177	-1.03873
H	2.22602	-3.14002	-1.79104
H	-2.56126	0.80373	-4.91676
H	-1.69805	-0.57578	-4.19202
H	-0.82641	0.94854	-4.5148
H	-4.69243	0.90434	-2.5205
H	-4.09189	0.6062	-0.86563
H	-3.93825	-0.66147	-2.10846
H	-2.7734	-3.20921	1.93006
H	-2.2708	-3.62118	3.59448
H	-1.11344	-3.7826	2.25011
H	0.81181	-2.09519	3.91888
H	-0.36353	-1.58425	5.16291
H	0.51652	-0.36116	4.20518
H	3.32316	2.16515	-2.2159
H	3.92096	3.5122	-1.2077
H	2.16808	3.30122	-1.47475
H	4.53391	-0.13524	-0.63492
H	4.56965	-0.08476	1.14931
H	5.50008	1.10745	0.19745

[W]-A-TS

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -61.00 cm^{-1}
Zero-point correction= 0.675502 (Hartree/Particle)
Thermal correction to Energy= 0.723675
Thermal correction to Enthalpy= 0.724619
Thermal correction to Gibbs Free Energy= 0.595066
Sum of electronic and zero-point Energies= -2557.434867
Sum of electronic and thermal Energies= -2557.386694
Sum of electronic and thermal Enthalpies= -2557.385750
Sum of electronic and thermal Free Energies= -2557.515303

C	-1.93329	1.17884	1.81177
C	-0.67718	1.44601	2.37106
C	0.26566	2.22987	1.69181
C	-0.06908	2.73579	0.42883
C	-1.32985	2.49572	-0.14858
C	-2.26591	1.74678	0.57709
C	-2.86949	0.22154	2.47242
C	-2.58716	-1.16899	2.47072
C	-3.50368	-2.02742	3.10994
C	-4.66077	-1.54411	3.72776
C	-4.93583	-0.17434	3.7025
C	-4.04452	0.69916	3.07407
C	-1.67047	3.0672	-1.486
C	-2.15938	2.29851	-2.5855

C	-2.4532	3.00478	-3.77335
C	-2.26751	4.38381	-3.90661
C	-1.76352	5.11397	-2.83101
C	-1.47356	4.45324	-1.63708
C	1.5637	2.5708	2.35817
C	2.83368	2.10138	1.93617
C	3.96612	2.52874	2.66322
C	3.87274	3.37679	3.76793
C	2.61448	3.81885	4.1844
C	1.47787	3.41475	3.48336
H	-0.42041	1.01965	3.34344
H	0.66673	3.32893	-0.11651
H	-3.25805	1.57659	0.16063
H	-3.32071	-3.10639	3.11849
H	-5.35076	-2.23649	4.21717
H	-5.84257	0.21542	4.1726
H	-4.25212	1.77237	3.05435
H	-2.82842	2.46404	-4.64346
H	-2.50971	4.87873	-4.85068
H	-1.60432	6.19226	-2.91347
H	-1.09899	5.02481	-0.78435
H	4.96025	2.18003	2.36324
H	4.77461	3.68559	4.30299
H	2.51665	4.47952	5.04983
H	0.49265	3.766	3.80119
O	-0.64046	-0.90146	0.35843
O	-0.83033	-0.34048	-2.45692
O	1.84098	0.47286	-0.27519
Si	-1.0959	-1.94771	1.59044
Si	-2.31143	0.38534	-2.73016
Si	3.22531	0.85417	0.55899
C	2.65864	-1.48167	-4.09644
C	2.20126	-0.20431	-3.55444
C	1.86789	0.92292	-3.23261
C	1.81843	-3.57022	-1.50799
C	1.23802	-2.22023	-1.37245
H	2.92046	-3.55454	-1.42295
H	1.56041	-4.0421	-2.47333
H	1.44322	-4.23468	-0.70855
H	3.36098	-1.97918	-3.41107
H	3.16902	-1.32335	-5.06066
H	1.81171	-2.16515	-4.25883
C	1.53359	2.31409	-2.94308
H	2.15264	2.99645	-3.54705
H	0.47473	2.52001	-3.15922
H	1.70544	2.53263	-1.88032
W	0.52102	-0.6319	-1.10853
C	-3.55796	-0.43215	-1.57795
H	-3.83056	-1.41334	-2.00112
H	-3.11461	-0.60273	-0.58711
H	-4.48111	0.15749	-1.45813
C	-2.77894	-0.0562	-4.50091
H	-2.78078	-1.15615	-4.57446
H	-3.78314	0.30136	-4.78139
H	-2.05098	0.32815	-5.23274
C	0.37872	-2.16577	2.73301
H	0.123	-2.76922	3.61896
H	1.19293	-2.67117	2.18806
H	0.75064	-1.18705	3.07355
C	-1.60343	-3.58176	0.81536
H	-0.77968	-3.94456	0.18043
H	-1.82853	-4.35661	1.56565
H	-2.49112	-3.44507	0.17744
C	3.91442	-0.719	1.32456
H	4.84686	-0.53925	1.88321
H	3.17514	-1.15662	2.01381
H	4.117	-1.45628	0.52997
C	4.45779	1.61743	-0.64049
H	5.41966	1.84162	-0.15201
H	4.64403	0.92081	-1.47403
H	4.06337	2.55511	-1.06292

[W]-B

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Zero-point correction= 0.677424 (Hartree/Particle)
Thermal correction to Energy= 0.725025
Thermal correction to Enthalpy= 0.725969
Thermal correction to Gibbs Free Energy= 0.598515
Sum of electronic and zero-point Energies= -2557.447293
Sum of electronic and thermal Energies= -2557.399692
Sum of electronic and thermal Enthalpies= -2557.398748
Sum of electronic and thermal Free Energies= -2557.526203

C	-1.67079	1.15232	1.96754
C	-0.37399	1.24506	2.48813
C	0.61847	1.99752	1.83509
C	0.28091	2.65709	0.64548
C	-1.00339	2.56017	0.09202
C	-1.97802	1.82867	0.78021
C	-2.71996	0.32526	2.63674
C	-2.66064	-1.09093	2.62505
C	-3.69365	-1.79956	3.2701
C	-4.75382	-1.1459	3.90473
C	-4.80913	0.2501	3.89252
C	-3.79886	0.9766	3.25752
C	-1.96117	-3.74055	1.18849
C	0.20163	-2.29822	2.85311
C	-1.33765	3.26528	-1.17833
C	-1.81306	2.57741	-2.3278
C	-2.14536	3.36197	-3.45211
C	-2.01016	4.75374	-3.4651
C	-1.51142	5.40852	-2.33788
C	-1.17786	4.66248	-1.2061
C	-3.32313	-0.15449	-1.63169
C	-2.06253	0.30546	-4.36357
C	1.98258	2.13075	2.4239
C	3.17937	1.93402	1.68006
C	4.40733	2.14008	2.34381
C	4.47882	2.5166	3.687
C	3.29829	2.68185	4.41397
C	2.06875	2.48824	3.78371
C	3.28636	2.63068	-1.42477
C	4.88105	0.27064	-0.28723
H	-0.1307	0.7189	3.41312
H	1.0275	3.26876	0.14026
H	-2.99038	1.77228	0.37921
H	-3.68254	-2.89357	3.26893
H	-5.5393	-1.72536	4.39701
H	-5.63735	0.77463	4.37627
H	-3.83649	2.06916	3.24568
H	-2.51046	2.87812	-4.36042
H	-2.28335	5.32092	-4.35897
H	-1.38907	6.49487	-2.33386
H	-0.80515	5.16917	-0.31185
H	5.34582	1.98945	1.80324
H	5.45069	2.66937	4.16313

H	3.33149	2.96958	5.46798
H	1.14567	2.64238	4.34769
W	0.67797	-0.99016	-0.70262
O	-0.91583	-1.22092	0.33718
O	-0.4268	0.07108	-1.97019
O	2.03008	0.24979	-0.39505
Si	-1.3005	-2.06877	1.73894
Si	-1.87676	0.67029	-2.51902
Si	3.31832	1.29813	-0.10221
C	-0.27854	-2.75789	-3.3276
C	0.55519	-2.52547	-2.11606
C	1.19179	-3.41372	-1.27791
C	1.24715	-4.91324	-1.33255
C	1.75256	-2.57707	-0.22331
H	-0.09868	-3.75267	-3.76974
H	-0.07754	-1.99375	-4.09386
H	-1.35495	-2.68287	-3.08968
H	0.76238	-5.31926	-2.23155
H	0.7549	-5.34398	-0.44364
H	2.29584	-5.25459	-1.30708
C	2.96937	-2.9161	0.57453
H	3.85271	-3.06004	-0.07771
H	3.21137	-2.13555	1.31044
H	2.8289	-3.86436	1.12706
H	4.83735	-0.26159	-1.25147
H	4.9652	-0.47763	0.5153
H	5.79135	0.89138	-0.28487
H	3.55673	2.18493	-2.39621
H	4.01861	3.42216	-1.19501
H	2.29529	3.09475	-1.5317
H	-3.01767	0.68846	-4.75978
H	-2.0554	-0.78315	-4.52361
H	-1.24209	0.74379	-4.9542
H	-4.24958	0.4376	-1.71459
H	-3.08373	-0.31627	-0.57248
H	-3.50778	-1.14246	-2.08692
H	0.8339	-3.12389	2.49541
H	-0.12253	-2.52365	3.88261
H	0.81869	-1.38712	2.87536
H	-2.89129	-3.62453	0.60995
H	-2.15624	-4.41866	2.03483
H	-1.21009	-4.21656	0.53754

[W]-B-TS-B'

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -135.61 cm^{-1}
Zero-point correction= 0.676479 (Hartree/Particle)
Thermal correction to Energy= 0.723579
Thermal correction to Enthalpy= 0.724523
Thermal correction to Gibbs Free Energy= 0.597659
Sum of electronic and zero-point Energies= -2557.441541
Sum of electronic and thermal Energies= -2557.394440
Sum of electronic and thermal Enthalpies= -2557.393496
Sum of electronic and thermal Free Energies= -2557.520361

C	-1.70413	1.10361	1.91525
C	-0.41632	1.19307	2.45882
C	0.57723	1.98577	1.85449
C	0.24846	2.68437	0.68373
C	-1.01858	2.575	0.09633
C	-1.99708	1.81171	0.74323
C	-2.76163	0.25566	2.5408
C	-2.66557	-1.15816	2.5692
C	-3.71665	-1.87744	3.17361
C	-4.82918	-1.23838	3.72748
C	-4.9211	0.15474	3.67262
C	-3.89419	0.89135	3.07868
C	-1.88669	-3.8089	1.18361
C	0.15648	-2.40557	3.00973
C	-1.32286	3.2485	-1.19782
C	-1.7296	2.50836	-2.34123
C	-2.03775	3.2393	-3.50666
C	-1.94139	4.63342	-3.5631
C	-1.50747	5.3411	-2.44044
C	-1.19957	4.64684	-1.26844
C	-3.17731	-0.25998	-1.6479
C	-1.69094	0.12144	-4.28763
C	1.93972	2.07834	2.45556
C	3.14004	1.97558	1.69618
C	4.36297	2.09944	2.38951
C	4.42912	2.30929	3.76916
C	3.24559	2.39244	4.50466
C	2.02019	2.27703	3.84858
C	3.34764	3.15404	-1.22735
C	4.91154	0.65836	-0.46825
H	-0.1805	0.62834	3.36244
H	0.99491	3.31588	0.20625
H	-2.99795	1.7482	0.31498
H	-3.67814	-2.97036	3.2031
H	-5.62644	-1.82701	4.18889
H	-5.79015	0.66867	4.09173
H	-3.95915	1.98177	3.03556
H	-2.3483	2.70953	-4.41073
H	-2.19187	5.16198	-4.4868
H	-1.41465	6.4299	-2.4723
H	-0.87497	5.19482	-0.37968
H	5.30446	2.01642	1.84003
H	5.39911	2.40066	4.26472
H	3.27295	2.55529	5.58523
H	1.09557	2.36784	4.42352
O	-0.72401	-1.32941	0.41769
O	-0.28659	0.05743	-1.79219
O	2.04402	0.63782	-0.68257
Si	-1.24939	-2.1433	1.785
Si	-1.70542	0.59779	-2.46086
Si	3.3084	1.60015	-0.1661
C	0.4762	-3.23918	-2.69941
C	1.18144	-2.51465	-1.60878
C	1.95285	-2.96652	-0.53466
C	2.36299	-4.40024	-0.30275
C	2.26323	-1.91615	0.44607
H	1.03733	-4.12257	-3.04721
H	0.31644	-2.56846	-3.55721
H	-0.52321	-3.57658	-2.36758
H	2.04223	-5.06292	-1.11768
H	1.92619	-4.75813	0.64426
H	3.45773	-4.4648	-0.195
C	3.34212	-2.06539	1.46109
H	4.31106	-2.33208	1.00049
H	3.47802	-1.13586	2.03366
H	3.10669	-2.86917	2.18305
H	4.87925	0.24262	-1.48884
H	5.03946	-0.1743	0.23795
H	5.79561	1.31286	-0.40061
H	3.63716	2.87991	-2.25551
H	4.09544	3.86653	-0.84131

H	2.37613	3.66673	-1.27963
H	-2.64346	0.35628	-4.79102
H	-1.53531	-0.9677	-4.36124
H	-0.87486	0.62099	-4.83353
H	-4.12055	0.29112	-1.79662
H	-2.99822	-0.3904	-0.57188
H	-3.29417	-1.26446	-2.0891
H	0.80196	-3.23719	2.68831
H	-0.24548	-2.64379	4.00814
H	0.78463	-1.5059	3.08672
H	-2.7664	-3.68223	0.533
H	-2.15798	-4.48236	2.01257
H	-1.09273	-4.29931	0.59612
W	0.89982	-0.8828	-0.51386

[W]-B'

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Zero-point correction= 0.677501 (Hartree/Particle)
Thermal correction to Energy= 0.725005
Thermal correction to Enthalpy= 0.725949
Thermal correction to Gibbs Free Energy= 0.598897
Sum of electronic and zero-point Energies= -2557.459719
Sum of electronic and thermal Energies= -2557.412216
Sum of electronic and thermal Enthalpies= -2557.411271
Sum of electronic and thermal Free Energies= -2557.538324

W	7.98351	3.25548	5.69037
Si	8.65285	-0.18677	6.02703
Si	6.25751	5.71952	3.87628
Si	11.33721	3.61209	4.67377
O	8.74831	1.45126	5.87621
O	7.36949	4.84213	4.72718
O	9.70959	3.72074	5.03744
C	8.5168	-1.11274	4.36513
C	8.54391	-2.5188	4.50531
H	8.66324	-2.95629	5.50184
C	8.42017	-3.3876	3.42017
H	8.44694	-4.46936	3.57597
C	8.26058	-2.85968	2.13662
H	8.16121	-3.52087	1.27175
C	8.22985	-1.47546	1.96569
H	8.10683	-1.05568	0.96368
C	8.35802	-0.5928	3.05619
C	8.30126	0.86852	2.7222
C	9.47029	1.61097	2.5081
H	10.4417	1.13076	2.6351
C	9.40905	2.9509	2.09674
C	8.15623	3.55092	1.90961
H	8.10878	4.59226	1.5894
C	6.97082	2.83912	2.13318
C	7.06248	1.48775	2.51128
H	6.15013	0.91121	2.6654
C	5.6341	3.47814	1.96139
C	5.25339	4.68118	2.61744
C	3.95598	5.17356	2.35656
H	3.62225	6.09422	2.84243
C	3.0573	4.52486	1.5061
H	2.06299	4.94573	1.33497
C	3.43867	3.33265	0.88762
H	2.74982	2.80554	0.22236
C	4.71532	2.82097	1.11944
H	5.02356	1.89661	0.62437
C	10.65262	3.72944	1.82344
C	11.59426	4.02686	2.84005
C	12.74972	4.74699	2.47523
H	13.49191	5.00209	3.23699
C	12.9773	5.16927	1.16244
H	13.88603	5.72416	0.9147
C	12.02845	4.89112	0.17553
H	12.18608	5.22414	-0.85371
C	10.87489	4.17885	0.50969
H	10.13346	3.94936	-0.26026
C	6.1186	2.50644	5.72331
C	6.25401	2.99233	7.01506
C	7.54436	3.67914	7.44903
C	4.97119	1.80943	5.09745
H	5.26431	0.79706	4.77467
H	4.10712	1.71259	5.77485
H	4.64189	2.34639	4.19433
C	5.20431	2.88842	8.0928
H	4.93836	3.89173	8.46008
H	4.29812	2.39093	7.72545
H	5.601	2.31921	8.94799
C	7.79696	4.23839	8.79974
H	7.0743	5.03242	9.05868
H	7.73792	3.46383	9.58495
H	8.80495	4.67654	8.83396
C	12.19474	4.91462	5.72808
H	13.29228	4.86815	5.63904
H	11.86534	5.92855	5.45054
H	11.93527	4.74535	6.78615
C	12.00132	1.91288	5.11938
H	13.05689	1.82133	4.81404
H	11.93696	1.75788	6.20779
H	11.42324	1.11588	4.63364
C	10.19749	-0.80523	6.91542
H	10.13086	-1.87842	7.15605
H	11.09926	-0.64473	6.30572
H	10.32248	-0.25119	7.86076
C	7.13979	-0.62987	7.06799
H	7.19973	-0.11965	8.04411
H	6.20747	-0.31301	6.57718
H	7.07886	-1.71509	7.25033
C	5.04816	6.42208	5.14576
H	5.63282	6.90266	5.94773
H	4.35571	7.17423	4.73582
H	4.45375	5.61099	5.59762
C	7.14234	7.12198	2.9845
H	7.59681	7.80734	3.71909
H	7.94715	6.74115	2.33649
H	6.44191	7.69968	2.35923

[W]-B-TS-ent-B

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -35.17 cm^{-1}
Zero-point correction= 0.676893 (Hartree/Particle)
Thermal correction to Energy= 0.723559
Thermal correction to Enthalpy= 0.724503
Thermal correction to Gibbs Free Energy= 0.599376
Sum of electronic and zero-point Energies= -2557.443042
Sum of electronic and thermal Energies= -2557.396376

Sum of electronic and thermal Enthalpies= -2557.395432
Sum of electronic and thermal Free Energies= -2557.520560

C	-1.72853	1.1171	1.95008
C	-0.42825	1.1612	2.46836
C	0.58252	1.91329	1.83857
C	0.25458	2.6133	0.66862
C	-1.02188	2.53309	0.0966
C	-2.01664	1.81669	0.77146
C	-2.80904	0.32578	2.61074
C	-2.81011	-1.09098	2.61208
C	-3.88124	-1.744	3.25713
C	-4.91834	-1.03985	3.87419
C	-4.91387	0.35705	3.84646
C	-3.86635	1.02937	3.21421
C	-2.32484	-3.7506	1.12982
C	-0.19495	-2.66934	3.06415
C	-1.30544	3.18065	-1.21547
C	-1.72882	2.42606	-2.34459
C	-1.99612	3.1449	-3.52846
C	-1.84553	4.53269	-3.61717
C	-1.39848	5.2509	-2.50697
C	-1.13003	4.57174	-1.31688
C	-3.32963	-0.21423	-1.5568
C	-1.93981	0.02133	-4.25908
C	1.97165	1.91824	2.38274
C	3.13088	1.77676	1.5657
C	4.38534	1.79405	2.21181
C	4.52246	1.93147	3.59526
C	3.37823	2.05359	4.38555
C	2.12256	2.04734	3.7784
C	3.38384	3.11624	-1.26245
C	4.74279	0.44661	-0.71379
H	-0.19391	0.58044	3.36264
H	1.01398	3.20969	0.16743
H	-3.02599	1.78072	0.36074
H	-3.91825	-2.8371	3.27236
H	-5.73174	-1.58041	4.36542
H	-5.72265	0.92308	4.31612
H	-3.85468	2.12232	3.19069
H	-2.32032	2.6096	-4.42384
H	-2.06592	5.04725	-4.55642
H	-1.26431	6.33449	-2.56233
H	-0.79368	5.12719	-0.43709
H	5.29703	1.68157	1.6193
H	5.51621	1.93821	4.05069
H	3.46009	2.16308	5.4701
H	1.2304	2.16901	4.39721
O	-0.81512	-1.42925	0.4721
O	-0.42651	-0.17261	-1.8528
O	1.89452	0.66032	-0.91584
Si	-1.49737	-2.18925	1.7867
Si	-1.81712	0.50636	-2.43453
Si	3.21463	1.49053	-0.32623
C	1.20549	-3.07462	-2.86079
C	1.35659	-2.35091	-1.57984
C	2.17364	-2.57952	-0.42574
C	3.1492	-3.73152	-0.3651
C	2.11348	-1.67716	0.76339
H	2.1703	-3.17208	-3.38773
H	0.51142	-2.51798	-3.5081
H	0.79599	-4.08803	-2.70536
H	3.08743	-4.35821	-1.26356
H	2.94717	-4.34633	0.5251
H	4.17326	-3.33805	-0.26728
C	2.99185	-1.83977	1.94507
H	4.06102	-1.80795	1.67104
H	2.8062	-1.02234	2.65665
H	2.81428	-2.79824	2.46333
H	4.6901	0.15095	-1.77478
H	4.77603	-0.47057	-0.10608
H	5.68732	0.99402	-0.56516
H	3.59117	2.90408	-2.3245
H	4.22404	3.70624	-0.86001
H	2.47595	3.73617	-1.21753
H	-2.89315	0.33183	-4.71814
H	-1.88153	-1.07817	-4.32456
H	-1.11258	0.44209	-4.85292
H	-4.21724	0.43392	-1.64494
H	-3.11106	-0.38387	-0.49362
H	-3.57386	-1.19159	-2.00685
H	0.48987	-3.43058	2.65738
H	-0.68309	-3.08972	3.95904
H	0.404	-1.80031	3.37551
H	-3.15268	-3.49381	0.44971
H	-2.71869	-4.39733	1.93036
H	-1.58257	-4.33347	0.5593
W	0.8289	-0.92622	-0.45766

[W]-C

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Zero-point correction= 0.678449 (Hartree/Particle)
Thermal correction to Energy= 0.725649
Thermal correction to Enthalpy= 0.726593
Thermal correction to Gibbs Free Energy= 0.600119
Sum of electronic and zero-point Energies= -2557.450847
Sum of electronic and thermal Energies= -2557.403648
Sum of electronic and thermal Enthalpies= -2557.402703
Sum of electronic and thermal Free Energies= -2557.529177

C	-1.2514	-2.71901	-1.49326
C	-2.25876	-2.39948	-0.57449
C	-3.02337	-1.2332	-0.7145
C	-2.7865	-0.39696	-1.81246
C	-1.78305	-0.69373	-2.74506
C	-1.03384	-1.86569	-2.58375
C	-0.45327	-3.96875	-1.33951
C	0.35645	-4.21589	-0.20026
C	1.0275	-5.45476	-0.13398
C	0.92331	-6.41459	-1.14463
C	0.14824	-6.14345	-2.27414
C	-0.53067	-4.9271	-2.366
C	-4.09895	-0.91194	0.26643
C	-4.089	0.2797	1.03767
C	-5.18236	0.50788	1.89878
C	-6.24194	-0.39638	2.01456
C	-6.22096	-1.57985	1.2737
C	-5.15373	-1.83106	0.40948
C	-1.54899	0.2028	-3.91326
C	-0.30893	0.85897	-4.12882
C	-0.1832	1.6467	-5.29218
C	-1.22841	1.79795	-6.20774
C	-2.45195	1.16995	-5.96589
C	-2.60562	0.38223	-4.82366
C	2.3705	-3.37621	1.94929

C	-0.58695	-2.86068	2.52838
C	-2.72815	2.43576	2.73577
C	-2.59743	2.76432	-0.30722
C	2.17117	2.40334	-3.21013
C	2.26609	-0.65022	-3.00607
C	2.19355	1.80438	0.84555
C	2.22525	0.70792	1.82726
C	1.25891	1.80857	1.98316
C	3.27841	0.09049	2.6818
H	-2.45366	-3.0699	0.26375
H	-3.39348	0.49972	-1.94584
H	-0.26843	-2.12016	-3.31839
H	1.66596	-5.68065	0.72353
H	1.45682	-7.36444	-1.05438
H	0.06578	-6.87805	-3.07951
H	-1.1529	-4.71566	-3.23955
H	-5.20923	1.41066	2.51377
H	-7.07311	-0.18179	2.6914
H	-7.0353	-2.30384	1.36192
H	-5.1394	-2.74791	-0.18568
H	0.7525	2.17443	-5.49169
H	-1.08954	2.41491	-7.09939
H	-3.28374	1.28732	-6.66545
H	-3.55575	-0.12431	-4.63485
W	0.62652	0.47795	0.51989
O	0.81107	-1.43395	0.4435
O	-1.22092	0.61639	1.03534
O	0.49772	0.91193	-1.35034
Si	0.71307	-2.9437	1.16894
Si	-2.63969	1.51137	1.09862
Si	1.14281	0.85751	-2.8991
C	3.18558	2.77149	0.29695
C	0.91323	2.75872	3.07762
H	0.38938	3.64721	2.68972
H	1.82409	3.10805	3.59601
H	0.26104	2.28476	3.82859
H	2.69288	3.55978	-0.29442
H	3.92002	2.27078	-0.35442
H	3.7452	3.26361	1.11255
H	3.90641	-0.60649	2.10417
H	2.83878	-0.47001	3.52266
H	3.94075	0.86505	3.10826
H	-2.18971	2.31182	-1.22279
H	-1.93632	3.60074	-0.02331
H	-3.59592	3.17598	-0.52699
H	-1.50877	-2.37553	2.17693
H	-0.19026	-2.26031	3.36482
H	-0.83877	-3.8619	2.91487
H	3.17495	-3.40867	1.19735
H	2.33631	-4.35142	2.46168
H	2.63016	-2.6174	2.70095
H	-1.85432	3.0961	2.83092
H	-2.73249	1.74215	3.59163
H	-3.62925	3.06766	2.7976
H	2.54503	-0.88483	-4.04628
H	1.78883	-1.53429	-2.55919
H	3.19144	-0.44741	-2.44027
H	2.63941	2.385	-4.20779
H	2.97906	2.46211	-2.46705
H	1.56105	3.3172	-3.13144

[W]-B-TS

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -191.45 cm^{-1}

Zero-point correction= 0.676752
(Hartree/Particle)
Thermal correction to Energy= 0.723761
Thermal correction to Enthalpy= 0.724705
Thermal correction to Gibbs Free Energy=
0.598409
Sum of electronic and zero-point Energies= -
2557.419417
Sum of electronic and thermal Energies= -
2557.372408
Sum of electronic and thermal Enthalpies= -
2557.371464
Sum of electronic and thermal Free Energies= -
2557.497760

C	-0.99979	-2.59292	-1.32717
C	-1.88427	-2.21958	-0.3063
C	-2.67119	-1.0594	-0.41462
C	-2.55637	-0.27803	-1.57208
C	-1.63285	-0.59542	-2.57415
C	-0.88634	-1.77236	-2.45642
C	-0.20397	-3.85261	-1.255
C	0.73852	-4.11055	-0.22807
C	1.41589	-5.34785	-0.25707
C	1.19176	-6.29827	-1.2562
C	0.27962	-6.01965	-2.27673
C	-0.4062	-4.80431	-2.27235
C	-3.64185	-0.68931	0.6534
C	-3.73117	0.62331	1.19878
C	-4.732	0.85415	2.16698
C	-5.60642	-0.14627	2.60039
C	-5.48896	-1.43398	2.07598
C	-4.51365	-1.6948	1.11319
C	-1.42103	0.32201	-3.72864
C	-0.16407	0.94926	-3.93316
C	-0.03322	1.78261	-5.06265
C	-1.08966	2.005	-5.95133
C	-2.32839	1.4032	-5.71678
C	-2.48857	0.56929	-4.60816
C	3.01975	-3.22621	1.60931
C	0.08329	-3.14335	2.6489
C	-2.75462	3.34737	2.24274
C	-2.77663	2.99277	-0.77509
C	2.27147	2.45013	-2.84228
C	2.45817	-0.59623	-3.08067
C	2.15076	1.72611	1.36325
C	1.21336	0.46333	2.71433
C	1.3188	1.91973	2.44563
C	2.04176	-0.19933	3.76513
H	-1.97318	-2.84681	0.58166
H	-3.18952	0.59881	-1.69403
H	-0.18965	-2.04669	-3.24988
H	2.15448	-5.5789	0.51534
H	1.73578	-7.24636	-1.24303
H	0.0984	-6.74676	-3.07265
H	-1.12921	-4.58567	-3.06248
H	-4.83355	1.84443	2.61557
H	-6.36823	0.08064	3.35068
H	-6.15895	-2.23231	2.40567
H	-4.43782	-2.69593	0.68196
H	0.91635	2.28946	-5.25463
H	-0.94821	2.65695	-6.81755
H	-3.16673	1.57756	-6.39644
H	-3.45088	0.08422	-4.42316
W	0.60842	0.49899	0.80634
O	1.11258	-1.33144	0.60575
O	-0.95827	1.55298	0.90397

O	0.70762	0.68343	-1.16653
Si	1.21733	-2.90648	1.1608
Si	-2.54782	2.08426	0.86141
Si	1.29392	0.83896	-2.70099
C	3.34309	2.41853	0.81103
C	0.7578	3.10552	3.15591
H	0.64907	3.96856	2.48095
H	1.41531	3.40413	3.99119
H	-0.22772	2.86271	3.57879
H	3.00311	3.33039	0.28614
H	3.88107	1.79767	0.0808
H	4.03346	2.73261	1.6109
H	1.59318	-0.00397	4.757
H	3.0682	0.20872	3.79787
H	2.09913	-1.28711	3.63595
H	2.75777	-0.61049	-4.1417
H	1.99676	-1.56387	-2.83367
H	3.37014	-0.49548	-2.46787
H	2.72646	2.58461	-3.8372
H	3.08769	2.44616	-2.10333
H	1.62774	3.32115	-2.63733
H	-1.96934	4.11224	2.13775
H	-2.66559	2.89491	3.24251
H	-3.72868	3.85945	2.17805
H	-2.1794	2.53644	-1.57795
H	-2.44003	4.03571	-0.65395
H	-3.83277	3.01151	-1.09014
H	-0.83686	-2.55222	2.52392
H	0.56224	-2.81811	3.58474
H	-0.19497	-4.20426	2.75651
H	3.64203	-3.25717	0.70073
H	3.15472	-4.1757	2.15224
H	3.39529	-2.41492	2.25133

[W]-D-TS

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -35.99 cm^{-1}
Zero-point correction= 0.676816 (Hartree/Particle)
Thermal correction to Energy= 0.723480
Thermal correction to Enthalpy= 0.724425
Thermal correction to Gibbs Free Energy= 0.601112
Sum of electronic and zero-point Energies= -2557.396992
Sum of electronic and thermal Energies= -2557.350328
Sum of electronic and thermal Enthalpies= -2557.349383
Sum of electronic and thermal Free Energies= -2557.472696

C	-1.25644	1.21666	2.08453
C	0.0868	1.59479	1.96596
C	0.56149	2.18625	0.79428
C	-0.36619	2.49271	-0.21999
C	-1.71484	2.13403	-0.12208
C	-2.15257	1.49639	1.04499
C	-1.6551	0.31461	3.20266
C	-1.74557	-1.07264	2.9277
C	-2.0915	-1.92924	3.99064
C	-2.33706	-1.4409	5.2782
C	-2.22979	-0.07075	5.5333
C	-1.88543	0.80188	4.49691
C	-2.67934	2.514	-1.20706
C	-2.9708	1.74613	-2.36663
C	-3.89411	2.30672	-3.28315
C	-4.51309	3.54165	-3.09002
C	-4.22289	4.27642	-1.93925
C	-3.31489	3.75859	-1.0171
C	2.01263	2.48201	0.58657
C	3.04578	1.49274	0.5666
C	4.34972	1.95754	0.27921
C	4.6511	3.29882	0.02406
C	3.6304	4.24733	0.05132
C	2.3282	3.82994	0.32819
H	0.78064	1.36313	2.77369
H	-0.02965	3.00791	-1.11706
H	-3.19479	1.18143	1.13294
H	-2.16653	-3.00725	3.8187
H	-2.60479	-2.13054	6.08326
H	-2.41373	0.31912	6.53804
H	-1.79797	1.87499	4.68724
H	-4.14647	1.75636	-4.19464
H	-5.21793	3.92395	-3.8331
H	-4.6961	5.24545	-1.76022
H	-3.07735	4.32936	-0.11551
H	5.17683	1.24753	0.24084
H	5.68065	3.59437	-0.19477
H	3.84052	5.30276	-0.14075
H	1.52031	4.56579	0.34919
W	0.47615	-0.81591	-1.41355
O	-0.39672	-0.83	0.32911
O	-1.36039	-0.88895	-2.11385
O	2.10034	-1.20932	-0.37534
Si	-1.42855	-1.80621	1.19682
Si	-2.38939	0.03694	-3.03193
Si	2.94895	-0.42584	0.82983
C	1.54602	-1.60835	-3.62489
C	1.04949	0.67444	-2.22922
C	1.00065	-2.38392	-2.79621
C	2.23349	-0.91911	2.50148
H	1.13868	-0.85496	2.4995
H	2.51419	-1.96579	2.70675
H	2.62498	-0.29386	3.32063
C	4.69748	-1.13517	0.75675
H	5.35639	-0.73702	1.5454
H	4.61144	-2.22395	0.90868
H	5.17975	-0.97243	-0.22028
C	-1.54491	0.36727	-4.69124
H	-0.69735	1.057	-4.55693
H	-1.15441	-0.58122	-5.09562
H	-2.22795	0.80738	-5.43441
C	-3.93506	-1.01497	-3.28314
H	-4.42635	-1.2009	-2.315
H	-4.67053	-0.55274	-3.95921
H	-3.64401	-1.99126	-3.70577
C	-3.07257	-2.01549	0.30683
H	-2.91238	-2.49515	-0.66984
H	-3.7631	-2.63009	0.90808
H	-3.54532	-1.03907	0.12375
C	-0.61012	-3.49513	1.39389
H	0.36002	-3.3973	1.90588
H	-1.23333	-4.20911	1.95599
H	-0.42658	-3.92421	0.39519
C	1.54728	1.92951	-2.79876
H	2.31298	1.72071	-3.56556
H	0.75269	2.52905	-3.27817
H	2.04153	2.54528	-2.03033
C	2.17842	-0.71004	-4.58443
H	1.45409	0.01482	-4.97963
H	3.02137	-0.17513	-4.1253

H	2.57595	-1.2907	-5.43638
C	0.63181	-3.79239	-2.47829
H	1.14751	-4.11542	-1.56085
H	-0.45166	-3.86342	-2.29619
H	0.90569	-4.46718	-3.30247

[W]-A-Ph

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Zero-point correction= 0.918026
(Hartree/Particle)
Thermal correction to Energy= 0.978882
Thermal correction to Enthalpy= 0.979826
Thermal correction to Gibbs Free Energy=
0.816105
Sum of electronic and zero-point Energies= -
3550.979886
Sum of electronic and thermal Energies= -
3550.919029
Sum of electronic and thermal Enthalpies= -
3550.918085
Sum of electronic and thermal Free Energies= -
3551.081806

C	-1.97202	1.66924	1.90319
C	-0.73637	1.81989	2.54852
C	0.31489	2.53379	1.95124
C	0.09357	3.14359	0.70823
C	-1.13488	3.01469	0.04022
C	-2.16219	2.28374	0.65495
C	-3.08423	0.88465	2.51858
C	-2.94309	-0.47336	2.91629
C	-4.05985	-1.11996	3.48117
C	-5.28416	-0.46798	3.6548
C	-5.41888	0.85867	3.2417
C	-4.32746	1.52192	2.67696
C	-1.83984	-3.33396	2.57082
C	-1.75312	-4.16786	3.70043
C	-2.11633	-5.51739	3.62791
C	-2.56682	-6.05635	2.41811
C	-2.65062	-5.24369	1.28134
C	-2.29025	-3.89524	1.35943
C	-0.03352	-1.15497	3.87119
C	-0.34106	-0.97872	5.23396
C	0.65318	-0.64343	6.15964
C	1.97434	-0.46615	5.73418
C	2.29821	-0.63646	4.38433
C	1.30354	-0.98241	3.46588
C	-1.32449	3.67897	-1.28415
C	-1.73569	2.9852	-2.45583
C	-1.87105	3.72376	-3.64866
C	-1.61059	5.09547	-3.70786
C	-1.1861	5.76201	-2.55756
C	-1.0454	5.05496	-1.36243
C	-3.61266	0.54069	-1.83081
C	-3.69621	-0.71549	-1.20186
C	-4.87008	-1.13016	-0.56681
C	-5.99323	-0.29594	-0.56431
C	-5.93735	0.94769	-1.20338
C	-4.7554	1.36235	-1.82674
C	-1.81793	0.55856	-4.36317
C	-2.91232	0.54243	-5.24748
C	-2.75513	0.14408	-6.57925
C	-1.49713	-0.2532	-7.04605
C	-0.39959	-0.25333	-6.17763
C	-0.56073	0.14885	-4.84797
C	1.63027	2.63801	2.65054
C	2.86007	2.25648	2.04557
C	4.03989	2.38325	2.80509
C	4.02999	2.86614	4.11671
C	2.81593	3.22009	4.70734
C	1.63173	3.10215	3.97742
C	2.87555	2.71806	-1.06353
C	2.09806	2.43943	-2.20349
C	1.91392	3.39674	-3.20451
C	2.51734	4.65308	-3.08883
C	3.30543	4.94561	-1.97014
C	3.47683	3.98752	-0.96483
C	4.61412	0.48519	0.22883
C	4.62595	-0.85758	0.65479
C	5.79965	-1.61607	0.60949
C	6.98511	-1.04211	0.1357
C	6.9903	0.28841	-0.29692
C	5.8126	1.04251	-0.25329
C	0.79402	-2.04474	-1.14144
C	1.29689	-3.29002	-1.75218
H	-0.57657	1.35896	3.52244
H	0.88991	3.72048	0.24056
H	-3.12459	2.17923	0.15661
H	-3.97963	-2.17042	3.77425
H	-6.13059	-0.99976	4.09687
H	-6.37231	1.38058	3.35766
H	-4.43228	2.56219	2.35886
H	-1.38964	-3.76384	4.65037
H	-2.04202	-6.15127	4.51563
H	-2.84773	-7.1113	2.35925
H	-2.99475	-5.66311	0.3321
H	-2.34825	-3.26932	0.46446
H	-1.37509	-1.07945	5.5792
H	0.39369	-0.5057	7.21278
H	2.74871	-0.18264	6.45159
H	3.32212	-0.47498	4.03865
H	1.57453	-1.0817	2.41332
H	-2.16674	3.21008	-4.567
H	-1.7257	5.63478	-4.65154
H	-0.96434	6.83196	-2.58646
H	-0.72047	5.57921	-0.4604
H	-2.82561	-1.37607	-1.19273
H	-4.90241	-2.09817	-0.06018
H	-6.90857	-0.61156	-0.0573
H	-6.81268	1.60275	-1.20257
H	-4.71616	2.35253	-2.29177
H	-3.90458	0.83724	-4.89152
H	-3.61616	0.13712	-7.25306
H	-1.37339	-0.56825	-8.08564
H	0.58303	-0.57083	-6.53687
H	0.29837	0.13427	-4.17109
H	4.99382	2.07479	2.36903
H	4.96489	2.95088	4.67657
H	2.78681	3.58762	5.73636
H	0.68221	3.38382	4.43919
H	1.59545	1.47525	-2.30144
H	1.27797	3.16828	-4.06318
H	2.36335	5.4078	-3.86431
H	3.77518	5.92813	-1.87315
H	4.06773	4.24601	-0.08014
H	3.70147	-1.31716	1.01597
H	5.78976	-2.65768	0.94161
H	7.90388	-1.63355	0.09882
H	7.91269	0.73755	-0.67493
H	5.82875	2.07768	-0.6081
W	0.21507	-0.56431	-0.38528
O	-0.80451	-1.11403	1.10748

O	-0.76183	0.34655	-1.73378
O	1.76669	0.37308	0.15519
Si	-1.38718	-1.51014	2.61348
Si	-1.97916	1.10934	-2.57207
Si	3.011	1.46189	0.33139
H	1.05107	-3.33972	-2.82829
H	0.85715	-4.17955	-1.26596
H	2.39523	-3.36487	-1.65606

[W]-A-TS-Ph

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -61.24 cm^{-1}
Zero-point correction= 1.004403 (Hartree/Particle)
Thermal correction to Energy= 1.070417
Thermal correction to Enthalpy= 1.071361
Thermal correction to Gibbs Free Energy= 0.900808
Sum of electronic and zero-point Energies= -3706.779892
Sum of electronic and thermal Energies= -3706.713879
Sum of electronic and thermal Enthalpies= -3706.712935
Sum of electronic and thermal Free Energies= -3706.883487

C	-1.9988	1.11472	1.78201
C	-0.76004	1.33221	2.39502
C	0.25886	2.05501	1.7568
C	-0.00516	2.59897	0.49095
C	-1.2619	2.438	-0.12788
C	-2.25447	1.70525	0.53929
C	-2.98586	0.17765	2.39067
C	-2.65004	-1.19036	2.57186
C	-3.61311	-2.04142	3.14433
C	-4.87404	-1.5713	3.52409
C	-5.20293	-0.23027	3.31284
C	-4.26329	0.63477	2.74636
C	-1.24328	-3.748	1.53212
C	-1.129	-4.7278	2.53758
C	-1.31935	-6.08357	2.25102
C	-1.61779	-6.48625	0.94446
C	-1.72041	-5.52914	-0.07079
C	-1.53445	-4.17446	0.22263
C	0.38334	-1.71661	3.17059
C	0.16952	-1.44018	4.53308
C	1.24689	-1.23196	5.40161
C	2.55859	-1.29505	4.91844
C	2.79004	-1.58124	3.56851
C	1.71014	-1.79505	2.70854
C	-1.54735	3.06524	-1.45297
C	-2.06941	2.3538	-2.57329
C	-2.32988	3.09451	-3.7457
C	-2.07291	4.46508	-3.84493
C	-1.52407	5.1396	-2.75458
C	-1.27008	4.43943	-1.57404
C	-3.83193	-0.11275	-1.76738
C	-3.75604	-1.26185	-0.96153
C	-4.85462	-1.69425	-0.21437
C	-6.05562	-0.98	-0.26278
C	-6.15232	0.16654	-1.06011
C	-5.04753	0.59736	-1.80215
C	-2.5087	0.04973	-4.55874
C	-3.75881	-0.01197	-5.20116
C	-3.8548	-0.29825	-6.5676
C	-2.69639	-0.53395	-7.31567
C	-1.44457	-0.48713	-6.69124
C	-1.35323	-0.19995	-5.32569
C	1.55304	2.22946	2.49131
C	2.82497	1.80508	2.02015
C	3.93725	1.98816	2.86782
C	3.82936	2.56418	4.13433
C	2.57601	2.97512	4.59132
C	1.45801	2.80288	3.77591
C	3.72365	2.37243	-0.85667
C	3.40344	3.72502	-0.63523
C	3.75322	4.71452	-1.56062
C	4.44764	4.36717	-2.72397
C	4.798	3.03079	-2.95139
C	4.44051	2.04766	-2.02486
C	4.60938	-0.25084	0.40321
C	5.95997	0.11456	0.56631
C	6.9753	-0.84731	0.57341
C	6.65977	-2.19978	0.39967
C	5.32755	-2.58104	0.20882
C	4.31566	-1.61483	0.20864
H	-0.56062	0.88966	3.37031
H	0.7738	3.15918	-0.02691
H	-3.22813	1.56301	0.07341
H	-3.38573	-3.10349	3.2735
H	-5.6032	-2.25547	3.96574
H	-6.19229	0.14472	3.58755
H	-4.51633	1.68519	2.5807
H	-0.87749	-4.43076	3.5607
H	-1.22752	-6.82827	3.04626
H	-1.76304	-7.54567	0.71679
H	-1.93972	-5.83821	-1.09628
H	-1.58874	-3.44336	-0.58648
H	-0.85196	-1.36343	4.9187
H	1.06258	-1.00837	6.45587
H	3.40016	-1.11365	5.59198
H	3.8096	-1.62276	3.17753
H	1.90311	-2.00316	1.65496
H	-2.72335	2.58119	-4.62577
H	-2.28905	4.9957	-4.77575
H	-1.30207	6.20824	-2.81466
H	-0.86286	4.97115	-0.71054
H	-2.81157	-1.80142	-0.89533
H	-4.76384	-2.57458	0.42546
H	-6.9118	-1.30827	0.33203
H	-7.08756	0.732	-1.09479
H	-5.13182	1.51137	-2.39905
H	-4.67489	0.15901	-4.62789
H	-4.83577	-0.34247	-7.0486
H	-2.76938	-0.75925	-8.38312
H	-0.53673	-0.67826	-7.27021
H	-0.37085	-0.17734	-4.84493
H	4.92353	1.64998	2.54151
H	4.71694	2.68235	4.76104
H	2.46535	3.42681	5.58055
H	0.47734	3.12491	4.13444
H	2.87943	4.01639	0.27952
H	3.48814	5.75802	-1.37088
H	4.72331	5.13736	-3.44927
H	5.34827	2.75536	-3.8551
H	4.71433	1.00749	-2.21889
H	6.23315	1.16909	0.67069
H	8.0164	-0.5408	0.70595
H	7.45237	-2.95279	0.40274
H	5.07367	-3.6337	0.05643
H	3.28204	-1.91875	0.03419

O	-0.61469	-1.09991	0.5462
O	-1.00299	-0.41233	-2.22022
O	1.86776	0.20398	-0.20225
Si	-1.02276	-1.92289	1.93863
Si	-2.32116	0.46071	-2.72632
Si	3.20468	1.00922	0.34398
C	2.99032	-1.62497	-3.63213
C	2.20692	-0.42815	-3.3354
C	1.69075	0.66918	-3.20314
C	1.50329	-3.79585	-1.53469
C	1.045	-2.40658	-1.35458
H	2.60507	-3.87625	-1.51167
H	1.15058	-4.22907	-2.48803
H	1.105	-4.42789	-0.7218
H	3.57176	-1.93864	-2.75171
H	3.69352	-1.41224	-4.4541
H	2.34985	-2.46658	-3.9329
C	1.2309	2.05406	-3.18639
H	2.03613	2.71366	-3.54485
H	0.34566	2.19285	-3.82258
H	0.96684	2.37472	-2.17205
W	0.44052	-0.79095	-0.99651

[W]-B-Ph

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Zero-point correction= 1.006845
(Hartree/Particle)
Thermal correction to Energy= 1.072263
Thermal correction to Enthalpy= 1.073207
Thermal correction to Gibbs Free Energy=
0.904075
Sum of electronic and zero-point Energies= -
3706.795399
Sum of electronic and thermal Energies= -
3706.729981
Sum of electronic and thermal Enthalpies= -
3706.729037
Sum of electronic and thermal Free Energies= -
3706.898169

C	-1.73316	1.1415	1.88232
C	-0.46675	1.22864	2.47683
C	0.57163	1.9569	1.87355
C	0.30407	2.64685	0.68378
C	-0.95604	2.58436	0.07344
C	-1.9705	1.83938	0.68887
C	-2.80543	0.2843	2.47154
C	-2.62264	-1.11001	2.68248
C	-3.6877	-1.84874	3.23061
C	-4.90674	-1.24903	3.56171
C	-5.08545	0.11636	3.32858
C	-4.04227	0.87091	2.78614
C	-1.48755	-3.82549	1.6977
C	-0.87617	-4.91086	2.35111
C	-1.18295	-6.23169	2.00123
C	-2.10572	-6.48951	0.98297
C	-2.71533	-5.42252	0.31201
C	-2.40705	-4.107	0.66643
C	0.32361	-1.94988	3.35205
C	0.09175	-2.41811	4.66107
C	1.08035	-2.33462	5.64714
C	2.32262	-1.7656	5.34544
C	2.56884	-1.28649	4.05506
C	1.5813	-1.38627	3.07116
C	-1.19178	3.31182	-1.20799
C	-1.5799	2.64433	-2.39883
C	-1.78448	3.42558	-3.55379
C	-1.60433	4.81197	-3.55496
C	-1.19114	5.45197	-2.38484
C	-0.98668	4.70221	-1.22486
C	-3.45697	0.19993	-1.98483
C	-3.56432	-0.71419	-0.92027
C	-4.81214	-1.08946	-0.41218
C	-5.98147	-0.56381	-0.97138
C	-5.89604	0.3455	-2.03255
C	-4.64453	0.72782	-2.52783
C	-1.50126	0.34141	-4.39523
C	-2.51441	-0.16283	-5.22853
C	-2.25188	-0.51125	-6.55922
C	-0.96375	-0.36196	-7.08174
C	0.06005	0.13977	-6.26841
C	-0.20993	0.48566	-4.94193
C	1.92295	2.01538	2.50136
C	3.12562	1.7449	1.78778
C	4.34737	1.87703	2.48116
C	4.4048	2.23607	3.8303
C	3.21784	2.4619	4.52898
C	1.99561	2.35231	3.86502
C	3.10845	2.44775	-1.31861
C	2.05108	2.41865	-2.24747
C	1.92152	3.41551	-3.21855
C	2.8534	4.45632	-3.28078
C	3.91251	4.50013	-2.36645
C	4.03598	3.50457	-1.39194
C	4.82986	0.12516	-0.21521
C	5.19596	-0.85107	0.73331
C	6.30843	-1.67189	0.53498
C	7.08378	-1.52946	-0.6219
C	6.73998	-0.56502	-1.57408
C	5.62222	0.25269	-1.37156
H	-0.27519	0.69756	3.40932
H	1.08706	3.24444	0.21811
H	-2.95227	1.7756	0.21936
H	-3.57354	-2.92676	3.37833
H	-5.71702	-1.849	3.98394
H	-6.03752	0.59727	3.56781
H	-4.18088	1.94009	2.60646
H	-0.14418	-4.72713	3.14185
H	-0.69629	-7.06036	2.52248
H	-2.34419	-7.51981	0.70605
H	-3.42886	-5.61666	-0.49306
H	-2.88555	-3.28972	0.1218
H	-0.88036	-2.84681	4.92548
H	0.87702	-2.70444	6.65569
H	3.09225	-1.68522	6.11756
H	3.52252	-0.80812	3.81836
H	1.79332	-0.98489	2.08098
H	-2.06993	2.93526	-4.48841
H	-1.77085	5.38538	-4.47068
H	-1.02958	6.53305	-2.37161
H	-0.67058	5.20043	-0.3047
H	-2.65162	-1.09083	-0.45728
H	-4.86853	-1.77165	0.4401
H	-6.95833	-0.85132	-0.57315
H	-6.80693	0.76652	-2.46717
H	-4.59948	1.46002	-3.34058
H	-3.52368	-0.30447	-4.83283
H	-3.05468	-0.90666	-7.18765
H	-0.7559	-0.63761	-8.11916
H	1.07096	0.25679	-6.66845
H	0.60625	0.86049	-4.31799
H	5.28625	1.67415	1.96012

H	5.37147	2.32622	4.33206
H	3.24027	2.73051	5.58823
H	1.06826	2.54978	4.40772
H	1.2987	1.63012	-2.18587
H	1.07592	3.38962	-3.90922
H	2.74916	5.24012	-4.03572
H	4.63997	5.31518	-2.40889
H	4.86526	3.55905	-0.67929
H	4.60603	-0.97263	1.64537
H	6.57082	-2.42482	1.28276
H	7.95574	-2.16977	-0.77949
H	7.34285	-0.44886	-2.47859
H	5.36409	0.9993	-2.12761
W	0.65446	-1.20066	-0.68221
O	-0.71187	-1.27344	0.64981
O	-0.56284	0.01824	-1.69686
O	1.98647	0.03588	-0.27595
Si	-1.07745	-2.02737	2.09249
Si	-1.75114	0.75504	-2.56608
Si	3.24665	1.12133	0.00032
C	-0.77548	-2.77684	-3.25955
C	0.20459	-2.62962	-2.14787
C	0.79115	-3.59411	-1.35984
C	0.56581	-5.07817	-1.33991
C	1.6135	-2.87983	-0.38005
H	-0.9246	-3.83402	-3.53728
H	-0.44671	-2.22926	-4.15607
H	-1.75648	-2.3529	-2.98764
H	-0.12605	-5.40695	-2.12715
H	0.15486	-5.38197	-0.36422
H	1.52684	-5.60487	-1.46513
C	2.72606	-3.50858	0.38923
H	3.5361	-3.85062	-0.28181
H	3.163	-2.82576	1.12818
H	2.35649	-4.39998	0.92941

[W]-B-TS-B'

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -115.91 cm^{-1}
Zero-point correction= 1.005410 (Hartree/Particle)
Thermal correction to Energy= 1.070377
Thermal correction to Enthalpy= 1.071321
Thermal correction to Gibbs Free Energy= 0.902417
Sum of electronic and zero-point Energies= -3706.782329
Sum of electronic and thermal Energies= -3706.717362
Sum of electronic and thermal Enthalpies= -3706.716418
Sum of electronic and thermal Free Energies= -3706.885323

Si	-0.14227	-3.42394	-0.04578
Si	-2.34	2.43986	-0.17611
Si	2.85599	1.06954	-0.31817
O	-0.02094	-1.8127	0.32882
O	-0.97175	1.58381	0.22103
O	1.40776	0.50042	0.20408
C	0.27332	-1.41729	-2.7361
C	-1.08532	-1.1133	-2.56541
H	-1.80677	-1.9185	-2.4247
C	-1.53477	0.21775	-2.5534
C	-0.59811	1.24657	-2.72312
H	-0.93006	2.28479	-2.73129
C	0.76856	0.97088	-2.83432
C	1.18891	-0.36424	-2.87128
H	2.25033	-0.5911	-2.9777
C	0.7788	-2.82116	-2.79774
C	0.63502	-3.75646	-1.74169
C	1.17403	-5.04727	-1.92281
H	1.09268	-5.78231	-1.11763
C	1.84149	-5.41847	-3.09143
H	2.24849	-6.42766	-3.19387
C	1.99645	-4.48309	-4.11733
H	2.52515	-4.75011	-5.03606
C	1.4705	-3.20026	-3.96426
H	1.58573	-2.46835	-4.76758
C	-2.977	0.54603	-2.36776
C	-3.42527	1.53626	-1.44819
C	-4.80186	1.8435	-1.43201
H	-5.17449	2.60768	-0.74439
C	-5.72319	1.18677	-2.25166
H	-6.78219	1.45404	-2.21016
C	-5.27882	0.17927	-3.11076
H	-5.98604	-0.35507	-3.7505
C	-3.91909	-0.12986	-3.166
H	-3.56688	-0.8908	-3.86678
C	1.75496	2.08645	-2.86045
C	2.7285	2.22185	-1.83708
C	3.63086	3.30034	-1.9328
H	4.38802	3.43753	-1.15605
C	3.57499	4.22447	-2.98098
H	4.29093	5.0497	-3.02159
C	2.58958	4.09542	-3.96239
H	2.52268	4.81945	-4.77863
C	1.68639	3.03271	-3.89607
H	0.91591	2.92306	-4.66374
C	0.82726	-4.3194	1.30536
C	1.80349	-3.62213	2.04366
H	1.97645	-2.56229	1.843
C	2.55654	-4.26482	3.03174
H	3.31204	-3.7054	3.5901
C	2.34449	-5.62066	3.30419
H	2.93317	-6.12437	4.07563
C	1.37215	-6.32846	2.58918
H	1.19582	-7.38611	2.80316
C	0.62075	-5.68057	1.6032
H	-0.14622	-6.24584	1.06496
C	-1.91606	-4.07075	-0.04282
C	-2.63557	-4.26758	-1.23749
H	-2.15279	-4.07762	-2.20011
C	-3.95832	-4.72197	-1.22243
H	-4.49787	-4.86209	-2.16286
C	-4.58594	-5.00429	-0.00451
H	-5.61946	-5.36043	0.01078
C	-3.8812	-4.84094	1.19338
H	-4.36209	-5.07177	2.14781
C	-2.56104	-4.38252	1.16976
H	-2.02162	-4.26756	2.11391
C	-3.32968	2.72684	1.4127
C	-4.36408	1.87465	1.84313
H	-4.68474	1.04536	1.2082
C	-4.99669	2.06419	3.07626
H	-5.79955	1.38962	3.38612
C	-4.59857	3.1121	3.91407
H	-5.09021	3.26139	4.87901
C	-3.56754	3.96739	3.50981
H	-3.25091	4.78837	4.15864
C	-2.94495	3.77583	2.27191
H	-2.14555	4.45812	1.96803

C	-1.6826	4.09301	-0.79804
C	-2.52831	5.15924	-1.1572
H	-3.61508	5.04791	-1.08379
C	-2.001	6.37263	-1.61084
H	-2.67227	7.19089	-1.88575
C	-0.61433	6.53868	-1.71621
H	-0.20282	7.48558	-2.07634
C	0.24114	5.48917	-1.3652
H	1.32424	5.60008	-1.45986
C	-0.29133	4.27989	-0.90687
H	0.37523	3.45527	-0.64748
C	3.60455	2.0955	1.08875
C	3.07294	3.36345	1.3994
H	2.2918	3.79533	0.76695
C	3.51739	4.08459	2.51114
H	3.08716	5.06495	2.73378
C	4.51047	3.54914	3.34052
H	4.85923	4.10958	4.21218
C	5.05739	2.29631	3.04567
H	5.83704	1.87509	3.68647
C	4.60783	1.58023	1.92953
H	5.04323	0.5999	1.71461
C	3.9751	-0.39918	-0.71108
C	5.32165	-0.26686	-1.09974
H	5.77881	0.72603	-1.16566
C	6.09393	-1.39097	-1.41191
H	7.1387	-1.26982	-1.71179
C	5.52837	-2.67088	-1.34784
H	6.13028	-3.54843	-1.59976
C	4.1906	-2.82148	-0.96786
H	3.73178	-3.81283	-0.92907
C	3.42775	-1.69382	-0.64957
H	2.37876	-1.80447	-0.37191
C	0.20192	0.42281	2.87372
C	-1.86363	-0.60579	2.12841
C	-1.1073	0.09674	3.19979
C	1.26261	1.17031	3.58582
C	-3.12266	-1.33151	2.42905
H	-3.85343	-0.66747	2.92158
H	-2.93706	-2.17207	3.12152
C	-1.79943	0.48596	4.48405
H	-2.63198	1.16954	4.25453
H	-2.22796	-0.40552	4.96803
H	1.30915	2.21777	3.24453
H	1.10881	1.16093	4.67748
H	2.2505	0.74004	3.36324
H	-1.11101	0.98001	5.18175
H	-3.5769	-1.74176	1.51775
W	-0.36202	-0.05622	1.03793

[W]-B'-Ph

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Zero-point correction= 1.006770 (Hartree/Particle)
Thermal correction to Energy= 1.071942
Thermal correction to Enthalpy= 1.072886
Thermal correction to Gibbs Free Energy= 0.903533
Sum of electronic and zero-point Energies= -3706.805211
Sum of electronic and thermal Energies= -3706.740038
Sum of electronic and thermal Enthalpies= -3706.739094
Sum of electronic and thermal Free Energies= -3706.908447

W	7.92707	3.09139	5.76336
Si	8.01716	-0.43855	5.89999
Si	6.54688	5.66527	3.85315
Si	11.18602	3.56901	4.45578
O	8.36367	1.17265	5.95615
O	7.54637	4.82131	4.86419
O	9.60987	3.21181	4.86156
C	8.70628	-1.25071	4.329
C	9.09213	-2.60079	4.46874
H	8.96856	-3.09581	5.43522
C	9.65746	-3.33286	3.42312
H	9.94545	-4.37602	3.5765
C	9.86235	-2.7127	2.18938
H	10.31005	-3.26281	1.35762
C	9.49069	-1.37898	2.02219
H	9.6457	-0.89521	1.05471
C	8.9058	-0.63296	3.06546
C	8.58476	0.79269	2.73909
C	9.62516	1.61801	2.2837
H	10.64509	1.23096	2.27084
C	9.38612	2.9442	1.9058
C	8.07451	3.42647	1.90526
H	7.88827	4.44494	1.5679
C	7.01536	2.64414	2.38485
C	7.28767	1.32634	2.80989
H	6.47478	0.70956	3.19531
C	5.63465	3.20727	2.41603
C	5.33812	4.50561	2.92557
C	5.50858	6.81663	4.93778
C	5.40764	8.1996	4.70466
H	5.92962	8.64507	3.85282
C	4.65093	9.02263	5.54832
H	4.58591	10.09566	5.3482
C	3.98266	8.47431	6.64712
H	3.3928	9.11564	7.30759
C	4.07245	7.0993	6.89829
H	3.55111	6.66358	7.7554
C	4.82699	6.28411	6.0511
H	4.88704	5.21298	6.25666
C	7.57961	6.69669	2.66743
C	8.94733	6.91092	2.91712
H	9.41223	6.45688	3.79388
C	9.7269	7.67439	2.04406
H	10.79114	7.81028	2.24665
C	9.14994	8.23864	0.90179
H	9.76106	8.82892	0.21367
C	7.7914	8.03427	0.63452
H	7.33782	8.46762	-0.26114
C	7.01574	7.2674	1.51035
H	5.95789	7.10303	1.28062
C	4.00032	4.94451	2.84792
H	3.73835	5.93116	3.23834
C	2.9781	4.14975	2.32057
H	1.95365	4.52907	2.28267
C	3.27666	2.86721	1.85845
H	2.49009	2.22566	1.45279
C	4.5943	2.4098	1.90501
H	4.83128	1.41536	1.51904
C	10.5097	3.88643	1.63614
C	11.36127	4.26567	2.70295
C	11.75357	4.86371	5.70527
C	13.09121	4.96688	6.12976
H	13.84093	4.26884	5.74515
C	13.48236	5.9414	7.05524

H	14.52659	6.00376	7.37335
C	12.53602	6.82798	7.57973
H	12.83894	7.58714	8.30588
C	11.19922	6.73613	7.175
H	10.45354	7.42346	7.58396
C	10.81309	5.76415	6.24656
H	9.76369	5.70312	5.94429
C	12.19637	1.98799	4.58039
C	11.60986	0.84227	5.14718
H	10.57904	0.9005	5.49704
C	12.31333	-0.363	5.23031
H	11.82904	-1.24241	5.66262
C	13.62432	-0.43994	4.74856
H	14.17722	-1.38135	4.80853
C	14.22403	0.68972	4.17816
H	15.24541	0.6307	3.79213
C	13.51273	1.89115	4.08974
H	13.98819	2.75531	3.61459
C	12.3913	5.18695	2.43676
H	13.0479	5.51424	3.24836
C	12.58278	5.71923	1.15792
H	13.39095	6.43288	0.97764
C	11.72204	5.3533	0.12026
H	11.85135	5.77773	-0.87869
C	10.6867	4.44677	0.36321
H	10.00531	4.16355	-0.44324
C	6.16015	-0.76323	6.00718
C	5.41411	-1.27522	4.93018
H	5.91888	-1.52926	3.99341
C	4.03244	-1.47391	5.03538
H	3.47125	-1.86992	4.18478
C	3.37213	-1.17012	6.2301
H	2.29321	-1.32456	6.3153
C	4.09868	-0.67279	7.31874
H	3.58749	-0.4375	8.25628
C	5.47683	-0.47303	7.20472
H	6.03216	-0.08416	8.06371
C	8.80798	-1.1917	7.44333
C	8.36849	-2.41204	7.99242
H	7.53465	-2.94807	7.52843
C	8.96857	-2.95051	9.13535
H	8.61228	-3.90012	9.54399
C	10.01996	-2.26947	9.75919
H	10.49059	-2.68765	10.65313
C	10.4602	-1.0475	9.23939
H	11.27516	-0.50607	9.72755
C	9.85657	-0.51472	8.09516
H	10.19904	0.44612	7.70449
C	5.98041	2.71317	5.97257
C	6.33172	3.16429	7.25183
C	7.74978	3.59067	7.55418
C	4.64456	2.29882	5.47818
H	4.73649	1.46438	4.77146
H	3.97965	1.97437	6.29241
H	4.15741	3.12555	4.93723
C	5.36647	3.27102	8.40576
H	5.27338	4.3246	8.71305
H	4.37478	2.8882	8.13604
H	5.74888	2.70765	9.27059
C	8.23753	4.09983	8.86135
H	7.64594	4.96573	9.20536
H	8.18862	3.32317	9.64474
H	9.28416	4.42201	8.76199

[W]-C-Ph

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Zero-point correction= 1.007112 (Hartree/Particle)
Thermal correction to Energy= 1.072424
Thermal correction to Enthalpy= 1.073368
Thermal correction to Gibbs Free Energy= 0.905894
Sum of electronic and zero-point Energies= -3706.804354
Sum of electronic and thermal Energies= -3706.739043
Sum of electronic and thermal Enthalpies= -3706.738098
Sum of electronic and thermal Free Energies= -3706.905572

C	-1.17886	-2.67462	-1.52464
C	-2.18083	-2.4138	-0.57956
C	-2.97583	-1.26171	-0.663
C	-2.78474	-0.38615	-1.74056
C	-1.79216	-0.624	-2.70207
C	-1.00933	-1.78149	-2.59252
C	-0.30326	-3.87739	-1.40796
C	0.46887	-4.15374	-0.2464
C	1.25064	-5.32637	-0.23601
C	1.29483	-6.20012	-1.32615
C	0.55677	-5.90222	-2.47335
C	-0.23136	-4.75046	-2.50756
C	-4.00501	-0.98237	0.38093
C	-4.02838	0.2264	1.12921
C	-5.05534	0.39585	2.07933
C	-6.02449	-0.58503	2.30891
C	-5.97226	-1.78149	1.59108
C	-4.96947	-1.97212	0.63863
C	-1.5823	0.34427	-3.81807
C	-0.32512	0.95694	-4.07441
C	-0.23268	1.84358	-5.16627
C	-1.33178	2.14058	-5.97731
C	-2.56892	1.55766	-5.69612
C	-2.68624	0.66961	-4.62542
C	2.29951	-3.28496	2.05903
C	3.4674	-3.17719	1.27698
C	4.73587	-3.30662	1.84733
C	4.86207	-3.5479	3.22105
C	3.71611	-3.65891	4.01402
C	2.44773	-3.52747	3.43584
C	-0.77253	-3.19733	2.49008
C	-0.99311	-4.42495	3.14421
C	-2.06827	-4.59028	4.02369
C	-2.95272	-3.53019	4.25405
C	-2.7536	-2.30596	3.6077
C	-1.66859	-2.1406	2.74122
C	-2.62497	2.46748	2.69346
C	-2.39723	1.71458	3.86346
C	-2.2535	2.33438	5.10698
C	-2.3356	3.72895	5.20577
C	-2.56271	4.49339	4.05759
C	-2.70471	3.86577	2.81404
C	-2.99082	2.79225	-0.37227
C	-4.16109	3.57423	-0.42444
C	-4.41107	4.42798	-1.50396
C	-3.4969	4.50456	-2.56111
C	-2.33247	3.73053	-2.52972
C	-2.07945	2.89024	-1.44083
C	2.26797	2.31127	-3.14107
C	1.69035	3.57073	-2.88073
C	2.45589	4.73867	-2.9119

C	3.82345	4.66979	-3.20579
C	4.41494	3.43066	-3.46815
C	3.64194	2.26376	-3.43462
C	2.20932	-0.77965	-3.37167
C	2.76726	-0.96797	-4.65115
C	3.46035	-2.14018	-4.97077
C	3.59507	-3.1551	-4.01638
C	3.04182	-2.98872	-2.74276
C	2.36481	-1.80777	-2.42264
C	2.26642	1.69805	0.81127
C	2.14161	0.71438	1.89486
C	1.25416	1.89208	1.86921
C	3.03547	0.06608	2.89445
H	-2.33545	-3.10739	0.24675
H	-3.40417	0.50671	-1.8242
H	-0.24141	-1.98388	-3.33903
H	1.86453	-5.55331	0.6397
H	1.91414	-7.09978	-1.28288
H	0.59056	-6.56562	-3.3415
H	-0.81759	-4.52215	-3.40119
H	-5.08641	1.3107	2.67736
H	-6.80588	-0.41975	3.05518
H	-6.71205	-2.56648	1.76838
H	-4.93393	-2.90384	0.06845
H	0.71902	2.33863	-5.37767
H	-1.22329	2.83463	-6.81476
H	-3.4429	1.78953	-6.31037
H	-3.65143	0.20422	-4.41051
H	3.38854	-2.97876	0.20471
H	5.6279	-3.21549	1.22189
H	5.85316	-3.64793	3.67161
H	3.80923	-3.84482	5.08741
H	1.56193	-3.60706	4.07193
H	-0.32397	-5.27222	2.96253
H	-2.22303	-5.5511	4.52211
H	-3.80341	-3.66236	4.92791
H	-3.46064	-1.48575	3.75454
H	-1.54336	-1.19046	2.21902
H	-2.32085	0.62536	3.80533
H	-2.07372	1.73059	6.00048
H	-2.22182	4.2176	6.17713
H	-2.62547	5.58261	4.12877
H	-2.87184	4.47939	1.92457
H	-4.89791	3.51383	0.38308
H	-5.32573	5.02667	-1.52604
H	-3.69803	5.15831	-3.41399
H	-1.63284	3.75662	-3.36876
H	-1.18247	2.26881	-1.44516
H	0.627	3.64359	-2.63737
H	1.98757	5.70415	-2.7027
H	4.42589	5.58182	-3.22893
H	5.48266	3.37099	-3.69572
H	4.12212	1.30132	-3.63114
H	2.65503	-0.19425	-5.41755
H	3.8863	-2.26738	-5.96972
H	4.12045	-4.07984	-4.26938
H	3.11124	-3.79171	-2.00493
H	1.91381	-1.70506	-1.43443
W	0.62381	0.47431	0.50564
O	0.59671	-1.43526	0.66435
O	-1.24388	0.8079	0.80044
O	0.66765	0.6741	-1.40195
Si	0.62415	-2.98835	1.24544
Si	-2.69438	1.57518	1.03335
Si	1.20623	0.76248	-2.96897
C	3.3599	2.50547	0.20168
C	0.88128	2.98363	2.81244
H	0.31804	3.77826	2.29887
H	1.78245	3.43914	3.26022
H	0.24292	2.60988	3.62674
H	2.95928	3.31437	-0.42676
H	4.00138	1.88333	-0.44164
H	3.99664	2.95747	0.98303
H	3.72563	-0.64397	2.41564
H	2.45313	-0.50048	3.63748
H	3.63457	0.82206	3.43264

[W]-B-TS-Ph

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -212.31 cm^{-1}
Zero-point correction= 1.004097 (Hartree/Particle)
Thermal correction to Energy= 1.069572
Thermal correction to Enthalpy= 1.070516
Thermal correction to Gibbs Free Energy= 0.899188
Sum of electronic and zero-point Energies= -3706.774043
Sum of electronic and thermal Energies= -3706.708568
Sum of electronic and thermal Enthalpies= -3706.707624
Sum of electronic and thermal Free Energies= -3706.878951

C	-0.94993	-2.58804	-1.42265
C	-1.84181	-2.26443	-0.39163
C	-2.62081	-1.09662	-0.43643
C	-2.51777	-0.26241	-1.55864
C	-1.62766	-0.55881	-2.59913
C	-0.86836	-1.73381	-2.53196
C	-0.07337	-3.79297	-1.34531
C	0.77142	-4.05403	-0.23188
C	1.57569	-5.20978	-0.26347
C	1.56456	-6.09129	-1.3483
C	0.74617	-5.81629	-2.44549
C	-0.05979	-4.67624	-2.43915
C	-3.55017	-0.77978	0.68517
C	-3.60333	0.48863	1.32956
C	-4.55727	0.65777	2.35731
C	-5.41638	-0.36651	2.76236
C	-5.33087	-1.6145	2.14433
C	-4.40726	-1.80926	1.1182
C	-1.44348	0.40838	-3.72041
C	-0.18695	1.02856	-3.94911
C	-0.08557	1.94653	-5.01193
C	-1.17815	2.25117	-5.83047
C	-2.41403	1.64919	-5.58158
C	-2.54223	0.73932	-4.52949
C	2.6839	-3.11653	2.00965
C	3.73502	-2.29535	1.55613
C	5.01837	-2.40397	2.09916
C	5.27385	-3.33859	3.10968
C	4.241	-4.15949	3.57508
C	2.95707	-4.0453	3.02983
C	-0.38215	-3.19892	2.52621
C	-0.77914	-4.51242	2.84442
C	-1.81353	-4.75242	3.75542
C	-2.48132	-3.67839	4.35433
C	-2.10695	-2.36724	4.04196
C	-1.06391	-2.13099	3.14199
C	-2.4534	3.00173	2.61289

C	-2.02753	2.35559	3.79199
C	-1.86866	3.06297	4.98513
C	-2.13293	4.43805	5.02267
C	-2.55566	5.09615	3.86401
C	-2.71298	4.38172	2.66955
C	-3.05887	3.05285	-0.45334
C	-4.32025	3.67397	-0.51568
C	-4.69868	4.41529	-1.64046
C	-3.82341	4.5383	-2.7263
C	-2.56869	3.92087	-2.68409
C	-2.19118	3.19047	-1.55433
C	2.37837	2.31856	-2.84737
C	1.84765	3.51106	-2.31346
C	2.62688	4.66517	-2.20153
C	3.96189	4.65124	-2.62524
C	4.50643	3.48069	-3.1617
C	3.72	2.3264	-3.26889
C	2.33554	-0.74222	-3.32276
C	2.81748	-0.93859	-4.63055
C	3.55183	-2.08265	-4.96212
C	3.80988	-3.0556	-3.98869
C	3.3335	-2.87944	-2.68523
C	2.6063	-1.73114	-2.35775
C	2.29439	1.63957	1.17704
C	1.19041	0.65006	2.61332
C	1.46523	2.05335	2.20442
C	1.88902	-0.0329	3.73939
H	-1.92185	-2.92026	0.47443
H	-3.12338	0.64104	-1.6208
H	-0.16438	-1.96367	-3.33258
H	2.24982	-5.41704	0.57232
H	2.20264	-6.97873	-1.34078
H	0.7329	-6.48767	-3.30803
H	-0.70434	-4.46562	-3.29615
H	-4.62234	1.61696	2.87588
H	-6.1387	-0.18975	3.56338
H	-5.98378	-2.43471	2.45359
H	-4.35456	-2.78078	0.62165
H	0.86664	2.45413	-5.19309
H	-1.06769	2.96726	-6.64912
H	-3.28077	1.88978	-6.20277
H	-3.50826	0.26811	-4.33009
H	3.53817	-1.55032	0.78042
H	5.82126	-1.75619	1.73652
H	6.27646	-3.42378	3.53728
H	4.43463	-4.88534	4.36948
H	2.1549	-4.68103	3.41711
H	-0.29074	-5.36434	2.36025
H	-2.10777	-5.77928	3.98888
H	-3.30023	-3.86381	5.05451
H	-2.6407	-1.52333	4.48686
H	-0.79269	-1.10197	2.89359
H	-1.80598	1.28408	3.77463
H	-1.53343	2.54446	5.88745
H	-2.00815	4.99504	5.95512
H	-2.76252	6.16944	3.8886
H	-3.03656	4.91138	1.76903
H	-5.02318	3.57689	0.31799
H	-5.68195	4.89234	-1.6737
H	-4.12461	5.10796	-3.60956
H	-1.88946	3.98522	-3.53738
H	-1.225	2.6819	-1.53555
H	0.81044	3.53872	-1.96727
H	2.19483	5.57725	-1.78063
H	4.57523	5.55195	-2.53616
H	5.5484	3.46355	-3.49293
H	4.16454	1.41389	-3.67642
H	2.61131	-0.19578	-5.40824
H	3.91712	-2.22056	-5.98363
H	4.37377	-3.95526	-4.25002
H	3.50745	-3.64496	-1.9249
H	2.2074	-1.60976	-1.34926
W	0.63306	0.54962	0.70197
O	0.93836	-1.32889	0.70176
O	-0.91072	1.64289	0.66612
O	0.7894	0.53116	-1.2764
Si	0.9723	-2.89416	1.25359
Si	-2.50457	2.01212	1.00975
Si	1.31246	0.75564	-2.81424
C	3.61729	2.05368	0.65265
C	1.07746	3.39314	2.7395
H	0.11454	3.7175	2.31546
H	1.83816	4.1455	2.47761
H	0.95533	3.36833	3.83206
H	4.37709	1.34545	1.0307
H	3.89784	3.06541	0.98901
H	3.64194	2.00253	-0.44566
H	1.51369	0.3646	4.70062
H	2.97824	0.15165	3.71921
H	1.7234	-1.1191	3.72652

[W]-D-TS-Ph

B3LYP-D3/def2SVP-LANL2DZ(W)-CPCM(benzene)
Imaginary frequency = -108.94 cm^{-1}
Zero-point correction= 1.004743 (Hartree/Particle)
Thermal correction to Energy= 1.069366
Thermal correction to Enthalpy= 1.070310
Thermal correction to Gibbs Free Energy= 0.903823
Sum of electronic and zero-point Energies= -3706.721912
Sum of electronic and thermal Energies= -3706.657289
Sum of electronic and thermal Enthalpies= -3706.656345
Sum of electronic and thermal Free Energies= -3706.822832

C	-1.20339	0.99331	2.3947
C	0.16738	1.25701	2.29183
C	0.6727	1.9636	1.19807
C	-0.23129	2.4379	0.22225
C	-1.60023	2.16724	0.29359
C	-2.07938	1.48891	1.4232
C	-1.69883	-0.01633	3.37025
C	-2.1128	-1.27705	2.86967
C	-2.64205	-2.20709	3.78547
C	-2.71132	-1.9309	5.1541
C	-2.24606	-0.70462	5.63794
C	-1.74859	0.24862	4.74577
C	-2.5816	2.62083	-0.75361
C	-2.86462	1.99137	-2.00842
C	-3.91548	2.56189	-2.76793
C	-4.64789	3.68052	-2.36662
C	-4.35416	4.28329	-1.14579
C	-3.3381	3.74332	-0.35887
C	2.14212	2.1848	1.00534
C	3.095	1.14311	0.76647
C	4.40817	1.54656	0.44284
C	4.802	2.88752	0.37816
C	3.87094	3.88813	0.64733

C	2.55553	3.5279	0.94825
H	0.84518	0.85198	3.04071
H	0.13971	3.00253	-0.63048
H	-3.14435	1.26795	1.51125
H	-3.00384	-3.17574	3.42869
H	-3.12204	-2.67464	5.84201
H	-2.28319	-0.48459	6.70811
H	-1.40418	1.21884	5.11324
H	-4.1905	2.11174	-3.72285
H	-5.44554	4.06707	-3.00611
H	-4.91181	5.15777	-0.80091
H	-3.11161	4.19814	0.60867
H	5.16171	0.78709	0.22705
H	5.83377	3.1406	0.12067
H	4.15679	4.94266	0.61354
H	1.81239	4.30762	1.13387
W	0.33753	-0.8111	-1.2668
O	-0.89379	-0.78698	0.23685
O	-1.26481	-0.7092	-2.39346
O	1.71584	-1.4889	-0.0429
Si	-1.94632	-1.78832	1.04497
Si	-2.07827	0.57269	-3.07834
Si	2.86118	-0.76312	0.92831
C	1.96561	-1.51547	-3.2775
C	1.11596	0.70499	-1.75561
C	1.13883	-2.43018	-3.25941
C	0.20798	-3.54198	-3.43325
H	0.44808	-4.07977	-4.36492
H	0.27488	-4.24683	-2.5938
H	-0.82421	-3.16302	-3.49537
C	1.77366	1.92968	-2.23756
H	1.15512	2.46202	-2.97633
H	2.02414	2.61836	-1.42039
H	2.73176	1.67638	-2.71511
C	3.1504	-0.74131	-3.66059
H	3.81475	-1.38026	-4.26345
H	2.86	0.13141	-4.26296
H	3.70833	-0.39255	-2.78059
C	-1.34288	-3.58566	0.90854
C	-1.4057	-4.18523	-0.36619
C	-0.83436	-4.36313	1.96436
C	-0.97936	-5.49987	-0.57737
H	-1.81163	-3.61657	-1.20807
C	-0.39459	-5.67595	1.76009
H	-0.77754	-3.94502	2.9701
C	-0.46619	-6.24898	0.48747
H	-1.05558	-5.94774	-1.57199
H	0.0019	-6.25232	2.60009
H	-0.13091	-7.27679	0.32582
C	-3.67161	-1.78802	0.25638
C	-4.46168	-2.95579	0.25202
C	-4.24053	-0.62316	-0.2874
C	-5.76036	-2.95412	-0.27038
H	-4.05994	-3.88927	0.65532
C	-5.53474	-0.61178	-0.81233
H	-3.65827	0.29187	-0.32815
C	-6.30204	-1.78005	-0.80397
H	-6.34936	-3.87549	-0.26374
H	-5.93193	0.30975	-1.24575
H	-7.31254	-1.77964	-1.22095
C	-0.93717	1.44523	-4.31079
C	-0.05014	0.6567	-5.06912
C	-0.92069	2.83622	-4.51783
C	0.83072	1.23427	-5.98729
H	-0.03522	-0.42558	-4.92349
C	-0.04439	3.42177	-5.44023
H	-1.59148	3.47987	-3.94312
C	0.83791	2.62247	-6.17297
H	1.51427	0.60175	-6.56067
H	-0.04657	4.50604	-5.58114
H	1.52757	3.07791	-6.88868
C	-3.414	-0.32275	-4.08692
C	-3.93126	-1.54745	-3.62043
C	-3.84334	0.13222	-5.34877
C	-4.86054	-2.27376	-4.37184
H	-3.60394	-1.93729	-2.65482
C	-4.77263	-0.58975	-6.10553
H	-3.43526	1.06119	-5.75963
C	-5.28705	-1.79495	-5.61531
H	-5.25448	-3.21591	-3.98102
H	-5.08986	-0.21499	-7.08263
H	-6.01325	-2.36218	-6.20403
C	4.47943	-1.63988	0.48235
C	5.61761	-1.60652	1.31153
C	4.55107	-2.39636	-0.70265
C	6.79026	-2.28199	0.96026
H	5.59182	-1.04845	2.25239
C	5.72193	-3.07471	-1.06026
H	3.6693	-2.46664	-1.34379
C	6.84647	-3.0148	-0.23129
H	7.66188	-2.24097	1.61921
H	5.75413	-3.6559	-1.98616
H	7.76259	-3.54394	-0.50731
C	2.47064	-1.10292	2.73784
C	3.10591	-0.38383	3.76916
C	1.49734	-2.05097	3.09073
C	2.7746	-0.60447	5.10947
H	3.84878	0.3822	3.52546
C	1.15147	-2.26579	4.42824
H	0.99104	-2.60291	2.29866
C	1.78959	-1.54272	5.44062
H	3.27347	-0.03319	5.89715
H	0.36607	-2.98081	4.68488
H	1.51209	-1.70174	6.48597

[Mo]-A

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 0.588330
(Hartree/Particle)
Thermal correction to Energy= 0.631455
Thermal correction to Enthalpy= 0.632399
Thermal correction to Gibbs Free Energy=
0.511970
Sum of electronic and zero-point Energies= -
2401.306719
Sum of electronic and thermal Energies= -
2401.263594
Sum of electronic and thermal Enthalpies= -
2401.262650
Sum of electronic and thermal Free Energies= -
2401.383078

C	-1.92094	1.83023	2.05946
C	-0.63837	2.02589	2.59184
C	0.34131	2.74522	1.89056
C	0.00897	3.29294	0.6424
C	-1.26544	3.11347	0.08273
C	-2.22511	2.39569	0.81218
C	-2.96552	1.07509	2.81446
C	-2.80029	-0.27171	3.23676
C	-3.85054	-0.85959	3.97242
C	-5.0253	-0.16959	4.28238

C	-5.18579	1.14448	3.83813
C	-4.16303	1.75377	3.10975
C	-1.94733	-3.17327	2.61993
C	0.03018	-1.34445	4.10401
C	-1.60103	3.72075	-1.23929
C	-2.08879	2.96726	-2.34199
C	-2.40873	3.67335	-3.5209
C	-2.25388	5.05771	-3.63237
C	-1.74671	5.78032	-2.55094
C	-1.42354	5.11117	-1.36967
C	-3.87621	0.41971	-1.75025
C	-2.06797	0.52639	-4.22504
C	1.69036	2.95838	2.4951
C	2.90412	2.59288	1.85206
C	4.11089	2.88783	2.52094
C	4.14282	3.50723	3.77297
C	2.94222	3.83571	4.40551
C	1.73214	3.55943	3.76785
C	3.179	2.79101	-1.27798
C	4.61319	0.56331	0.27825
C	0.73301	-1.87026	-0.97929
C	1.2102	-3.12461	-1.5835
H	-0.39507	1.60694	3.5692
H	0.75581	3.86863	0.09445
H	-3.22776	2.27383	0.40099
H	-3.7609	-1.89741	4.3056
H	-5.81477	-0.66084	4.85711
H	-6.10174	1.6978	4.06143
H	-4.2793	2.78765	2.77434
H	-2.77887	3.12805	-4.39291
H	-2.51702	5.56522	-4.56409
H	-1.60826	6.86234	-2.62171
H	-1.04347	5.67611	-0.51459
H	5.06379	2.61376	2.05997
H	5.10034	3.72049	4.25523
H	2.94503	4.31163	5.38962
H	0.79126	3.83244	4.25256
Mo	0.17214	-0.3851	-0.26298
O	-0.69078	-0.90697	1.35183
O	-1.00487	0.37289	-1.55931
O	1.74796	0.65177	0.01101
Si	-1.33179	-1.40393	2.80724
Si	-2.24425	1.06838	-2.42981
Si	3.0713	1.64264	0.20925
H	0.7744	-3.27081	-2.58833
H	0.93124	-3.99485	-0.96233
H	2.31022	-3.12047	-1.68794
H	-2.93682	0.81179	-4.84022
H	-1.98509	-0.57269	-4.25196
H	-1.16206	0.95056	-4.68667
H	-4.72851	0.99019	-2.15485
H	-3.91202	0.47352	-0.65209
H	-4.00211	-0.63645	-2.04164
H	-2.7918	-3.22853	1.91448
H	-2.2674	-3.61311	3.57836
H	-1.12664	-3.79384	2.22355
H	0.79577	-2.10457	3.87547
H	-0.37378	-1.55508	5.10807
H	0.52474	-0.36179	4.1298
H	3.41007	2.20622	-2.18395
H	3.97868	3.53721	-1.13846
H	2.23372	3.32664	-1.45259
H	4.61658	-0.10279	-0.6004
H	4.6215	-0.06311	1.18459
H	5.5446	1.15189	0.25566

[Mo]-A-TS

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Imaginary frequency = -108.38 cm^{-1}
Zero-point correction= 0.675093 (Hartree/Particle)
Thermal correction to Energy= 0.722735
Thermal correction to Enthalpy= 0.723679
Thermal correction to Gibbs Free Energy= 0.596955
Sum of electronic and zero-point Energies= -2557.096285
Sum of electronic and thermal Energies= -2557.048643
Sum of electronic and thermal Enthalpies= -2557.047699
Sum of electronic and thermal Free Energies= -2557.174423

C	-1.50459	0.51978	1.87354
C	-0.20628	0.96812	2.14388
C	0.41621	1.918	1.31862
C	-0.29676	2.41604	0.21797
C	-1.58722	1.96077	-0.09282
C	-2.18679	1.02105	0.75458
C	-2.17536	-0.456	2.79244
C	-2.12064	-1.85623	2.58888
C	-2.78874	-2.68369	3.51526
C	-3.48814	-2.1636	4.60657
C	-3.53443	-0.77961	4.79572
C	-2.88153	0.0623	3.89288
C	-2.33646	-3.96874	0.35485
C	0.30755	-3.62489	1.88149
C	-2.31252	2.55587	-1.25927
C	-2.63182	1.8352	-2.44094
C	-3.32431	2.53031	-3.45546
C	-3.68985	3.87358	-3.33209
C	-3.35231	4.5732	-2.17226
C	-2.66635	3.9138	-1.15083
C	-3.34454	-1.15658	-1.91845
C	-2.28251	-0.28454	-4.65768
C	1.7744	2.46461	1.61882
C	2.94548	1.66671	1.72136
C	4.15711	2.32651	2.02044
C	4.23717	3.70896	2.20366
C	3.08228	4.48383	2.07687
C	1.86866	3.86095	1.78545
C	4.74416	-0.57895	0.61602
C	3.005	-1.09072	3.10924
H	0.3216	0.58414	3.0187
H	0.16382	3.17106	-0.42035
H	-3.20208	0.67812	0.54792
H	-2.76442	-3.77064	3.38309
H	-3.99539	-2.83433	5.30524
H	-4.07817	-0.35501	5.64384
H	-2.91597	1.14567	4.03617
H	-3.5832	2.01281	-4.38241
H	-4.22813	4.3716	-4.14301
H	-3.62269	5.62646	-2.05932
H	-2.40446	4.45355	-0.23678
H	5.07978	1.74533	2.10394
H	5.19726	4.17754	2.43557
H	3.12263	5.56816	2.20969
H	0.96004	4.46243	1.69998
Mo	0.73299	-1.02095	-1.11044
O	-0.70038	-1.59413	0.06644
O	-0.5992	-0.28367	-2.34554

O	1.90059	-0.78272	0.44299
Si	-1.18848	-2.72164	1.18071
Si	-2.16483	0.01735	-2.7977
Si	3.08433	-0.21656	1.44151
C	3.48394	-1.48218	-3.46249
C	2.53848	-0.71257	-2.631
C	2.11295	0.3734	-2.15571
C	1.69299	-3.82418	-2.38329
C	1.32512	-2.50473	-1.86574
H	2.73071	-4.10415	-2.13153
H	1.54905	-3.91012	-3.4744
H	1.02446	-4.5594	-1.90012
H	4.08082	-2.17958	-2.85518
H	4.17215	-0.77448	-3.95152
H	2.97149	-2.06275	-4.24372
C	2.15568	1.84587	-2.08436
H	1.17816	2.26133	-2.37286
H	2.36876	2.1789	-1.05775
H	2.93038	2.24699	-2.75765
H	-4.39341	-0.88041	-2.1166
H	-3.167	-1.14017	-0.83541
H	-3.18318	-2.18858	-2.2703
H	-1.67455	0.43795	-5.22595
H	-3.31751	-0.23952	-5.0343
H	-1.89443	-1.29517	-4.86806
H	-3.24537	-3.48093	-0.02819
H	-2.63842	-4.76626	1.05334
H	-1.81765	-4.4408	-0.49641
H	0.82887	-4.17004	1.07676
H	0.01531	-4.34797	2.66039
H	1.01633	-2.90593	2.31597
H	3.22341	-2.16545	2.99945
H	2.00965	-0.98886	3.569
H	3.74593	-0.65822	3.80194
H	4.77568	-1.64999	0.35467
H	5.61279	-0.36282	1.25809
H	4.84588	0.00027	-0.31605

[Mo]-B

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 0.677811
(Hartree/Particle)
Thermal correction to Energy= 0.725151
Thermal correction to Enthalpy= 0.726095
Thermal correction to Gibbs Free Energy=
0.599392
Sum of electronic and zero-point Energies= -
2557.107330
Sum of electronic and thermal Energies= -
2557.059989
Sum of electronic and thermal Enthalpies= -
2557.059045
Sum of electronic and thermal Free Energies= -
2557.185748

C	-1.66755	1.21213	2.02127
C	-0.38171	1.35061	2.55857
C	0.60301	2.09975	1.89201
C	0.27274	2.7138	0.6772
C	-1.00304	2.57599	0.11103
C	-1.97187	1.84794	0.81066
C	-2.71061	0.38372	2.69878
C	-2.63317	-1.03219	2.71809
C	-3.66492	-1.7387	3.3677
C	-4.73994	-1.08472	3.97701
C	-4.81214	0.30968	3.93467
C	-3.80369	1.03439	3.29471
C	-1.84301	-3.75065	1.4613
C	0.2787	-2.11362	2.98059
C	-1.33295	3.23613	-1.18397
C	-1.80679	2.51264	-2.31299
C	-2.12657	3.26497	-3.46328
C	-1.98214	4.65471	-3.52136
C	-1.4881	5.34332	-2.41284
C	-1.16683	4.63142	-1.25613
C	-3.31085	-0.2002	-1.50235
C	-2.20491	0.20981	-4.28078
C	1.96056	2.27348	2.48446
C	3.15702	1.98747	1.77187
C	4.38465	2.24365	2.41758
C	4.45215	2.75455	3.71626
C	3.26998	3.00394	4.41669
C	2.04055	2.76155	3.80223
C	3.18859	2.3143	-1.4031
C	4.82347	0.10921	-0.01925
H	-0.13865	0.86297	3.50475
H	1.019	3.31919	0.16212
H	-2.9787	1.76297	0.4016
H	-3.64087	-2.832	3.39175
H	-5.52348	-1.66343	4.47331
H	-5.65169	0.83443	4.3983
H	-3.85426	2.12592	3.25866
H	-2.48998	2.75706	-4.35834
H	-2.24572	5.19312	-4.43574
H	-1.35967	6.42857	-2.4426
H	-0.79753	5.16462	-0.37604
H	5.32366	2.02533	1.9015
H	5.42301	2.94427	4.18117
H	3.30241	3.39382	5.43741
H	1.11436	2.97615	4.34129
Mo	0.65997	-1.09284	-0.69246
O	-0.90756	-1.2348	0.42328
O	-0.40555	0.01483	-1.98012
O	1.97085	0.07068	-0.04526
Si	-1.24621	-2.01387	1.87192
Si	-1.88843	0.59604	-2.45463
Si	3.26015	1.15231	0.07126
C	0.07695	-2.40488	-3.73366
C	0.66364	-2.43764	-2.37059
C	1.20078	-3.47497	-1.6554
C	1.34662	-4.93102	-1.98886
C	1.58975	-2.81308	-0.4279
H	0.48599	-3.2078	-4.37149
H	0.24537	-1.43372	-4.22069
H	-1.01806	-2.54097	-3.68714
H	1.06632	-5.14581	-3.02991
H	0.70608	-5.53908	-1.3265
H	2.38435	-5.26562	-1.8221
C	2.63295	-3.28291	0.52981
H	3.57226	-3.52342	-0.00403
H	2.85703	-2.54639	1.31391
H	2.30372	-4.21541	1.02608
H	4.77757	-0.51539	-0.92654
H	4.90722	-0.5569	0.85388
H	5.7367	0.72294	-0.07861
H	3.49729	1.77076	-2.31144
H	3.87119	3.16901	-1.26619
H	2.17303	2.70131	-1.57097
H	-3.16029	0.64556	-4.6177
H	-2.27994	-0.87856	-4.42139
H	-1.40327	0.58552	-4.93664
H	-4.23282	0.40081	-1.57307

H	-3.04675	-0.34782	-0.44769
H	-3.51862	-1.19242	-1.93844
H	0.88447	-3.00032	2.74087
H	-0.02473	-2.18371	4.03807
H	0.91388	-1.22195	2.86531
H	-2.78166	-3.72157	0.8854
H	-2.00269	-4.36726	2.36076
H	-1.07501	-4.24575	0.84368

[Mo]-B-TS-B'

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Imaginary frequency = -200.55 cm^{-1}
Zero-point correction= 0.676296 (Hartree/Particle)
Thermal correction to Energy= 0.723269
Thermal correction to Enthalpy= 0.724213
Thermal correction to Gibbs Free Energy= 0.598902
Sum of electronic and zero-point Energies= -2557.092269
Sum of electronic and thermal Energies= -2557.045296
Sum of electronic and thermal Enthalpies= -2557.044352
Sum of electronic and thermal Free Energies= -2557.169664

C	-1.69733	1.07146	1.89987
C	-0.40182	1.1351	2.42911
C	0.59129	1.93463	1.83258
C	0.25406	2.66807	0.68666
C	-1.01965	2.58261	0.11067
C	-1.99717	1.81058	0.74832
C	-2.76111	0.22871	2.52248
C	-2.69385	-1.18713	2.52387
C	-3.75366	-1.89509	3.12701
C	-4.84666	-1.24406	3.70514
C	-4.90991	0.15132	3.67777
C	-3.87429	0.87701	3.08581
C	-1.9807	-3.8548	1.13875
C	0.09587	-2.48684	2.94334
C	-1.32615	3.28564	-1.16684
C	-1.72141	2.56591	-2.3265
C	-2.02521	3.31875	-3.47908
C	-1.93548	4.71431	-3.50646
C	-1.5139	5.40189	-2.36665
C	-1.20997	4.6856	-1.20689
C	-3.20089	-0.18209	-1.67535
C	-1.71551	0.21392	-4.31201
C	1.96314	2.00367	2.41375
C	3.14855	1.92411	1.628
C	4.38337	2.03113	2.30295
C	4.47503	2.19753	3.68718
C	3.30572	2.25324	4.44766
C	2.06857	2.15771	3.81074
C	3.28641	3.16387	-1.27494
C	4.9143	0.70427	-0.59653
H	-0.16129	0.54795	3.31705
H	0.99855	3.3097	0.22003
H	-3.00336	1.76631	0.33034
H	-3.73815	-2.98874	3.13685
H	-5.65086	-1.82506	4.16424
H	-5.76318	0.67537	4.11633
H	-3.91698	1.96915	3.06355
H	-2.32796	2.80613	-4.39551
H	-2.18209	5.2602	-4.42113
H	-1.42701	6.49164	-2.37601
H	-0.89305	5.21643	-0.30499
H	5.31485	1.96771	1.73459
H	5.4541	2.27655	4.1669
H	3.35328	2.38064	5.53232
H	1.15453	2.23001	4.40496
Mo	0.87238	-0.93404	-0.56383
O	-0.77971	-1.40692	0.33292
O	-0.29211	0.06303	-1.8453
O	2.03763	0.60735	-0.77723
Si	-1.30438	-2.19267	1.71437
Si	-1.70625	0.65503	-2.47362
Si	3.27875	1.58199	-0.24927
C	0.61813	-3.45103	-2.59572
C	1.25171	-2.61751	-1.54535
C	1.99172	-2.9351	-0.41248
C	2.42406	-4.33133	-0.0262
C	2.2531	-1.80018	0.49889
H	1.15573	-4.40006	-2.75856
H	0.58299	-2.90167	-3.54955
H	-0.42737	-3.68703	-2.32534
H	2.17093	-5.06934	-0.79862
H	1.93622	-4.62185	0.91838
H	3.51108	-4.35276	0.15023
C	3.32469	-1.82955	1.52296
H	4.29796	-2.13392	1.09791
H	3.44232	-0.84795	2.0038
H	3.08128	-2.56341	2.31342
H	4.87983	0.31719	-1.62841
H	5.09282	-0.1427	0.08154
H	5.77413	1.39048	-0.52727
H	3.60654	2.92225	-2.30224
H	4.00224	3.89177	-0.85783
H	2.29966	3.64508	-1.33881
H	-2.67307	0.46479	-4.7982
H	-1.56706	-0.87465	-4.40864
H	-0.90299	0.71918	-4.85806
H	-4.12235	0.41386	-1.78255
H	-3.01058	-0.36846	-0.6095
H	-3.36768	-1.15946	-2.15951
H	0.75193	-3.3045	2.60646
H	-0.32125	-2.76614	3.92492
H	0.71519	-1.58696	3.06953
H	-2.86427	-3.71859	0.49526
H	-2.25832	-4.51119	1.97943
H	-1.20415	-4.37139	0.55047

[Mo]-B'

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 0.677674 (Hartree/Particle)
Thermal correction to Energy= 0.724866
Thermal correction to Enthalpy= 0.725810
Thermal correction to Gibbs Free Energy= 0.599312
Sum of electronic and zero-point Energies= -2557.108581
Sum of electronic and thermal Energies= -2557.061389
Sum of electronic and thermal Enthalpies= -2557.060444
Sum of electronic and thermal Free Energies= -2557.186942

Si	8.78502	-0.1563	5.97636
Si	6.43877	5.79954	3.84384

Si	10.96344	3.92159	4.64312
O	8.77564	1.47697	5.81058
O	6.8931	4.88363	5.14539
O	9.30312	3.86099	4.82329
C	8.50166	-1.11291	4.35028
C	8.49993	-2.51733	4.50484
H	8.68138	-2.94787	5.49509
C	8.26924	-3.39207	3.44206
H	8.27857	-4.47285	3.60694
C	8.02341	-2.87128	2.16897
H	7.8379	-3.53739	1.32219
C	8.01949	-1.48844	1.98469
H	7.83213	-1.0743	0.9903
C	8.26028	-0.60053	3.05187
C	8.23295	0.85848	2.70631
C	9.41567	1.57016	2.45821
H	10.38041	1.07895	2.60069
C	9.36973	2.89436	2.00298
C	8.12694	3.51228	1.81336
H	8.09422	4.53148	1.4322
C	6.93309	2.85267	2.12316
C	7.00453	1.50722	2.53012
H	6.08512	0.95597	2.72578
C	5.61607	3.54208	2.00255
C	5.32918	4.79668	2.61976
C	4.04009	5.3295	2.39714
H	3.76736	6.28611	2.84565
C	3.06796	4.67984	1.63041
H	2.08577	5.13931	1.49073
C	3.35949	3.44288	1.05576
H	2.61333	2.91576	0.45538
C	4.62503	2.88743	1.24584
H	4.86749	1.92896	0.77977
C	10.6149	3.67818	1.74291
C	11.39232	4.18621	2.81243
C	12.53956	4.9393	2.49171
H	13.15719	5.35384	3.29382
C	12.9133	5.18982	1.16827
H	13.80958	5.77798	0.95381
C	12.12822	4.69435	0.12403
H	12.40425	4.88912	-0.9157
C	10.98428	3.94697	0.41464
H	10.36489	3.55697	-0.39754
C	6.02304	2.29224	5.81444
C	6.20141	2.63216	7.15618
C	7.43264	3.37853	7.59123
C	4.90187	1.60603	5.1414
H	5.21248	0.60356	4.80222
H	4.02446	1.48798	5.79819
H	4.59406	2.17099	4.24723
C	5.2309	2.27497	8.25438
H	4.91437	3.18196	8.79195
H	4.34495	1.76351	7.85885
H	5.72574	1.61252	8.98197
C	7.7575	3.76653	8.98148
H	6.99016	4.44072	9.40174
H	7.82235	2.88227	9.64075
H	8.72422	4.28896	9.01381
C	11.54903	5.40912	5.64087
H	12.64592	5.51592	5.64045
H	11.108	6.34017	5.25022
H	11.22195	5.28871	6.68714
C	11.78931	2.35785	5.27041
H	12.88326	2.43668	5.15481
H	11.55174	2.18739	6.3312
H	11.4355	1.48478	4.70613
C	10.43697	-0.72144	6.69435
H	10.43539	-1.80263	6.90872
H	11.26688	-0.51057	6.00305
H	10.63721	-0.18611	7.63758
C	7.41171	-0.66597	7.17806
H	7.54108	-0.12742	8.13228
H	6.41635	-0.41506	6.77951
H	7.43035	-1.74717	7.39032
C	5.39849	7.21903	4.53385
H	6.01038	7.73812	5.29012
H	5.11967	7.95848	3.76494
H	4.47985	6.86604	5.02934
C	7.97419	6.57699	3.06208
H	8.26006	7.461	3.65663
H	8.81965	5.87518	3.07553
H	7.7996	6.90784	2.02505
Mo	7.77422	3.2115	5.77077

[Mo]-B-TS-ent-B

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Imaginary frequency = -93.60 cm^{-1}
Zero-point correction= 0.675593 (Hartree/Particle)
Thermal correction to Energy= 0.723002
Thermal correction to Enthalpy= 0.723946
Thermal correction to Gibbs Free Energy= 0.597023
Sum of electronic and zero-point Energies= -2557.101177
Sum of electronic and thermal Energies= -2557.053768
Sum of electronic and thermal Enthalpies= -2557.052824
Sum of electronic and thermal Free Energies= -2557.179746

C	-1.59678	0.97631	1.67245
C	-0.49788	1.3696	2.44671
C	0.44066	2.28953	1.96579
C	0.21902	2.89398	0.72105
C	-0.89525	2.55649	-0.06166
C	-1.79208	1.59584	0.42589
C	-2.50852	-0.11661	2.11323
C	-2.02845	-1.36245	2.6114
C	-2.99167	-2.32485	2.98173
C	-4.36601	-2.09844	2.87049
C	-4.82076	-0.87943	2.36456
C	-3.89561	0.09506	1.99023
C	-0.13878	-3.8057	2.53719
C	0.49718	-1.56643	4.48387
C	-1.09351	3.21545	-1.38655
C	-1.22493	2.48712	-2.59725
C	-1.41446	3.22208	-3.78705
C	-1.46881	4.61784	-3.80299
C	-1.31757	5.32366	-2.60658
C	-1.12892	4.6231	-1.41471
C	-2.89434	-0.09697	-2.84016
C	-0.30585	0.18432	-4.44439
C	1.67316	2.57151	2.75493
C	2.96784	2.30359	2.2373
C	4.07224	2.61813	3.05649
C	3.92394	3.15977	4.33635
C	2.64226	3.3881	4.84273
C	1.52946	3.09171	4.05379
C	3.68364	2.77128	-0.76429
C	4.88399	0.38264	0.77524

H	-0.34022	0.91758	3.42449
H	0.93974	3.61981	0.34153
H	-2.64541	1.30377	-0.1874
H	-2.6639	-3.29645	3.36117
H	-5.07553	-2.87378	3.1713
H	-5.8917	-0.6832	2.26672
H	-4.25097	1.05615	1.61005
H	-1.51382	2.69395	-4.73948
H	-1.61957	5.15005	-4.74583
H	-1.35069	6.41627	-2.59882
H	-1.02339	5.17119	-0.475
H	5.08617	2.42381	2.69525
H	4.80627	3.39035	4.9393
H	2.5077	3.8002	5.84629
H	0.5234	3.27981	4.4382
Mo	0.843	-0.95569	-0.26858
O	0.78348	-1.1968	1.65854
O	-0.22144	-0.12419	-1.62741
O	2.12651	0.48272	0.04891
Si	-0.20971	-1.93419	2.77565
Si	-1.14635	0.59832	-2.80812
Si	3.3572	1.47291	0.56163
C	-1.97222	-2.89093	-0.86478
C	-0.5352	-2.5943	-0.67419
C	0.55808	-3.11855	-1.31529
C	0.63336	-3.87714	-2.61746
C	1.73799	-2.59281	-0.61778
H	-2.26356	-3.68533	-0.15312
H	-2.21716	-3.26322	-1.87662
H	-2.59956	-2.01866	-0.63137
H	-0.34257	-4.29376	-2.90462
H	1.35983	-4.70297	-2.54803
H	0.97685	-3.20854	-3.42569
C	2.96693	-3.30427	-0.19045
H	3.37208	-3.93582	-1.00105
H	3.74893	-2.60552	0.14166
H	2.72549	-3.97147	0.6589
H	5.05697	-0.16875	-0.16401
H	4.71901	-0.35312	1.57936
H	5.80028	0.94902	1.00641
H	4.01557	2.28372	-1.69618
H	4.47011	3.47483	-0.44447
H	2.7754	3.35056	-0.9907
H	-0.91195	0.46244	-5.32132
H	-0.13373	-0.90414	-4.48349
H	0.6707	0.68819	-4.5235
H	-3.47548	0.43131	-3.61473
H	-3.42126	0.01985	-1.8813
H	-2.88158	-1.16809	-3.0937
H	1.47083	-2.07484	4.58431
H	-0.17084	-1.94898	5.27339
H	0.66302	-0.49353	4.65964
H	-0.68439	-4.13672	1.64211
H	-0.53954	-4.34411	3.41142
H	0.91811	-4.09656	2.42082

[Mo]-C

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 0.678894
(Hartree/Particle)
Thermal correction to Energy= 0.725931
Thermal correction to Enthalpy= 0.726875
Thermal correction to Gibbs Free Energy=
0.601238
Sum of electronic and zero-point Energies= -
2557.123525
Sum of electronic and thermal Energies= -
2557.076489
Sum of electronic and thermal Enthalpies= -
2557.075544
Sum of electronic and thermal Free Energies= -
2557.201181

C	-1.23123	-2.70761	-1.49465
C	-2.24449	-2.40442	-0.57714
C	-3.0143	-1.2399	-0.70802
C	-2.78139	-0.39333	-1.79856
C	-1.7751	-0.67686	-2.73314
C	-1.01961	-1.84558	-2.57989
C	-0.4157	-3.94596	-1.34411
C	0.40241	-4.17815	-0.20713
C	1.09701	-5.40444	-0.14824
C	1.00679	-6.36398	-1.16106
C	0.22109	-6.10682	-2.28615
C	-0.48067	-4.90305	-2.37218
C	-4.08633	-0.92947	0.2799
C	-4.06899	0.25167	1.06743
C	-5.1577	0.46673	1.93812
C	-6.21728	-0.43856	2.04752
C	-6.203	-1.61074	1.2891
C	-5.14106	-1.84965	0.41499
C	-1.54024	0.23219	-3.89067
C	-0.29025	0.86945	-4.1095
C	-0.16528	1.67259	-5.2622
C	-1.21891	1.85785	-6.1622
C	-2.45064	1.24827	-5.91604
C	-2.6043	0.44434	-4.78511
C	2.29286	-3.42654	2.08077
C	-0.65911	-2.72601	2.43281
C	-2.77512	2.46269	2.73718
C	-2.56731	2.71705	-0.29829
C	2.30162	2.27952	-3.29958
C	2.19956	-0.74813	-2.91708
C	2.17516	1.88645	0.87217
C	2.28005	0.77258	1.79725
C	1.29246	1.81435	2.02095
C	3.33327	0.03752	2.54554
H	-2.43711	-3.08194	0.25572
H	-3.39137	0.50245	-1.92345
H	-0.25201	-2.09007	-3.31514
H	1.74288	-5.62201	0.70537
H	1.55913	-7.30346	-1.07493
H	0.14841	-6.84166	-3.0923
H	-1.11039	-4.70074	-3.24258
H	-5.1824	1.36038	2.56578
H	-7.04386	-0.23274	2.73275
H	-7.01778	-2.33495	1.37133
H	-5.13062	-2.75763	-0.19376
H	0.77682	2.18634	-5.46621
H	-1.07932	2.48687	-7.04534
H	-3.28851	1.39202	-6.60336
H	-3.56081	-0.04897	-4.59333
Mo	0.64122	0.4992	0.51931
O	0.97518	-1.41374	0.43079
O	-1.19822	0.59924	1.13423
O	0.52853	1.02597	-1.34584
Si	0.73013	-2.89645	1.16807
Si	-2.61713	1.48736	1.13075
Si	1.16772	0.83147	-2.88099
C	3.05279	2.88029	0.2004
C	0.82623	2.68082	3.13531

H	0.28259	3.56025	2.75774
H	1.68664	3.04346	3.72508
H	0.15717	2.13159	3.81545
H	2.46716	3.56896	-0.42805
H	3.79945	2.38627	-0.43963
H	3.59619	3.48248	0.9498
H	3.85832	-0.67833	1.89435
H	2.90598	-0.52183	3.39174
H	4.08224	0.74113	2.94996
H	-2.10232	2.26892	-1.18814
H	-1.95834	3.58905	-0.0044
H	-3.57413	3.0783	-0.56449
H	-1.4283	-2.0275	2.07227
H	-0.24797	-2.31762	3.37175
H	-1.13222	-3.69512	2.6607
H	3.1562	-3.51388	1.40204
H	2.15303	-4.39471	2.58935
H	2.53606	-2.68332	2.8538
H	-1.92685	3.15499	2.83467
H	-2.78459	1.80118	3.61817
H	-3.69591	3.0688	2.75036
H	2.30673	-1.14933	-3.93814
H	1.75276	-1.52072	-2.27431
H	3.20928	-0.53101	-2.52869
H	2.73858	2.16931	-4.30584
H	3.13496	2.31269	-2.58304
H	1.7704	3.24369	-3.25724

[Mo]-B-TS

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Imaginary frequency = -179.76 cm^{-1}
Zero-point correction= 0.676178
(Hartree/Particle)
Thermal correction to Energy= 0.723241
Thermal correction to Enthalpy= 0.724185
Thermal correction to Gibbs Free Energy=
0.598258
Sum of electronic and zero-point Energies= -
2557.086727
Sum of electronic and thermal Energies= -
2557.039664
Sum of electronic and thermal Enthalpies= -
2557.038719
Sum of electronic and thermal Free Energies= -
2557.164647

C	-1.15611	-2.5882	-1.21194
C	-2.13465	-2.19475	-0.29083
C	-2.86708	-1.01006	-0.4815
C	-2.59314	-0.21925	-1.60572
C	-1.57953	-0.56608	-2.50972
C	-0.89076	-1.76878	-2.31564
C	-0.44596	-3.89829	-1.08001
C	0.67724	-4.08467	-0.24036
C	1.25606	-5.37197	-0.20566
C	0.76062	-6.43534	-0.96377
C	-0.34076	-6.23064	-1.79844
C	-0.93361	-4.96819	-1.85285
C	-3.95913	-0.62532	0.45769
C	-3.99758	0.63821	1.10667
C	-5.11159	0.92517	1.92179
C	-6.15074	0.0095	2.11052
C	-6.08436	-1.24161	1.4939
C	-4.99508	-1.55111	0.67722
C	-1.2587	0.30703	-3.67462
C	0.04003	0.85216	-3.85992
C	0.26001	1.62335	-5.01911
C	-0.74833	1.86622	-5.95714
C	-2.02825	1.34995	-5.7429
C	-2.27632	0.57769	-4.60615
C	3.33076	-3.12661	0.88749
C	0.71302	-2.98318	2.60168
C	-2.75382	3.05085	2.56479
C	-2.31503	2.90263	-0.46053
C	2.61266	2.19903	-2.85509
C	2.46541	-0.82926	-2.6723
C	1.66863	2.27852	1.37263
C	1.74167	0.47244	2.47205
C	1.30047	1.88229	2.62552
C	3.02562	-0.02578	3.04172
H	-2.33853	-2.82131	0.58082
H	-3.17985	0.68247	-1.78295
H	-0.13801	-2.07861	-3.04147
H	2.12645	-5.5557	0.4303
H	1.23721	-7.41772	-0.90747
H	-0.73807	-7.04917	-2.40453
H	-1.79675	-4.79899	-2.50227
H	-5.17055	1.88436	2.44236
H	-7.00045	0.26877	2.74742
H	-6.88213	-1.97444	1.64081
H	-4.95018	-2.52162	0.17648
H	1.24443	2.06503	-5.19526
H	-0.53686	2.46763	-6.84543
H	-2.83061	1.54091	-6.46054
H	-3.27124	0.15552	-4.44057
Mo	0.60784	0.55677	0.86688
O	1.24132	-1.23192	0.30555
O	-1.15386	0.98987	1.36215
O	0.73691	0.94929	-1.07143
Si	1.472	-2.76965	0.88702
Si	-2.56421	1.88211	1.10273
Si	1.43598	0.74685	-2.55794
C	2.17013	3.51524	0.73772
C	0.7048	2.56403	3.81362
H	0.50873	3.62826	3.61729
H	1.37796	2.48112	4.68296
H	-0.24513	2.07497	4.08202
H	1.75072	3.63745	-0.2714
H	3.26637	3.43773	0.62155
H	1.96358	4.40708	1.35468
H	3.07294	0.1758	4.12697
H	3.89318	0.47982	2.57858
H	3.14721	-1.10491	2.88667
H	2.75833	-1.03647	-3.71529
H	1.92583	-1.69357	-2.26524
H	3.38437	-0.70305	-2.07573
H	3.18722	2.09748	-3.79069
H	3.33632	2.2375	-2.02371
H	2.07347	3.15982	-2.88287
H	-1.85146	3.67846	2.63653
H	-2.87427	2.50706	3.51471
H	-3.61776	3.72345	2.43614
H	-1.64552	2.37864	-1.15936
H	-1.84384	3.86379	-0.19468
H	-3.26621	3.11928	-0.97275
H	-0.36679	-2.76529	2.5561
H	1.16067	-2.30267	3.34183
H	0.8382	-4.02027	2.9544
H	3.67998	-3.26951	-0.14792
H	3.59189	-4.02846	1.46448
H	3.8903	-2.28026	1.31327

[Mo]-D-TS

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Imaginary frequency = -249.08 cm^{-1}
Zero-point correction= 0.675819 (Hartree/Particle)
Thermal correction to Energy= 0.722782
Thermal correction to Enthalpy= 0.723726
Thermal correction to Gibbs Free Energy= 0.599520
Sum of electronic and zero-point Energies= -2557.055119
Sum of electronic and thermal Energies= -2557.008156
Sum of electronic and thermal Enthalpies= -2557.007212
Sum of electronic and thermal Free Energies= -2557.131419

C	-1.27163	1.26698	2.10035
C	0.07119	1.63004	1.94508
C	0.53439	2.16299	0.74045
C	-0.40273	2.42407	-0.2798
C	-1.76079	2.12112	-0.12611
C	-2.18481	1.53892	1.07449
C	-1.66506	0.40838	3.2538
C	-1.81094	-0.98259	3.02178
C	-2.15167	-1.7959	4.11956
C	-2.34107	-1.26333	5.39919
C	-2.17965	0.10875	5.6111
C	-1.8381	0.93932	4.53976
C	-2.75902	2.49925	-1.17914
C	-3.0528	1.74445	-2.34412
C	-4.01144	2.28682	-3.23324
C	-4.66596	3.49696	-3.00237
C	-4.37752	4.21813	-1.84205
C	-3.43311	3.71592	-0.94789
C	1.9847	2.45862	0.53134
C	3.02612	1.48252	0.61343
C	4.33496	1.93961	0.33768
C	4.63151	3.26279	-0.00305
C	3.60146	4.19902	-0.07865
C	2.29489	3.78913	0.18763
H	0.77514	1.43327	2.75293
H	-0.07435	2.87161	-1.21824
H	-3.23383	1.26208	1.19993
H	-2.26571	-2.87525	3.98137
H	-2.60627	-1.92061	6.23171
H	-2.31861	0.53286	6.60915
H	-1.7079	2.01359	4.69621
H	-4.26405	1.74245	-4.14828
H	-5.3988	3.87048	-3.72249
H	-4.8806	5.16618	-1.63444
H	-3.19652	4.27731	-0.04016
H	5.16899	1.23771	0.3777
H	5.665	3.55469	-0.20781
H	3.80886	5.24019	-0.33925
H	1.48077	4.51654	0.13504
O	-0.45343	-0.878	0.43694
O	-1.40975	-0.82245	-2.01018
O	2.0455	-1.22428	-0.20387
Si	-1.55015	-1.77926	1.30695
Si	-2.39258	0.0696	-3.00561
Si	2.91387	-0.42147	0.96717
C	1.50846	-1.22888	-3.44714
C	1.17979	0.39839	-2.27439
C	1.15138	-2.40771	-3.08442
C	2.20799	-0.8467	2.66283
H	1.11142	-0.80154	2.65837
H	2.50412	-1.87969	2.91187
H	2.59005	-0.18246	3.45551
C	4.65785	-1.14544	0.90941
H	5.31681	-0.73595	1.69252
H	4.5656	-2.23041	1.08319
H	5.14427	-1.00412	-0.06883
C	-1.47404	0.46185	-4.61153
H	-2.14716	0.90387	-5.36344
H	-0.65893	1.17861	-4.42674
H	-1.03584	-0.45792	-5.03225
C	-3.88401	-1.02857	-3.36719
H	-4.4348	-1.23458	-2.43549
H	-4.58441	-0.58812	-4.09347
H	-3.53194	-1.9924	-3.77145
C	-3.20345	-1.91503	0.41503
H	-3.07046	-2.44013	-0.54271
H	-3.93157	-2.46603	1.03364
H	-3.6166	-0.9203	0.19238
C	-0.8312	-3.50818	1.54806
H	0.12327	-3.45758	2.09594
H	-1.51208	-4.18291	2.09204
H	-0.63295	-3.95503	0.55894
C	1.01031	-3.85519	-3.28786
H	1.43859	-4.15293	-4.26123
H	1.52714	-4.41676	-2.49341
H	-0.05115	-4.1506	-3.26712
C	1.87655	1.59737	-2.75605
H	2.96139	1.41962	-2.84446
H	1.49374	1.95725	-3.72542
H	1.75239	2.39992	-2.01809
C	2.16753	-0.6451	-4.65698
H	1.53254	0.11364	-5.13581
H	3.13298	-0.17835	-4.41597
H	2.3465	-1.45498	-5.38002
Mo	0.42758	-0.90836	-1.29835

[Mo]-A-Ph

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 0.917179 (Hartree/Particle)
Thermal correction to Energy= 0.978141
Thermal correction to Enthalpy= 0.979086
Thermal correction to Gibbs Free Energy= 0.814927
Sum of electronic and zero-point Energies= -3550.648228
Sum of electronic and thermal Energies= -3550.587266
Sum of electronic and thermal Enthalpies= -3550.586322
Sum of electronic and thermal Free Energies= -3550.750480

C	-1.97192	1.65265	1.8911
C	-0.74162	1.80585	2.54519
C	0.31719	2.5101	1.94939
C	0.10785	3.1058	0.69779
C	-1.11514	2.97293	0.01986
C	-2.15086	2.25368	0.63452
C	-3.08795	0.87232	2.50422
C	-2.9488	-0.48695	2.89739
C	-4.06686	-1.13204	3.46151
C	-5.28935	-0.47709	3.63795
C	-5.42157	0.85098	3.22836

C	-4.32893	1.51299	2.66446
C	-1.85663	-3.34759	2.56489
C	-1.74377	-4.17738	3.69523
C	-2.12066	-5.52423	3.64074
C	-2.61221	-6.06542	2.44816
C	-2.72374	-5.25711	1.31056
C	-2.3491	-3.91165	1.37118
C	-0.04697	-1.17322	3.86104
C	-0.37179	-0.97746	5.2172
C	0.61226	-0.64139	6.15342
C	1.9411	-0.48198	5.74526
C	2.28261	-0.67267	4.40252
C	1.2979	-1.02086	3.47387
C	-1.2928	3.62912	-1.30991
C	-1.7008	2.93187	-2.48092
C	-1.83023	3.67124	-3.67481
C	-1.56406	5.04184	-3.73638
C	-1.14098	5.70974	-2.58663
C	-1.0088	5.00422	-1.38985
C	-3.59377	0.50507	-1.84167
C	-3.6959	-0.73932	-1.19244
C	-4.87623	-1.12738	-0.55183
C	-5.98816	-0.27885	-0.56366
C	-5.91467	0.95337	-1.22284
C	-4.72665	1.34116	-1.85153
C	-1.89298	0.56567	-4.42772
C	-3.05202	0.42398	-5.21228
C	-2.9679	0.09118	-6.56912
C	-1.71783	-0.11095	-7.16331
C	-0.55362	0.01781	-6.3964
C	-0.64318	0.35196	-5.04188
C	1.62769	2.61711	2.65662
C	2.86237	2.24146	2.05748
C	4.03661	2.37227	2.8254
C	4.01691	2.85225	4.13803
C	2.79805	3.20005	4.72225
C	1.61919	3.07893	3.98448
C	2.91777	2.7214	-1.04813
C	2.14791	2.46473	-2.19859
C	1.98808	3.434	-3.1926
C	2.60907	4.68008	-3.06012
C	3.38891	4.95118	-1.93037
C	3.5353	3.98168	-0.93197
C	4.66349	0.51134	0.25966
C	4.71535	-0.81135	0.74237
C	5.90787	-1.54078	0.71979
C	7.07453	-0.9573	0.21179
C	7.04094	0.3531	-0.27679
C	5.84384	1.07768	-0.25521
C	0.83049	-2.0596	-1.08821
C	1.34686	-3.32673	-1.62484
H	-0.59195	1.35324	3.52469
H	0.90938	3.67638	0.23134
H	-3.11067	2.14916	0.13137
H	-3.98915	-2.18319	3.75262
H	-6.13672	-1.00779	4.07965
H	-6.37382	1.37464	3.34634
H	-4.43077	2.55415	2.34809
H	-1.34998	-3.77151	4.63216
H	-2.02573	-6.15406	4.52941
H	-2.90462	-7.11794	2.40335
H	-3.10196	-5.67756	0.37474
H	-2.43239	-3.28934	0.47556
H	-1.41181	-1.06317	5.5481
H	0.33883	-0.48843	7.20095
H	2.70771	-0.19671	6.47027
H	3.31313	-0.52517	4.07028
H	1.5834	-1.13912	2.42671
H	-2.12925	3.15889	-4.59257
H	-1.67513	5.57922	-4.6817
H	-0.91491	6.77877	-2.61676
H	-0.68702	5.52917	-0.48711
H	-2.83538	-1.41252	-1.16877
H	-4.92189	-2.08623	-0.02902
H	-6.90797	-0.57388	-0.05235
H	-6.7809	1.62036	-1.23406
H	-4.67459	2.32276	-2.33322
H	-4.03697	0.57135	-4.75863
H	-3.87983	-0.01508	-7.16294
H	-1.65023	-0.37282	-8.22267
H	0.42527	-0.14472	-6.85567
H	0.27277	0.44289	-4.45044
H	4.99491	2.06995	2.39489
H	4.94825	2.93984	4.70344
H	2.7611	3.56552	5.75178
H	0.66588	3.35678	4.44069
H	1.6324	1.50849	-2.31163
H	1.35674	3.22317	-4.05928
H	2.47492	5.44364	-3.83068
H	3.87211	5.92572	-1.81949
H	4.12106	4.22339	-0.03914
H	3.80718	-1.27888	1.13384
H	5.9281	-2.56677	1.09725
H	8.0084	-1.52551	0.1929
H	7.94843	0.81	-0.68075
H	5.83048	2.09733	-0.65222
Mo	0.23445	-0.57417	-0.40582
O	-0.80625	-1.13791	1.08447
O	-0.72714	0.23888	-1.85339
O	1.81693	0.34189	0.13875
Si	-1.3909	-1.5237	2.58884
Si	-1.96251	1.05387	-2.60888
Si	3.03331	1.45158	0.33933
H	1.11913	-3.42363	-2.70142
H	0.89458	-4.18676	-1.09912
H	2.44295	-3.38597	-1.49946

[Mo]-A-TS-Ph

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Imaginary frequency = -96.26 cm^{-1}
Zero-point correction= 1.004448 (Hartree/Particle)
Thermal correction to Energy= 1.069819
Thermal correction to Enthalpy= 1.070764
Thermal correction to Gibbs Free Energy= 0.901741
Sum of electronic and zero-point Energies= -3706.439514
Sum of electronic and thermal Energies= -3706.374143
Sum of electronic and thermal Enthalpies= -3706.373198
Sum of electronic and thermal Free Energies= -3706.542221

C	-1.92727	1.13775	1.76482
C	-0.69346	1.37816	2.38221
C	0.30595	2.13015	1.74485
C	0.03745	2.66252	0.47504
C	-1.21327	2.47539	-0.14726
C	-2.19275	1.73062	0.52571
C	-2.91577	0.18854	2.35823

C	-2.60241	-1.19054	2.48806
C	-3.5721	-2.04126	3.05094
C	-4.82059	-1.56342	3.46128
C	-5.12793	-0.21073	3.29927
C	-4.17944	0.65555	2.74962
C	-1.15397	-3.71919	1.36819
C	-0.09104	-4.62457	1.55765
C	-0.14038	-5.92213	1.03621
C	-1.26229	-6.34403	0.31409
C	-2.33437	-5.46501	0.12401
C	-2.2772	-4.16972	0.64807
C	0.32693	-1.84164	3.28345
C	0.1148	-2.46492	4.52793
C	1.07217	-2.38244	5.54388
C	2.26045	-1.67092	5.33211
C	2.48607	-1.04439	4.10248
C	1.52544	-1.13377	3.09007
C	-1.50137	3.06831	-1.486
C	-2.07008	2.33156	-2.56705
C	-2.32261	3.0321	-3.76568
C	-2.01637	4.38656	-3.92679
C	-1.42758	5.08552	-2.87284
C	-1.17979	4.42638	-1.66793
C	-4.0026	0.01708	-1.71788
C	-4.04132	-1.1183	-0.88922
C	-5.19652	-1.4497	-0.17659
C	-6.33871	-0.65004	-0.28536
C	-6.32003	0.48308	-1.10625
C	-5.15844	0.81489	-1.81206
C	-2.57765	-0.039	-4.44971
C	-3.81952	-0.11742	-5.10599
C	-3.90247	-0.46526	-6.4593
C	-2.73849	-0.74724	-7.18185
C	-1.49388	-0.68327	-6.54438
C	-1.41723	-0.33443	-5.19254
C	1.59344	2.37833	2.46801
C	2.87899	1.99634	1.99763
C	3.99236	2.29652	2.81061
C	3.87114	2.93905	4.04406
C	2.60206	3.29273	4.5061
C	1.48307	3.01047	3.72268
C	3.8331	2.24613	-0.92844
C	3.56575	3.62505	-0.84728
C	3.92427	4.49486	-1.88316
C	4.57183	3.99844	-3.01916
C	4.86454	2.6323	-3.11126
C	4.49814	1.76896	-2.07505
C	4.69567	-0.19021	0.70056
C	6.05163	0.19006	0.70398
C	7.06743	-0.74928	0.91048
C	6.74421	-2.09647	1.10835
C	5.404	-2.49775	1.09215
C	4.39251	-1.55327	0.88782
H	-0.48387	0.93285	3.35589
H	0.81266	3.23298	-0.03891
H	-3.1668	1.57616	0.06477
H	-3.35753	-3.10909	3.15368
H	-5.55529	-2.24884	3.89189
H	-6.10643	0.17281	3.59984
H	-4.41548	1.71548	2.62406
H	0.79431	-4.3099	2.11795
H	0.69771	-6.60628	1.19514
H	-1.30332	-7.35692	-0.09537
H	-3.21706	-5.78868	-0.43398
H	-3.12593	-3.50068	0.49227
H	-0.81054	-3.02026	4.71341
H	0.89137	-2.87063	6.50561
H	3.0065	-1.60272	6.1286
H	3.40345	-0.47675	3.92749
H	1.68837	-0.63422	2.13597
H	-2.75047	2.49773	-4.61687
H	-2.22804	4.88603	-4.87577
H	-1.17	6.14241	-2.98058
H	-0.7431	4.98035	-0.83338
H	-3.13925	-1.72553	-0.78716
H	-5.20219	-2.31698	0.48759
H	-7.23898	-0.90212	0.28118
H	-7.20857	1.11515	-1.18765
H	-5.15084	1.71886	-2.42973
H	-4.74019	0.09065	-4.55284
H	-4.87822	-0.52082	-6.94975
H	-2.80101	-1.02093	-8.2386
H	-0.58102	-0.9087	-7.10302
H	-0.44027	-0.29663	-4.70287
H	4.99143	1.99782	2.48269
H	4.76058	3.1495	4.64345
H	2.48037	3.78808	5.47291
H	0.49009	3.29334	4.08075
H	3.07305	4.02991	0.04166
H	3.70174	5.56219	-1.80215
H	4.85403	4.67565	-3.8297
H	5.37752	2.24086	-3.99402
H	4.72902	0.7032	-2.16158
H	6.32472	1.2352	0.52729
H	8.11373	-0.43156	0.91079
H	7.53654	-2.83266	1.26883
H	5.14531	-3.55007	1.23917
H	3.34969	-1.87741	0.86618
Mo	0.52058	-0.68886	-1.06209
O	-0.39867	-1.05047	0.60635
O	-1.18438	-0.4734	-2.0165
O	1.99211	0.13588	-0.06613
Si	-0.95285	-1.91585	1.90311
Si	-2.41171	0.44486	-2.62746
Si	3.28286	1.03251	0.40982
C	2.62205	-1.58327	-3.90038
C	1.81624	-0.67491	-3.06301
C	1.37412	0.46888	-2.77718
C	1.52173	-3.65656	-1.80117
C	1.11576	-2.27143	-1.5642
H	2.61499	-3.79392	-1.73832
H	1.15859	-4.04048	-2.76979
H	1.05646	-4.26581	-1.00494
H	3.42745	-2.06173	-3.32296
H	3.0797	-0.9902	-4.70818
H	2.01014	-2.37597	-4.35622
C	1.26034	1.89948	-3.12679
H	2.10842	2.19973	-3.76028
H	0.32255	2.07806	-3.67252
H	1.24925	2.53992	-2.23791

[Mo]-B-Ph

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 1.006303 (Hartree/Particle)
Thermal correction to Energy= 1.071843
Thermal correction to Enthalpy= 1.072787
Thermal correction to Gibbs Free Energy= 0.904069
Sum of electronic and zero-point Energies= -3706.455213

Sum of electronic and thermal Energies= -3706.389672
Sum of electronic and thermal Enthalpies= -3706.388728
Sum of electronic and thermal Free Energies= -3706.557447

C	-1.71897	1.16108	1.88056
C	-0.45917	1.27474	2.48385
C	0.5783	1.99616	1.87013
C	0.31587	2.6514	0.66033
C	-0.93909	2.56309	0.04133
C	-1.95294	1.82714	0.6683
C	-2.78714	0.30695	2.48236
C	-2.60043	-1.08536	2.70336
C	-3.65983	-1.81925	3.26911
C	-4.87692	-1.21789	3.60445
C	-5.05979	0.14491	3.35956
C	-4.02176	0.89538	2.80181
C	-1.47031	-3.80991	1.7317
C	-0.72888	-4.88549	2.25474
C	-1.02381	-6.2087	1.90434
C	-2.06707	-6.4809	1.01428
C	-2.81015	-5.42469	0.47321
C	-2.51268	-4.10672	0.8295
C	0.35032	-1.94419	3.36916
C	0.17429	-2.52185	4.64247
C	1.17899	-2.45557	5.61339
C	2.38161	-1.79683	5.33281
C	2.57213	-1.20872	4.07847
C	1.56792	-1.28992	3.10909
C	-1.17396	3.27044	-1.25122
C	-1.56532	2.59378	-2.43646
C	-1.77757	3.37294	-3.59247
C	-1.59706	4.75921	-3.60294
C	-1.1776	5.40605	-2.43933
C	-0.96989	4.66136	-1.27715
C	-3.44976	0.17035	-1.98146
C	-3.56586	-0.71698	-0.89553
C	-4.81607	-1.04246	-0.35872
C	-5.97929	-0.4973	-0.91167
C	-5.88562	0.3827	-1.99646
C	-4.63175	0.71704	-2.51904
C	-1.5919	0.32583	-4.45912
C	-2.61262	-0.25904	-5.22783
C	-2.4136	-0.57833	-6.57703
C	-1.1823	-0.31674	-7.18496
C	-0.15177	0.26789	-6.43793
C	-0.3588	0.58317	-5.09269
C	1.92571	2.07647	2.50393
C	3.13058	1.77058	1.80863
C	4.34778	1.91326	2.50781
C	4.39835	2.32039	3.84378
C	3.20873	2.58376	4.52448
C	1.99044	2.46093	3.85521
C	3.12588	2.3966	-1.30212
C	2.08784	2.35666	-2.25274
C	1.95876	3.36239	-3.2152
C	2.87346	4.41951	-3.25169
C	3.91547	4.47196	-2.31869
C	4.03592	3.47057	-1.34978
C	4.86538	0.1148	-0.1196
C	5.15194	-0.90457	0.81157
C	6.28361	-1.71156	0.67597
C	7.1586	-1.51144	-0.39897
C	6.89397	-0.50418	-1.33173
C	5.75545	0.29909	-1.19307
H	-0.27114	0.76748	3.43056
H	1.0983	3.24285	0.18593
H	-2.93142	1.74661	0.19485
H	-3.54311	-2.89526	3.42844
H	-5.68246	-1.81479	4.03996
H	-6.01059	0.62678	3.6019
H	-4.16257	1.96271	2.61297
H	0.09485	-4.69187	2.94673
H	-0.43435	-7.0278	2.32489
H	-2.29799	-7.5129	0.73727
H	-3.62245	-5.62901	-0.22923
H	-3.10274	-3.29808	0.39184
H	-0.76412	-3.0287	4.88954
H	1.01967	-2.91091	6.59457
H	3.16303	-1.73228	6.09458
H	3.49175	-0.65994	3.85986
H	1.73	-0.80173	2.14866
H	-2.07222	2.88155	-4.52295
H	-1.7702	5.32664	-4.52121
H	-1.01584	6.48716	-2.43201
H	-0.65263	5.16457	-0.36013
H	-2.65802	-1.10987	-0.43632
H	-4.87998	-1.69826	0.51354
H	-6.95691	-0.74615	-0.48991
H	-6.79106	0.81879	-2.42766
H	-4.57874	1.42746	-3.3504
H	-3.57816	-0.48453	-4.7671
H	-3.22174	-1.03711	-7.15348
H	-1.02389	-0.56775	-8.23727
H	0.81481	0.47521	-6.90536
H	0.46215	1.02896	-4.5235
H	5.28829	1.67964	2.00281
H	5.36201	2.41774	4.35007
H	3.22594	2.89007	5.57359
H	1.0601	2.68383	4.38297
H	1.3457	1.55638	-2.21703
H	1.12326	3.33382	-3.91821
H	2.76783	5.20951	-3.99995
H	4.62969	5.29947	-2.33997
H	4.84751	3.53604	-0.61787
H	4.48401	-1.06842	1.6617
H	6.48493	-2.49734	1.40895
H	8.04637	-2.14018	-0.50737
H	7.57449	-0.34363	-2.17217
H	5.55877	1.07846	-1.93451
O	-0.67925	-1.25205	0.67326
O	-0.52319	-0.04817	-1.80538
O	2.03722	-0.03878	-0.2029
Si	-1.05519	-2.00459	2.1103
Si	-1.74811	0.6991	-2.60675
Si	3.25985	1.08928	0.03845
C	-0.58066	-2.70293	-3.46399
C	0.24913	-2.66491	-2.2347
C	0.74158	-3.69353	-1.47323
C	0.51858	-5.17419	-1.56085
C	1.47883	-2.99997	-0.43958
H	-0.64776	-3.72458	-3.87585
H	-0.18364	-2.03546	-4.24309
H	-1.60427	-2.34748	-3.25896
H	-0.00606	-5.45967	-2.48328
H	-0.08271	-5.51173	-0.70064
H	1.48014	-5.71204	-1.51536
C	2.49916	-3.59714	0.4667
H	3.3164	-4.05998	-0.11691
H	2.93712	-2.87328	1.1659
H	2.0281	-4.40227	1.06078

Mo 0.67268 -1.22708 -0.69606

[Mo]-B-TS-B'-Ph

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Imaginary frequency = -211.97 cm^{-1}
Zero-point correction= 1.004988
(Hartree/Particle)
Thermal correction to Energy= 1.070033
Thermal correction to Enthalpy= 1.070977
Thermal correction to Gibbs Free Energy=
0.901728
Sum of electronic and zero-point Energies= -
3706.433662
Sum of electronic and thermal Energies= -
3706.368617
Sum of electronic and thermal Enthalpies= -
3706.367673
Sum of electronic and thermal Free Energies= -
3706.536923

Mo	-0.36202	-0.05622	1.03793
Si	-0.14227	-3.42394	-0.04578
Si	-2.34	2.43986	-0.17611
Si	2.85599	1.06954	-0.31817
O	-0.02094	-1.8127	0.32882
O	-0.97175	1.58381	0.22103
O	1.40776	0.50042	0.20408
C	0.27332	-1.41729	-2.7361
C	-1.08532	-1.1133	-2.56541
H	-1.80677	-1.9185	-2.4247
C	-1.53477	0.21775	-2.5534
C	-0.59811	1.24657	-2.72312
H	-0.93006	2.28479	-2.73129
C	0.76856	0.97088	-2.83432
C	1.18891	-0.36424	-2.87128
H	2.25033	-0.5911	-2.9777
C	0.7788	-2.82116	-2.79774
C	0.63502	-3.75646	-1.74169
C	1.17403	-5.04727	-1.92281
H	1.09268	-5.78231	-1.11763
C	1.84149	-5.41847	-3.09143
H	2.24849	-6.42766	-3.19387
C	1.99645	-4.48309	-4.11733
H	2.52515	-4.75011	-5.03606
C	1.4705	-3.20026	-3.96426
H	1.58573	-2.46835	-4.76758
C	-2.977	0.54603	-2.36776
C	-3.42527	1.53626	-1.44819
C	-4.80186	1.8435	-1.43201
H	-5.17449	2.60768	-0.74439
C	-5.72319	1.18677	-2.25166
H	-6.78219	1.45404	-2.21016
C	-5.27882	0.17927	-3.11076
H	-5.98604	-0.35507	-3.7505
C	-3.91909	-0.12986	-3.166
H	-3.56688	-0.8908	-3.86678
C	1.75496	2.08645	-2.86045
C	2.7285	2.22185	-1.83708
C	3.63086	3.30034	-1.9328
H	4.38802	3.43753	-1.15605
C	3.57499	4.22447	-2.98098
H	4.29093	5.0497	-3.02159
C	2.58958	4.09542	-3.96239
H	2.52268	4.81945	-4.77863
C	1.68639	3.03271	-3.89607
H	0.91591	2.92306	-4.66374
C	0.82726	-4.3194	1.30536
C	1.80349	-3.62213	2.04366
H	1.97645	-2.56229	1.843
C	2.55654	-4.26482	3.03174
H	3.31204	-3.7054	3.5901
C	2.34449	-5.62066	3.30419
H	2.93317	-6.12437	4.07563
C	1.37215	-6.32846	2.58918
H	1.19582	-7.38611	2.80316
C	0.62075	-5.68057	1.6032
H	-0.14622	-6.24584	1.06496
C	-1.91606	-4.07075	-0.04282
C	-2.63557	-4.26758	-1.23749
H	-2.15279	-4.07762	-2.20011
C	-3.95832	-4.72197	-1.22243
H	-4.49787	-4.86209	-2.16286
C	-4.58594	-5.00429	-0.00451
H	-5.61946	-5.36043	0.01078
C	-3.8812	-4.84094	1.19338
H	-4.36209	-5.07177	2.14781
C	-2.56104	-4.38252	1.16976
H	-2.02162	-4.26756	2.11391
C	-3.32968	2.72684	1.4127
C	-4.36408	1.87465	1.84313
H	-4.68474	1.04536	1.2082
C	-4.99669	2.06419	3.07626
H	-5.79955	1.38962	3.38612
C	-4.59857	3.1121	3.91407
H	-5.09021	3.26139	4.87901
C	-3.56754	3.96739	3.50981
H	-3.25091	4.78837	4.15864
C	-2.94495	3.77583	2.27191
H	-2.14555	4.45812	1.96803
C	-1.6826	4.09301	-0.79804
C	-2.52831	5.15924	-1.1572
H	-3.61508	5.04791	-1.08379
C	-2.001	6.37263	-1.61084
H	-2.67227	7.19089	-1.88575
C	-0.61433	6.53868	-1.71621
H	-0.20282	7.48558	-2.07634
C	0.24114	5.48917	-1.3652
H	1.32424	5.60008	-1.45986
C	-0.29133	4.27989	-0.90687
H	0.37523	3.45527	-0.64748
C	3.60455	2.0955	1.08875
C	3.07294	3.36345	1.3994
H	2.2918	3.79533	0.76695
C	3.51739	4.08459	2.51114
H	3.08716	5.06495	2.73378
C	4.51047	3.54914	3.34052
H	4.85923	4.10958	4.21218
C	5.05739	2.29631	3.04567
H	5.83704	1.87509	3.68647
C	4.60783	1.58023	1.92953
H	5.04323	0.5999	1.71461
C	3.9751	-0.39918	-0.71108
C	5.32165	-0.26686	-1.09974
H	5.77881	0.72603	-1.16566
C	6.09393	-1.39097	-1.41191
H	7.1387	-1.26982	-1.71179
C	5.52837	-2.67088	-1.34784
H	6.13028	-3.54843	-1.59976
C	4.1906	-2.82148	-0.96786
H	3.73178	-3.81283	-0.92907
C	3.42775	-1.69382	-0.64957
H	2.37876	-1.80447	-0.37191

C	0.20192	0.42281	2.87372
C	-1.86363	-0.60579	2.12841
C	-1.1073	0.09674	3.19979
C	1.26261	1.17031	3.58582
C	-3.12266	-1.33151	2.42905
H	-3.85343	-0.66747	2.92158
H	-2.93706	-2.17207	3.12152
C	-1.79943	0.48596	4.48405
H	-2.63198	1.16954	4.25453
H	-2.22796	-0.40552	4.96803
H	1.30915	2.21777	3.24453
H	1.10881	1.16093	4.67748
H	2.2505	0.74004	3.36324
H	-1.11101	0.98001	5.18175
H	-3.5769	-1.74176	1.51775

[Mo]-B'-Ph

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 1.005955
(Hartree/Particle)
Thermal correction to Energy= 1.071363
Thermal correction to Enthalpy= 1.072308
Thermal correction to Gibbs Free Energy=
0.902130
Sum of electronic and zero-point Energies= -
3706.454986
Sum of electronic and thermal Energies= -
3706.389578
Sum of electronic and thermal Enthalpies= -
3706.388634
Sum of electronic and thermal Free Energies= -
3706.558812

Si	8.03239	-0.43035	5.93475
Si	6.57605	5.67964	3.87888
Si	11.16152	3.57304	4.46675
O	8.41369	1.16213	6.03958
O	7.58299	4.88057	4.90566
O	9.58568	3.17745	4.81059
C	8.67329	-1.24808	4.33936
C	9.01416	-2.61201	4.46787
H	8.87608	-3.10957	5.43084
C	9.55213	-3.35719	3.41707
H	9.80357	-4.4107	3.56425
C	9.7781	-2.73718	2.1871
H	10.20681	-3.29669	1.35159
C	9.44978	-1.39123	2.02885
H	9.61709	-0.90743	1.06341
C	8.88952	-0.63247	3.07682
C	8.59601	0.79802	2.74787
C	9.64288	1.60668	2.27672
H	10.65835	1.2078	2.26053
C	9.41699	2.93466	1.89636
C	8.11119	3.43332	1.90251
H	7.93447	4.45337	1.56427
C	7.04614	2.66467	2.38937
C	7.30651	1.34803	2.82367
H	6.48879	0.73691	3.20838
C	5.6681	3.23564	2.40654
C	5.36634	4.52006	2.94555
C	5.52181	6.84501	4.94064
C	5.46878	8.23359	4.7256
H	6.02651	8.67398	3.8941
C	4.71498	9.0688	5.5602
H	4.68862	10.14586	5.3731
C	3.99981	8.52785	6.63266
H	3.41193	9.17849	7.28574
C	4.03938	7.14728	6.86574
H	3.48001	6.71625	7.70107
C	4.79191	6.32123	6.0274
H	4.80832	5.2458	6.21952
C	7.58256	6.70694	2.66281
C	8.9549	6.92749	2.87915
H	9.4398	6.48849	3.75257
C	9.71505	7.67727	1.97713
H	10.78339	7.81654	2.15452
C	9.11334	8.22272	0.83859
H	9.70883	8.8023	0.12797
C	7.74931	8.01353	0.6047
H	7.27569	8.43245	-0.2875
C	6.99398	7.25976	1.50912
H	5.93165	7.09121	1.30432
C	4.02887	4.96	2.86085
H	3.76143	5.9376	3.26951
C	3.01416	4.18006	2.29804
H	1.99034	4.56083	2.25641
C	3.31955	2.91229	1.80063
H	2.53945	2.28383	1.36316
C	4.63656	2.45405	1.85387
H	4.88126	1.47097	1.444
C	10.54693	3.8728	1.63421
C	11.36899	4.2721	2.717
C	11.69693	4.86649	5.73399
C	13.01686	4.94499	6.21583
H	13.76933	4.23324	5.86352
C	13.38672	5.91221	7.15784
H	14.41761	5.95467	7.51984
C	12.43619	6.8168	7.6421
H	12.72226	7.57039	8.38084
C	11.1166	6.75028	7.17979
H	10.36751	7.45266	7.55596
C	10.75149	5.78577	6.23498
H	9.71444	5.74548	5.88884
C	12.20688	2.01189	4.5936
C	11.64263	0.8454	5.14038
H	10.60764	0.87471	5.48222
C	12.37443	-0.34361	5.21683
H	11.90736	-1.23938	5.63463
C	13.69202	-0.38365	4.7487
H	14.26688	-1.31214	4.80385
C	14.26984	0.7669	4.19804
H	15.29627	0.73742	3.82203
C	13.53019	1.95158	4.11569
H	13.98906	2.83184	3.65414
C	12.39687	5.19953	2.46612
H	13.02972	5.54155	3.29066
C	12.61657	5.71722	1.18561
H	13.42255	6.43616	1.0166
C	11.78744	5.32838	0.13055
H	11.94007	5.73978	-0.8706
C	10.75305	4.4165	0.35867
H	10.09483	4.11759	-0.46131
C	6.16859	-0.72967	6.07949
C	5.38557	-1.2112	5.01496
H	5.86041	-1.45148	4.05899
C	4.0054	-1.39862	5.15574
H	3.41602	-1.77104	4.31358
C	3.38222	-1.11414	6.37502
H	2.30482	-1.26097	6.48834
C	4.14527	-0.64803	7.45295
H	3.66435	-0.43077	8.41071
C	5.52178	-0.45905	7.30225

H	6.10635	-0.09913	8.15472
C	8.83056	-1.25859	7.44135
C	8.33481	-2.45521	7.9947
H	7.45072	-2.92997	7.55793
C	8.94317	-3.0485	9.10597
H	8.54086	-3.97821	9.51779
C	10.06231	-2.44812	9.69339
H	10.54004	-2.90906	10.56222
C	10.5623	-1.25164	9.16809
H	11.43223	-0.7732	9.62649
C	9.9487	-0.66349	8.05672
H	10.34115	0.2765	7.66253
C	6.01438	2.6994	5.90748
C	6.32677	3.16789	7.20828
C	7.7037	3.59548	7.54803
C	4.69688	2.27238	5.39097
H	4.8144	1.57979	4.5507
H	4.09879	1.7661	6.16323
H	4.13006	3.14021	5.01522
C	5.29906	3.27043	8.30906
H	5.19625	4.3232	8.6161
H	4.32099	2.89289	7.98892
H	5.63749	2.70067	9.18818
C	8.17799	4.11943	8.8475
H	7.56527	4.9763	9.17775
H	8.12489	3.34356	9.63183
H	9.2213	4.45548	8.76123
Mo	7.93135	3.09084	5.7654

[Mo]-C-Ph

B3LYP-D3/def2SVP-LANL2DZ(Mo)-CPCM(benzene)
Zero-point correction= 1.006905
(Hartree/Particle)
Thermal correction to Energy= 1.072289
Thermal correction to Enthalpy= 1.073233
Thermal correction to Gibbs Free Energy=
0.905359
Sum of electronic and zero-point Energies= -
3706.475869
Sum of electronic and thermal Energies= -
3706.410485
Sum of electronic and thermal Enthalpies= -
3706.409541
Sum of electronic and thermal Free Energies= -
3706.577415

C	-1.14759	-2.65128	-1.50179
C	-2.14902	-2.39448	-0.55513
C	-2.94821	-1.24472	-0.63667
C	-2.75977	-0.36656	-1.71248
C	-1.76684	-0.59975	-2.6752
C	-0.982	-1.75614	-2.56897
C	-0.27576	-3.85752	-1.39317
C	0.49869	-4.14484	-0.23566
C	1.26895	-5.32537	-0.2351
C	1.30182	-6.19392	-1.32992
C	0.56306	-5.88379	-2.47325
C	-0.21553	-4.72545	-2.49768
C	-3.98373	-0.97342	0.40284
C	-4.02513	0.23754	1.147
C	-5.06334	0.39819	2.08675
C	-6.02341	-0.59264	2.312
C	-5.95174	-1.79132	1.59973
C	-4.93942	-1.9731	0.6559
C	-1.56381	0.36843	-3.79239
C	-0.30781	0.97902	-4.06058
C	-0.22586	1.86147	-5.15697
C	-1.33212	2.15816	-5.95849
C	-2.5675	1.57837	-5.66418
C	-2.67491	0.69281	-4.59056
C	2.33388	-3.34424	2.0871
C	3.50858	-3.25732	1.31215
C	4.77131	-3.41646	1.88788
C	4.88561	-3.66804	3.26092
C	3.73313	-3.76073	4.04688
C	2.4706	-3.59961	3.4628
C	-0.73667	-3.19879	2.50044
C	-0.96786	-4.43708	3.13068
C	-2.05028	-4.61473	3.99883
C	-2.93259	-3.55573	4.2419
C	-2.72379	-2.32101	3.61899
C	-1.63124	-2.1436	2.76409
C	-2.68951	2.50543	2.72066
C	-2.49234	1.76073	3.90161
C	-2.38015	2.38811	5.1447
C	-2.46468	3.78333	5.23259
C	-2.66469	4.53997	4.07414
C	-2.77535	3.90423	2.83129
C	-2.99361	2.80973	-0.35123
C	-4.17447	3.57496	-0.41611
C	-4.42633	4.42487	-1.49828
C	-3.50285	4.51491	-2.54626
C	-2.32755	3.75812	-2.50247
C	-2.07306	2.92147	-1.41091
C	2.31237	2.32297	-3.2009
C	1.75173	3.5953	-2.96665
C	2.5293	4.75389	-3.03399
C	3.89314	4.663	-3.33953
C	4.46792	3.41123	-3.57844
C	3.68234	2.25406	-3.50904
C	2.22098	-0.76742	-3.37633
C	2.7405	-0.97062	-4.66973
C	3.41561	-2.15036	-5.00008
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[Mo]-B-TS

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Sum of electronic and thermal Energies= -3706.373289
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[Mo]-D-TS-Ph

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H	5.64833	-0.84102	2.21168
C	5.78989	-3.11999	-0.93136
H	3.72011	-2.58206	-1.23597
C	6.92148	-2.96956	-0.12398
H	7.73854	-2.03248	1.64875
H	5.82559	-3.77221	-1.80858
H	7.84661	-3.49846	-0.36863
C	2.48338	-1.0788	2.72487
C	3.10211	-0.35353	3.76172
C	1.51465	-2.03488	3.06882
C	2.75785	-0.57464	5.09869
H	3.84077	0.41871	3.52483
C	1.15527	-2.24982	4.40264
H	1.02163	-2.59179	2.27169
C	1.77627	-1.51982	5.42045
H	3.24334	0.0019	5.8909
H	0.37117	-2.96861	4.65236
H	1.48752	-1.67851	6.46275
Mo	0.33558	-0.85829	-1.28972

Appendix 7: Methods, Experimental Data, Supplementary Figures, HPLC Traces and NMR Spectra of Structures from Chapter 7 (Iron-Catalyzed Multicomponent Cross-Coupling of Vinyl Aryl- and Alkyl Ethers with Grignard Reagents and (Fluoro)Alkyl Halides)

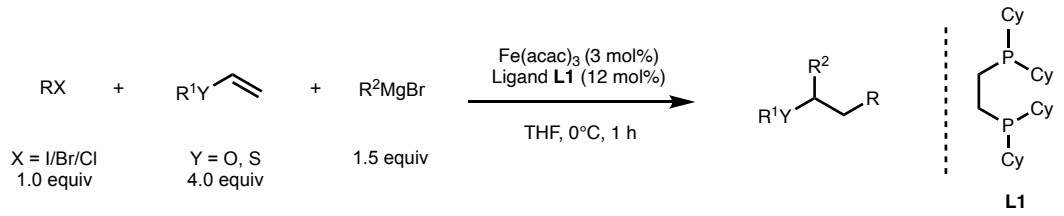
A7.1 Methods

A7.1.1 General

All non-aqueous reactions were carried out under a nitrogen atmosphere in oven- (150 °C) or flame-dried glassware. When necessary, solvents and reagents were dried prior to use. Tetrahydrofuran (THF) was dried by passage through activated alumina in Inert's PureSolv PS-MD-3 solvent purification system. All reagent grade solvents were purchased from VWR, Sigma-Aldrich, or Fisher and Organometallic reagents were purchased from Sigma-Aldrich. Analytical thin layer chromatography (TLC) was performed on Silicycle 250 μm silica-gel F-254 plates. Silica gel (230-400 mesh) was used for column chromatography. NMR (^{1}H, ^{13}C and ^{19}F) spectra were recorded on Bruker AV III HD NanoBay (400 MHz) NMR spectrometer. Chemical shifts (δ) are reported in parts per million (ppm) relative to the internal residual solvent resonance peak δ 7.26 ($CDCl_3$) and δ 0.00 (TMS) for all ^{1}H and δ 77.16 ($CDCl_3$) and δ 0.00 (TMS) for all ^{13}C. Other data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd= doublet of doublets), coupling constants (*J*) are reported in Hertz (Hz), and number of protons. High Resolution Mass (HRMS) spectra using DART modes were recorded on JEOL AccuTOF-CS. Agilent 7820A GC system and 5977B MSD was used to measure GC-MS. IR spectra were recorded on a Thermo Nicolet NEXUS 670 FTIR and are

reported in wavenumbers (cm^{-1}). Enantiomeric ratio (er) values were determined by HPLC with the Daicel Chiralcel OJ-H column (Hexane/*i*-PrOH 99.5:0.5, 0.7 mL/min, 214 nm). Melting points were obtained and are uncorrected.

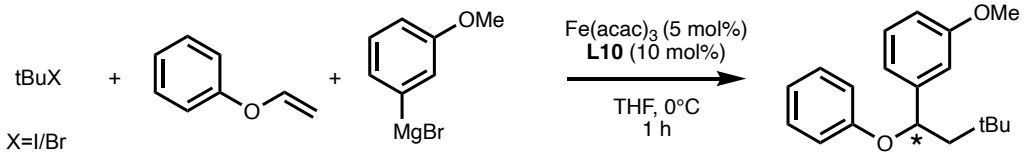
A7.1.2 General Procedure for Iron-Catalyzed Multicomponent Cross-Coupling Reaction



A flame-dried 5 mL microwave vial with a stir bar was transferred into an argon-filled glovebox and the vial was charged with $Fe(acac)_3$ (2.1 mg, 3 mol %), 1,2-bis(dicyclohexylphosphanyl)ethane L1 (10.1 mg, 12 mol %), alkyl halide (0.2 mmol, 1.0 equiv) and alkene (0.8 mmol, 4.0 equiv) (using oven-dried glass pipette to transfer alkyl halide and alkene to the vial). The vial was sealed with a Teflon cap and brought out of the glovebox without solvent. THF (0.2 mL) was then added into the reaction mixture. The resulting red solution was stirred at room temperature for 5 min. The reaction mixture was then cooled to 0 °C and a RMgBr solution (0.5–1.0 M solution in THF, 1.5 equiv) was added slowly for 1 h using a syringe pump. Over which time the heterogeneous solution turned from red to colorless or yellow, brown, grass green or orange color (depending on ArMgBr and substrate). The resulting reaction mixture was then stirred at 0 °C for an additional 10 min. After completion, reaction mixture was quenched with a 1.0 M aqueous solution of hydrochloric acid (0.5 mL) and water (0.5 mL) and then extracted with ethyl acetate (3 x 2 mL). The combined organic

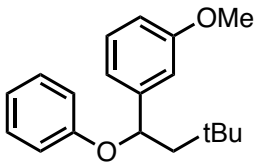
solution was filtered through a short pad of silica and evaporation of solvent gave a residue that was purified on silica gel column chromatography with hexane/CH_2Cl_2 to obtain product.

A7.1.2 General Procedure for Asymmetric Iron-Catalyzed Multicomponent Cross-Coupling Reaction



A flame-dried 5 mL microwave vial with a stir bar was transferred into an argon-filled glovebox and the vial was charged with $Fe(acac)_3$ (3.5 mg, 5 mol %), 1,2-bis(tert-butyl(methyl)phosphanyl)benzene L10 (5.6 mg, 10 mol %), alkyl halide (0.2 mmol, 1.0 equiv) and alkene (0.8 mmol, 4.0 equiv) (using oven-dried glass pipette to transfer alkyl halide and alkene to the vial). The vial was sealed with a Teflon cap and brought out of the glovebox without solvent. THF (0.2 mL) was then added into the reaction mixture. The resulting red solution was stirred at room temperature for 5 min. The reaction mixture was then cooled to 0 °C and a ArMgBr solution (1.0 M solution in THF, 1.5 equiv) was added slowly for 1 h using a syringe pump. The resulting reaction mixture was then stirred at 0 °C for an additional 10 min. After completion, reaction mixture was quenched with a 1.0 M aqueous solution of hydrochloric acid (0.5 mL) and water (0.5 mL) and then extracted with ethyl acetate (3 x 2 mL). The combined organic solution was filtered through a short pad of silica and evaporation of solvent gave a residue that was purified on silica gel column chromatography with hexane/CH_2Cl_2 to obtain product.

A7.2 Experimental Data



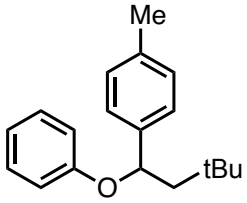
1-(3,3-dimethyl-1-phenoxybutyl)-3-methoxybenzene (4): Compound **4** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 3-methoxyphenylmagnesium bromide (0.3 mL, 1.0 M solution in THF, 0.3 mmol). The product **4** was obtained as a colorless liquid (40 mg, 71% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (9:1) to hexane/CH_2Cl_2 (22:3)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.28-7.18 (m, 3H), 6.95-6.84 (m, 5H), 6.78 (dd, *J* = 8.0, 2.4 Hz, 1H), 5.19 (dd, *J* = 9.6, 2.0 Hz, 1H), 3.80 (s, 3H), 2.06 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.61 (dd, *J* = 14.8, 2.0 Hz, 1H), 1.05 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.01, 158.16, 145.68, 129.79, 129.40 (2C), 120.61, 118.07, 115.88 (2C), 112.52, 111.39, 78.03, 53.31, 52.88, 30.93, 30.28 (3C);

IR (film) 2953, 2835, 1598, 1585, 1491, 1364, 1234, 1064, 750, 690 cm^{-1};

HRMS (DART) calcd for $C_{19}H_{24}O_2$ $[M+NH_4]^+$ m/z = 302.2120; found: 302.2125.



1-(3,3-dimethyl-1-phenoxybutyl)-4-methylbenzene (5): Compound **5** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and *p*-tolylmagnesium bromide (0.3 mL, 1.0 M solution in THF, 0.3 mmol). The product **5** was obtained as

a white solid (37 mg, 70% yield) after purification by column chromatography on silica gel with hexane to hexane/CH_2Cl_2 (99:1).

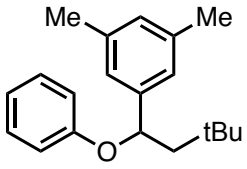
mp: 55-56 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.23-7.11 (m, 6H), 6.86-6.81 (m, 3H), 5.18 (dd, *J* = 9.6, 2.0 Hz, 1H), 2.31 (s, 3H), 2.03 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.57 (dd, *J* = 14.8, 2.4 Hz, 1H), 1.02 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.21, 140.85, 136.88, 129.41, 129.38 (2C), 125.67 (2C), 120.49, 115.90 (2C), 77.92, 53.02, 30.90 (2C), 30.30 (3C), 21.25;

IR (film) 2954, 2866, 1598, 1494, 1237, 1052, 815, 751, 690 cm^{-1};

HRMS (DART) calcd for $C_{19}H_{24}O$ $[M+NH_4]^+$ m/z = 286.2171; found: 286.2175.



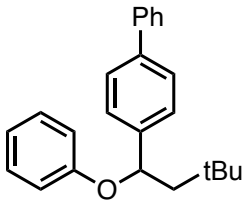
1-(3,3-dimethyl-1-phenoxybutyl)-3,5-dimethylbenzene (6): Compound **6** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and (3,5-dimethylphenyl) magnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **6** was obtained as a colorless liquid (32 mg, 57% yield) after purification by column chromatography on silica gel with hexane to hexane/CH_2Cl_2 (99:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.21-7.17 (m, 2H), 6.95 (s, 2H), 6.88-6.83 (m, 4H), 5.13 (dd, *J* = 9.6, 1.6 Hz, 1H), 2.30 (s, 6H), 2.03 (dd, *J* = 14.8, 10 Hz, 1H), 1.56 (dd, *J* = 14.8, 2.0 Hz, 1H), 1.03 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.36, 143.92, 138.23 (2C), 129.39 (2C), 128.99, 123.38 (2C), 120.45, 115.88 (2C), 78.25, 53.10, 30.95, 30.31 (3C), 21.52 (2C);

IR (film) 2952, 2866, 1597, 1586, 1493, 1237, 1057, 847, 751, 689 cm^{-1};

HRMS (DART) calcd for $C_{20}H_{26}O$ $[M+NH_4]^+$ m/z =300.2327; found: 300.2319.



4-(3,3-dimethyl-1-phenoxybutyl)-1,1'-biphenyl (7): Compound **7** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **7** was obtained as a white solid (37 mg, 56% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (49:1) to hexane/CH_2Cl_2(24:1).

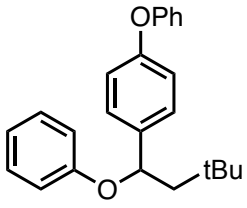
mp: 140-141 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.58-7.54 (m, 4H), 7.45-7.40 (m, 4H), 7.35-7.32 (m, 1H), 7.22-7.18 (m, 2H), 6.90-6.86 (m, 3H), 5.27 (dd, *J* = 9.6, 2.0 Hz, 1H), 2.10 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.64 (dd, *J* = 14.8, 2.0 Hz, 1H), 1.06 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.15, 142.89, 140.97, 140.23, 129.45 (2C), 128.86 (2C), 127.51 (2C), 127.34, 127.18 (2C), 126.16 (2C), 120.64, 115.92 (2C), 77.85, 52.95, 30.99, 30.32 (3C);

IR (film) 3028, 2953, 1597, 1492, 1364, 1236, 1172, 1053, 751, 691 cm^{-1};

HRMS (DART) calcd for $C_{24}H_{26}O$ $[M+NH_4]^+$ m/z = 348.2327; found: 348.2330.



1-(3,3-dimethyl-1-phenoxybutyl)-4-phenoxybenzene (8): Compound **8** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide

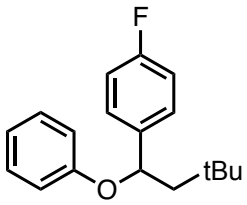
(36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and (4-phenoxyphenyl) magnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **8** was obtained as a colorless liquid (42 mg, 61% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (43:7) to hexane/CH_2Cl_2 (21:4).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.34-7.28 (m, 4H), 7.21-7.17 (m, 2H), 7.11-7.07 (m, 1H), 7.00-6.94 (m, 4H), 6.89-6.82 (m, 3H), 5.20 (dd, *J* = 9.6, 2.4 Hz, 1H), 2.05 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.59 (dd, *J* = 14.4, 2.4 Hz, 1H), 1.03 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.10, 157.25, 156.46, 138.58, 129.85 (2C), 129.43 (2C), 127.17 (2C), 123.40, 120.63, 119.08 (2C), 118.99 (2C), 115.93 (2C), 77.64, 52.93, 30.91, 30.31 (3C);

IR (film) 2953, 2866, 1587, 1504, 1487, 1230, 1165, 1052, 871, 750, 689 cm^{-1};

HRMS (DART) calcd for $C_{24}H_{26}O_2$ $[M-H]^-$ m/z = 345.1845; found: 345.1858.



1-(3,3-dimethyl-1-phenoxybutyl)-4-fluorobenzene (9): Compound **9** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-fluorophenylmagnesium bromide (0.3 mL, 1.0 M solution in THF, 0.3 mmol). The product **9** was obtained as a colorless liquid (25 mg, 46% yield) after purification by column chromatography on silica gel with hexane to hexane/CH_2Cl_2 (99:1).

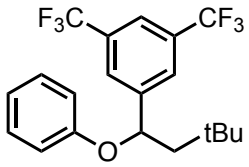
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.31-7.27 (m, 2H), 7.19-7.15 (m, 2H), 7.01-6.97 (m, 2H), 6.88-6.84 (m, 1H), 6.79 (dd, *J* = 8.8, 1.2 Hz, 2H), 5.19 (dd, *J* = 9.6, 2.4 Hz, 1H), 2.02 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.55 (dd, *J* = 14.8, 2.0 Hz, 1H), 1.02 (s, 9H);.

^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.24 (J_{C-F} = 243.6 Hz), 157.93, 139.55(J_{C-F} = 3.2 Hz), 129.45 (2C), 127.41 (J_{C-F} = 8.0 Hz, 2C), 120.77, 115.91 (2C), 115.72 (J_{C-F} = 21.3 Hz, 2C), 77.36, 52.92, 30.90, 30.28 (3C);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -115.530;

IR (film) 2954, 2868, 1598, 1509, 1494, 1365, 1223, 1155, 1053, 834, 752, 690 cm^{-1};

HRMS (DART) calcd for $C_{18}H_{21}FO$ $[M+NH_4]^+$ m/z = 290.1920; found: 290.1919.



1-(3,3-dimethyl-1-phenoxybutyl)-3,5-bis(trifluoromethyl)benzene (10): Compound **10** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 3,5-Bis(trifluoromethyl)phenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **10** was obtained as a white solid (22 mg, 28% yield) after purification by column chromatography on silica gel with hexane to hexane/CH_2Cl_2 (99:1).

mp: 54-55 °C;

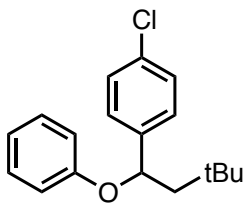
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (s, 2H), 7.76 (s, 1H), 7.23-7.19 (m, 2H), 6.94-6.90 (m, 1H), 6.80-6.77 (m, 2H), 5.32 (dd, *J* = 10, 2.0 Hz, 1H), 2.05 (dd, *J* = 14.8, 10 Hz, 1H), 1.54 (dd, *J* = 14.8, 2.0 Hz, 1H), 1.05 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.35, 146.73, 132.18 (q, $J_{C\text{-}F}$ = 33.1Hz, 2C), 129.74 (4C), 125.96 (2C), 121.51 (2C), 115.79 (2C), 77.21, 52.82, 31.14, 30.25 (3C);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -105.67, -105.82;

IR (film) 2958, 1590, 1494, 1348, 1276, 1234, 1168, 1130, 895, 752, 682 cm^{-1};

HRMS (DART) calcd for $C_{20}H_{20}F_6O$ $[M+NH_4]^+$ m/z = 408.1762; found: 408.1769.



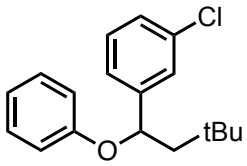
1-chloro-4-(3,3-dimethyl-1-phenoxybutyl)benzene (11): Compound **11** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and (4-chlorophenyl)magnesium bromide (0.3 mL, 1.0 M solution in diethyl ether, 0.3 mmol). The product **11** was obtained as a colorless liquid (38 mg, 66% yield) after purification by column chromatography on silica gel with hexane to hexane/CH_2Cl_2 (99:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.30-7.27 (m, 4H), 7.20-7.16 (m, 2H), 6.89-6.85 (m, 1H), 6.80-6.78 (m, 2H), 5.18 (dd, *J* = 9.6, 2.4 Hz, 1H), 2.02 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.55 (dd, *J* = 14.8, 2.4 Hz, 1H), 1.02 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ =157.85, 142.37, 132.97, 129.48 (2C), 128.94 (2C), 127.18 (2C), 120.84, 115.87 (2C), 77.43, 52.84, 30.94, 30.27 (3C);

IR (film) 2954, 2866, 1598, 1587, 1491, 1235, 1172, 1087, 1053, 883, 822, 751, 690 cm^{-1};

HRMS (DART) calcd for $C_{18}H_{21}ClO$ $[M+NH_4]^+$ m/z =306.1624; found: 306.1613.



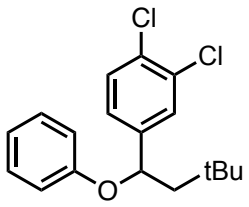
1-chloro-3-(3,3-dimethyl-1-phenoxybutyl)benzene (12): Compound **12** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and (3-chlorophenyl)magnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **12** was obtained as a colorless liquid (36 mg, 62% yield) after purification by column chromatography on silica gel with hexane to hexane/CH_2Cl_2 (99:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ =7.34 (s, 1H), 7.24-7.18 (m, 5H), 6.89 (t, *J* = 7.2 Hz, 1H), 6.82 (d, *J* = 8.4 Hz, 2H), 5.18 (dd, *J* = 9.6, 2.0 Hz, 1H), 2.03 (dd, *J* = 14.8, 10.0 Hz, 1H), 1.57 (dd, *J* = 14.4, 2.4 Hz, 1H), 1.04 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ =157.84, 146.08, 134.67, 130.10, 129.51 (2C), 127.54, 125.92, 123.90, 120.89, 115.83 (2C), 77.49, 52.82, 30.98, 30.26 (3C);

IR (film) 2954, 2867, 1596, 1586, 1492, 1475, 1234, 1077, 1053, 885, 785, 751, 689 cm^{-1};

HRMS (DART) calcd for $C_{18}H_{21}ClO$ $[M+NH_4]^+$ m/z =306.1624; found: 306.1627.



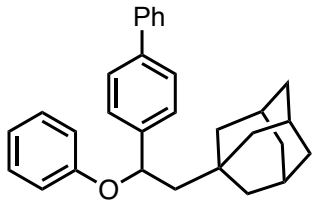
1,2-dichloro-4-(3,3-dimethyl-1-phenoxybutyl)benzene (13): Compound **13** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and (3,4-dichlorophenyl)magnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **13** was obtained as a colorless liquid (22 mg, 34% yield) after purification by column chromatography on silica gel with hexane to hexane/CH_2Cl_2 (99:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.42 (d, *J* = 2.0 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.22-7.16 (m, 3H), 6.91-6.87 (m, 1H), 6.79-6.77 (m, 2H), 5.14 (dd, *J* = 10.0, 2.0 Hz, 1H), 2.00 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.52 (dd, *J* = 14.8, 2.4 Hz, 1H), 1.02 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ =157.62, 144.28, 132.91, 131.25, 130.83, 129.58 (2C), 127.81, 125.16, 121.11, 115.80 (2C), 76.95, 52.74, 30.99, 30.24 (3C);

IR (film) 2954, 2868, 1598, 1587, 1493, 1472, 1234, 1152, 1055, 1029, 887, 751, 689;

HRMS (DART) calcd for $C_{18}H_{20}Cl_2O$ $[M+NH_4]^+$ m/z =340.1234; found: 340.1232.



1-(2-([1,1'-biphenyl]-4-yl)-2-phenoxyethyl)adamantine (14): Compound **14** was synthesized following the general procedure 1 (standard-scale), using iodoadamantane (52.4 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **14** was obtained as a white solid (40 mg, 49% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (23:2) to hexane/CH_2Cl_2 (9:1).

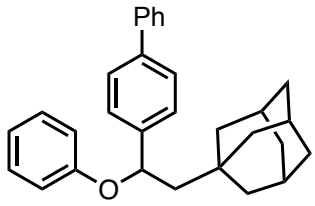
mp: 143-144 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.58-7.54 (m, 4H), 7.44-7.38 (m, 4H), 7.35-7.31 (m, 1H), 7.23-7.19 (m, 2H), 6.90-6.86 (m, 3H), 5.32 (dd, *J* = 9.6, 1.6 Hz, 1H), 2.02-1.96 (m, 4H), 1.74-1.64 (m, 12H), 1.49 (dd, *J* = 15.2, 2.0 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.06, 143.07, 140.98, 140.14, 129.44 (2C), 128.55 (2C), 127.48 (2C), 127.31, 127.17 (2C), 126.17 (2C), 120.59, 115.98 (2C), 76.27, 54.04, 43.13 (3C), 37.19 (3C), 32.95, 28.91 (3C);

IR (film) 3027, 2898, 2845, 1598, 1586, 1492, 1448, 1234, 1171, 1007, 751, 691 cm^{-1};

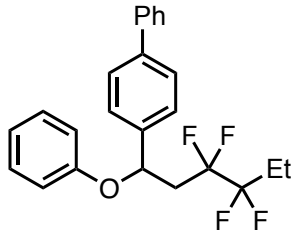
HRMS (DART) calcd for $C_{30}H_{32}O$ $[M-H]^-$ m/z =407.2374; found: 407.2382.



1-(2-([1,1'-biphenyl]-4-yl)-2-phenoxyethyl)adamantine (15): Compound **15** was synthesized following the general procedure 1 (standard-scale), using bromoadamantane (43 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **15** was obtained as a white solid (30 mg, 37% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (23:2) to hexane/CH_2Cl_2 (9:1).

mp: 143-144 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.57-7.52 (m, 4H), 7.43-7.37 (m, 4H), 7.34-7.30 (m, 1H), 7.22-7.17 (m, 2H), 6.88-6.84 (m, 3H), 5.30 (dd, *J* = 9.6, 2.0 Hz, 1H), 2.00-1.94 (m, 4H), 1.72-1.62 (m, 12H), 1.47 (dd, *J* = 14.8, 2.0 Hz, 1H); Spectral data matched compound **14**.



4-(3,3,4,4-tetrafluoro-1-phenoxyhexyl)-1,1'-biphenyl (16): Compound **16** was synthesized following the general procedure 1 (standard-scale), using 1-bromo-1,1,2,2-tetrafluorobutane (41.7 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **16** was obtained as a white solid (70 mg, 87% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (24:1) to hexane/CH_2Cl_2 (47:3).

mp: 88-89 °C;

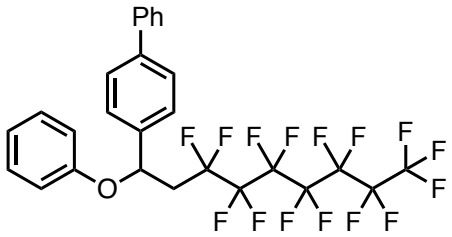
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.60-7.56 (m, 4H), 7.49-7.41 (m, 4H), 7.36-7.33 (m, 1H), 7.23-7.20 (m, 2H), 6.93-6.89 (m, 3H), 5.61 (dd, *J* = 8.8, 3.6 Hz, 1H), 2.94-2.79 (m, 1H), 2.60-2.46 (m, 1H), 2.14-1.99 (m, 2H), 1.11 (t, *J* = 7.6 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.75, 141.16, 140.71, 140.15, 129.51 (2C), 128.92 (2C), 127.74 (2C), 127.55, 127.21 (2C), 126.49 (2C), 122.22-115.28 (2C), 121.39, 116.30 (2C), 74.10, 39.18 (t, *J*= 21.5 Hz), 23.39 (t, *J* = 23.4 Hz), 4.99 (t, *J* = 5.2 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -112.84 to -113.58 (m, 1F), -113.96 to -114.70 (m, 1F), -117.33 to -117.36 (m, 2F);

IR (film) 3030, 2991, 2950, 1598, 1492, 1289, 1235, 1172, 1101, 1084, 1003, 851, 752, 689 cm^{-1};

HRMS (DART) calcd for $C_{24}H_{22}F_4O$ $[M+NH_4]^+$ m/z = 420.1951; found: 420.1954.



4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-pentadecafluoro-1-phenoxynonyl)-1,1'-biphenyl (17): Compound **17** was synthesized following the general procedure 1 (standard-scale), using 1-bromo-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoroheptane (89.7 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **17** was obtained as a white solid (82 mg, 64% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (9:1) to hexane/CH_2Cl_2 (22:3).

mp: 95-96 °C;

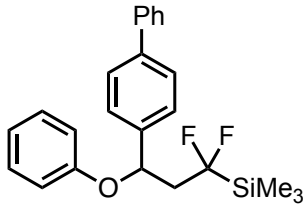
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.61-7.56 (m, 4H), 7.49-7.42 (m, 4H), 7.37-7.33 (m, 1H), 7.24-7.20 (m, 2H), 6.95-6.88 (m, 3H), 5.61 (dd, *J* = 8.8, 3.2 Hz, 1H), 3.02-2.87 (m, 1H), 2.62-2.49 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.45, 141.54, 140.56, 139.32, 129.58 (2C), 128.96 (2C), 127.94 (2C), 127.68, 127.23 (2C), 126.40 (2C), 121.68 , 119.98-108.42 (7C) 116.27 (2C), 73.57, 39.97 (t, *J* = 20.7 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -111.86 to -113.61 (m, 2F), -121.46 to -123.46 (m, 10F), -126.05 to -126.14 (m, 3F);

IR (film) 3016, 2926, 2862, 2604, 2359, 2337, 2186, 2032, 1215, 771, 667 cm^{-1};

HRMS (DART) calcd for $C_{27}H_{17}F_{15}O$ $[M+NH_4]^+$ m/z = 660.1383; found: 660.1364.



(3-([1,1'-biphenyl]-4-yl)-1,1-difluoro-3-phenoxypropyl)trimethylsilane (18): Compound **18** was synthesized following the general procedure 1 (standard-scale), using (bromodifluoromethyl)trimethylsilane (40.6 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **18** was obtained as a colorless liquid (52 mg, 65% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (23:2) to hexane/CH_2Cl_2 (9:1).

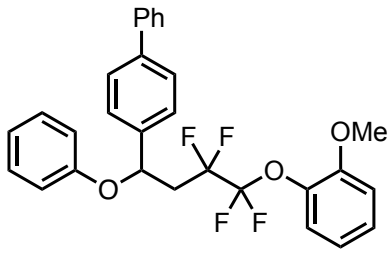
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.58-7.56 (m, 4H), 7.47-7.41 (m, 4H), 7.36-7.32 (m, 1H), 7.23-7.19 (m, 2H), 6.91-6.88 (m, 3H), 5.59 (dd, *J* = 8.8, 2.8 Hz, 1H), 2.78-2.61 (m, 1H), 2.39-2.24 (m, 1H), 0.22 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.42, 140.80, 140.77 (2C), 129.50 (2C), 128.88 (2C), 127.63 (2C), 127.47, 127.18 (2C), 126.46 (2C), 121.13 (2C), 116.19 (2C), 74.01 (dd, *J* = 10.4, 4.2 Hz), 45.84 (t, *J* = 20.4 Hz), - 4.23 (3C);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -107.82 to -108.69 (m, 1F), -113.16 to -114.02 (m, 1F);

IR (film) 3030, 2959, 1598, 1489, 1232, 1172, 1082, 1063, 1007, 956, 844, 752, 690 cm^{-1};

HRMS (DART) calcd for $C_{24}H_{26}F_2OSi$ $[M+NH_4]^+$ m/z = 414.2064; found: 414.2059.



4-(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-phenoxybutyl)-1,1'-biphenyl (19): Compound **19** was synthesized following the general procedure 1 (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.6 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **19** was obtained as a colorless liquid (91 mg, 92% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (43:7) to hexane/CH_2Cl_2 (21:4).

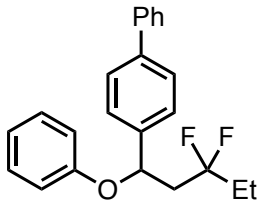
^{1}H NMR (400 MHz, $CDCl_3$) δ =7.61-7.51 (m, 6H), 7.45-7.41 (m, 2H), 7.36-7.33 (m, 1H), 7.25-7.19 (m, 4H), 6.98-6.89 (m, 5H), 5.73 (dd, *J* = 8.8, 3.6 Hz, 1H), 3.81 (s, 3H), 3.12-2.97 (m, 1H), 2.81-2.67 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.77, 152.53, 141.15, 140.71, 140.10, 137.86, 129.49 (2C), 128.93 (2C), 127.73 (2C), 127.64, 127.57, 127.21 (2C), 126.55 (2C), 124.02, 121.40, 120.74, 120.24-113.60 (2C), 116.39 (2C), 112.91, 74.06, 56.09, 40.33 (t, *J* = 20.9 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -114.29 to -115.01 (m, 2F), -116.04 to -116.74 (m, 2F);

IR (film) 3030, 2925, 2841, 1598, 1501, 1493, 1456, 1261, 1237, 1189, 1170, 1105, 1025, 1007, 750, 692 cm^{-1};

HRMS (DART) calcd for $C_{29}H_{24}F_4O_3$ $[M+NH_4]^+$ m/z = 514.2005; found: 514.1995.



4-(3,3-difluoro-1-phenoxypentyl)-1,1'-biphenyl (20): Compound **20** was synthesized following the general procedure 1 (standard-scale), using 1-bromo-1,1-difluoropropane (31.7 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **20** was obtained as a colorless liquid (37 mg, 52% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (22:3) to hexane/CH_2Cl_2 (43:7).

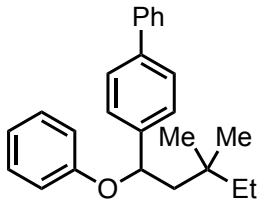
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.58-7.56 (m, 4H), 7.46-7.41 (m, 4H), 7.36-7.32 (m, 1H), 7.23- 7.19 (m, 2H), 6.93-6.87 (m, 3H), 5.46 (dd, *J* = 9.2, 2.8 Hz, 1H), 2.76-2.61 (m, 1H), 2.39-2.27 (m, 1H), 2.06-1.92 (m, 2H), 1.09 (t, *J* = 7.6 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.64, 140.95, 140.72, 140.41, 129.58 (2C), 128.91 (2C), 127.70 (2C), 127.52, 127.20 (2C), 126.36 (2C), 124.54, 121.30, 116.04 (2C), 75.12 (dd, *J* = 8.5, 3.3 Hz), 45.00 (t, *J* = 26 Hz), 30.19 (t, *J* = 25.4 Hz), 6.79 (dd, *J* = 6.8, 4.8 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -95.07 (d, *J* = 64.8 Hz, 1F), -97.98 (d, *J* = 64.8 Hz, 1F);

IR (film) 3030, 2941, 2853, 1598, 1492, 1377, 1235, 1007, 965, 887, 754, 691 cm^{-1};

HRMS (DART) calcd for $C_{23}H_{22}F_2O$ $[M+NH_4]^+$ m/z = 370.1982; found: 370.1996.



4-(3,3-dimethyl-1-phenoxypentyl)-1,1'-biphenyl (21): Compound **21** was synthesized following the general procedure 1 (standard-scale), using 2-bromo-2-methylbutane (30.2 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **21** was obtained as a white solid (35 mg, 51% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (24:1) to hexane/CH_2Cl_2 (47:3).

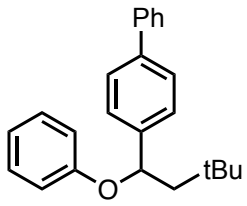
mp: 81-82 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.58-7.54 (m, 4H), 7.44-7.39 (m, 4H), 7.35-7.31 (m, 1H), 7.22-7.18 (m, 2H), 6.87-6.84 (m, 3H), 5.25 (dd, *J* = 9.6, 2.0 Hz, 1H), 2.09 (dd, *J* = 15.2, 9.6 Hz, 1H), 1.60 (dd, *J* = 15.2, 2.0 Hz, 1H), 1.46-1.31 (m, 2H), 1.01 (d, *J* = 3.2 Hz, 6H), 0.90 (t, *J* = 7.6 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.15, 143.04, 140.97, 140.21, 129.44 (2C), 128.86 (2C), 127.51 (2C), 127.34, 127.18 (2C), 126.13 (2C), 120.62, 115.88 (2C), 77.55, 50.47, 35.08, 33.49, 27.53, 27.48, 8.66;

IR (film) 3028, 2969, 1597, 1492, 1300, 1236, 1171, 1077, 1006, 765, 752, 690 cm^{-1};

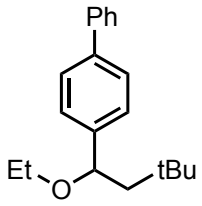
HRMS (DART) calcd for $C_{25}H_{28}O$ $[M+NH_4]^+$ m/z =362.2483; found: 362.2484.



4-(3,3-dimethyl-1-phenoxybutyl)-1,1'-biphenyl (22): Compound **22** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl chloride (18.5 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **22** was obtained as a white solid (26 mg, 39% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (49:1) to hexane/CH_2Cl_2 (24:1).

mp: 140-141 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.60-7.56 (m, 4H), 7.46-7.42 (m, 4H), 7.37-7.33 (m, 1H), 7.24-7.20 (m, 2H), 6.91-6.87 (m, 3H), 5.28 (dd, *J* = 10.0, 2.0 Hz, 1H), 2.11 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.66 (dd, *J* = 14.8, 2.4 Hz, 1H), 1.08 (s, 9H); Spectral data matched compound **7**.



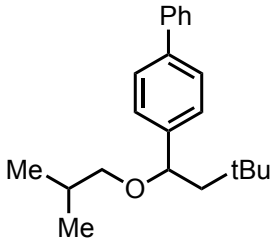
4-(1-ethoxy-3,3-dimethylbutyl)-1,1'-biphenyl (23): Compound **23** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), ethyl vinyl ether (57.6 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **23** was obtained as a colorless liquid (20 mg, 36% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (23:2) to hexane/CH_2Cl_2 (9:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.60-7.55 (m, 4H), 7.45-7.41 (m, 2H), 7.36-7.31 (m, 3H), 4.36 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.40-3.29 (m, 2H), 1.83 (dd, *J* = 14.4, 9.2 Hz, 1H), 1.46 (dd, *J* = 14.4, 3.2 Hz, 1H), 1.18 (t, *J* = 7.2 Hz, 3H), 0.99 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.87, 141.15, 140.15, 128.86 (2C), 127.27, 127.23 (2C), 127.20 (2C), 126.93 (2C), 79.92, 64.13, 52.34, 30.82, 30.35 (3C), 15.62;

IR (film) 2917, 2849, 1486, 1364, 1215, 1091, 838, 751, 697, 668 cm^{-1};

HRMS (DART) calcd for $C_{20}H_{26}O$ $[M+ NH_4]^+$ m/z = 300.2327; found: 300.2331.



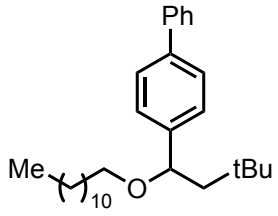
4-(1-isobutoxy-3,3-dimethylbutyl)-1,1'-biphenyl (24): Compound **24** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), isobutyl vinyl ether (80.1 mg, 0.4 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **24** was obtained as a colorless liquid (20 mg, 33% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (24:1) to hexane/CH_2Cl_2 (47:3).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.61-7.54 (m, 4H), 7.45-7.41 (m, 2H), 7.35-7.31 (m, 3H), 4.32 (dd, *J* = 9.2, 2.8 Hz, 1H), 3.09 (dd, *J* = 8.8, 6.0 Hz, 1H), 2.98 (dd, *J* = 8.8, 6.8 Hz, 1H), 1.87-1.79 (m, 2H), 1.44 (dd, *J* = 14.8, 2.4 Hz, 1H), 1.00 (s, 9H), 0.90 (dd, *J* = 14.0, 6.8 Hz, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 144.09, 141.17, 140.05, 128.85 (2C), 127.25, 127.19 (4C), 126.94 (2C), 80.20, 75.86, 52.61, 30.79, 30.42 (3C), 28.94, 19.90, 19.80;

IR (film) 2954, 2917, 2849, 1486, 1472, 1364, 1215, 1099, 838, 754, 697 cm^{-1};

HRMS (DART) calcd for $C_{22}H_{30}O$ $[M+ NH_4]^+$ m/z = 328.2640; found: 328.2632.



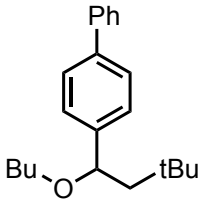
4-(1-(dodecyloxy)-3,3-dimethylbutyl)-1,1'-biphenyl (25): Compound **25** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), 1-(vinyloxy)dodecane (169.6 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **25** was obtained as a colorless liquid (25 mg, 29% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (23:2) to hexane/CH_2Cl_2 (9:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.61-7.55 (m, 4H), 7.45-7.41 (m, 2H), 7.36-7.32 (m, 3H), 4.34 (dd, *J* = 9.2, 2.8 Hz, 1H), 3.33-3.19 (m, 2H), 1.83 (dd, *J* = 14.4, 9.2 Hz, 1H), 1.58-1.52 (m, 2H), 1.46 (dd, *J* = 14.8, 2.8 Hz, 1H), 1.30-1.25 (m, 18H), 1.00 (s, 9H), 0.88 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.99, 141.16, 140.09, 128.85 (2C), 127.25, 127.20 (2C), 127.19 (2C), 126.94 (2C), 80.11, 68.96, 52.45, 32.08, 30.80, 30.39 (3C), 30.22, 29.82, 29.79, 29.77, 29.76, 29.62, 29.51, 26.48, 22.85, 14.27;

IR (film) 3028, 2923, 2853, 1486, 1465, 1363, 1101, 1008, 838, 753, 696 cm^{-1};

HRMS (DART) calcd for $C_{30}H_{46}O$ $[M+NH_4]^+$ m/z = 440.3892; found: 440.3886.



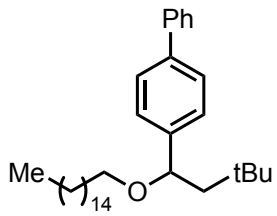
4-(1-butoxy-3,3-dimethylbutyl)-1,1'-biphenyl (26): Compound **26** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), 1-(vinyloxy)butane (80.1 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **26** was obtained as a colorless liquid (26 mg, 42% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (22:3) to hexane/CH_2Cl_2 (43:7).

^{1}H NMR (400 MHz, $CDCl_3$) δ =7.61-7.55 (m, 4H), 7.45-7.41 (m, 2H), 7.36-7.31 (m, 3H), 4.34 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.33-3.20 (m, 2H), 1.82 (dd, *J* = 14.8, 8.8 Hz, 1H), 1.57-1.50 (m, 2H), 1.45 (dd, *J* = 14.4, 2.8 Hz, 1H), 1.40-1.34 (m, 2H), 1.00 (s, 9H), 0.89 (t, *J* = 7.6 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.99, 141.16, 140.09, 128.85 (2C), 127.26, 127.21 (2C), 127.19 (2C), 126.93 (2C), 80.11, 68.67, 52.46, 32.35, 30.80, 30.38 (3C), 19.70, 14.09;

IR (film) 3028, 2954, 2929, 2865, 1600, 1486, 1464, 1363, 1098, 1008, 837, 769, 753, 696 cm^{-1};

HRMS (DART) calcd for $C_{22}H_{30}O$ $[M+NH_4]^+$ m/z = 328.2640; found: 328.2638.



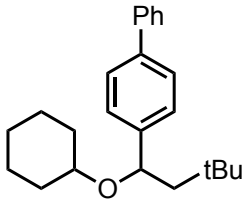
4-(1-(hexadecyloxy)-3,3-dimethylbutyl)-1,1'-biphenyl (27): Compound **27** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), 1-(vinyloxy)hexadecane (214.7 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **27** was obtained as a colorless liquid (28 mg, 29% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (9:1) to hexane/CH_2Cl_2 (22:3).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.61-7.55 (m, 4H), 7.45-7.41 (m, 2H), 7.36-7.31 (m, 3H), 4.33 (dd, *J* = 9.2, 2.8 Hz, 1H), 3.32-3.19 (m, 2H), 1.82 (dd, *J* = 14.4, 8.8 Hz, 1H), 1.59 -1.51 (m, 2H), 1.45 (dd, *J* = 14.4, 2.8 Hz, 1H), 1.28-1.25 (m, 26H), 1.00 (s, 9H), 0.88 (t, *J* = 6.8 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.99, 141.16, 140.09, 128.85 (2C), 127.25, 127.20 (4C), 126.94 (2C), 80.11, 68.97, 52.44, 32.08, 30.80, 30.38 (3C), 30.21, 29.85 (4C), 29.84 (2C), 29.77, 29.76, 29.62, 29.52, 26.47, 22.85, 14.27;

IR (film) 3028, 2922, 2852, 1600, 1486, 1465, 1363, 1100, 1008, 838, 753, 696 cm^{-1};

HRMS (DART) calcd for $C_{34}H_{54}O$ $[M+NH_4]^+$ m/z = 496.4518; found: 496.4529.



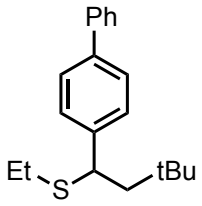
4-(1-(cyclohexyloxy)-3,3-dimethylbutyl)-1,1'-biphenyl (28): Compound **28** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), (vinyloxy)cyclohexane (100.9 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **28** was obtained as a colorless liquid (28 mg, 41% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (21:4) to hexane/CH_2Cl_2 (41:9).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.61-7.54 (m, 4H), 7.45-7.41 (m, 2H), 7.37-7.31 (m, 3H), 4.60 (dd, *J* = 9.2, 2.8 Hz, 1H), 3.17-3.10 (m, 1H), 2.05-2.02 (m, 1H), 1.83-1.62 (m, 4H), 1.42 (dd, *J* = 14.4, 2.8 Hz, 1H), 1.37-1.27 (m, 2H), 1.22-1.07 (m, 4H), 1.00 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 144.94, 141.15, 139.91, 128.85 (2C), 127.23, 127.17 (2C), 127.12 (2C), 126.96 (2C), 76.48, 75.11, 52.89, 34.05, 31.80, 30.89, 30.43 (3C), 26.01, 24.61, 24.47;

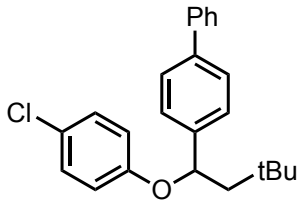
IR (film) 3027, 2929, 2855, 1600, 1486, 1449, 1362, 1258, 1087, 1064, 838, 754, 696 cm^{-1};

HRMS (DART) calcd for $C_{24}H_{32}O$ $[M+NH_4]^+$ m/z = 354.2796; found: 354.2796.

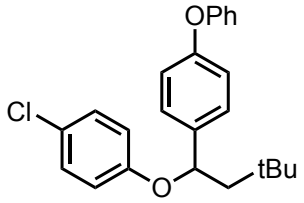


(1-([1,1'-biphenyl]-4-yl)-3,3-dimethylbutyl)(ethyl)sulfane (29): Compound **29** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), ethyl vinyl sulfide (70.5 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **29** was obtained as a colorless liquid (18 mg, 31% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (49:1) to hexane/CH_2Cl_2 (24:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.61-7.52 (m, 4H), 7.45-7.41 (m, 2H), 7.38-7.30 (m, 3H), 3.94 (dd, *J* = 8.4, 4.4 Hz, 1H), 2.30-2.17 (m, 2H), 1.98 (dd, *J* = 14.4, 8.4 Hz, 1H), 1.81 (dd, *J* = 14.0, 4.4 Hz, 1H), 1.16 (t, *J* = 7.2 Hz, 3H), 0.86 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$) δ = 143.73, 140.92, 139.63, 128.87 (2C), 128.54 (2C), 127.30, 127.12 (2C), 127.08 (2C), 50.09, 45.55, 31.83, 30.18 (3C), 25.42, 14.51;
IR (film) 3027, 2955, 2926, 2865, 1601, 1486, 1364, 1265, 1007, 843, 762, 696 cm^{-1};
HRMS (DART) calcd for $C_{20}H_{26}S$ $[M+NH_4]^+$ m/z = 316.2099; found: 316.2092.



4-(1-(4-chlorophenoxy)-3,3-dimethylbutyl)-1,1'-biphenyl (30): Compound **30** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), 1-chloro-4-(vinyloxy)benzene (123.2 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **30** was obtained as a colorless liquid (52 mg, 71% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (24:1) to hexane/CH_2Cl_2 (47:3).
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.58-7.55 (m, 4H), 7.45-7.32 (m, 5H), 7.16 (d, *J* = 9.2 Hz, 2H), 6.80 (d, *J* = 8.8Hz, 2H), 5.20 (dd, *J* = 9.6, 2.0 Hz, 1H), 2.08 (dd, *J* = 15.2, 9.6 Hz, 1H), 1.64 (dd, *J* = 14.8, 2.0 Hz, 1H), 1.05 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$) δ = 156.71, 142.28, 140.85, 140.47, 129.37 (2C), 128.89 (2C), 127.59 (2C), 127.42, 127.18 (2C), 126.12 (2C), 125.55, 117.18 (2C), 78.40, 52.82, 30.96, 30.29 (3C);
IR (film) 3028, 2953, 2866, 1596, 1487, 1364, 1235, 1168, 1052, 1006, 990, 821, 752, 696, 665 cm^{-1};
HRMS (DART) calcd for $C_{24}H_{25}ClO$ $[M+NH_4]^+$ m/z = 382.1937; found: 382.1935.



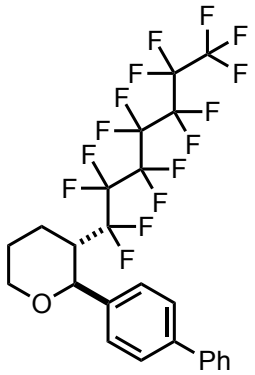
1-chloro-4-(3,3-dimethyl-1-(4-phenoxyphenyl)butoxy)benzene (31): Compound **31** was synthesized following the general procedure 1 (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), 1-chloro-4-(vinyloxy)benzene (123.2 mg, 0.8 mmol) and 4-Phenoxyphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **31** was obtained as a colorless liquid (50 mg, 66% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (24:1) to hexane/CH_2Cl_2 (47:3).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35-7.30 (m, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.15-7.08 (m, 3H), 7.01-6.94 (m, 4H), 6.76 (d, *J* = 8.8 Hz, 2H), 5.14 (dd, *J* = 9.6, 2.0 Hz, 1H), 2.03 (dd, *J* = 14.8, 9.2 Hz, 1H), 1.59 (dd, *J* = 14.8, 2.0 Hz, 1H), 1.02 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.11, 156.66, 137.92, 129.89 (2C), 129.34 (2C), 127.13 (2C), 125.54, 123.52 (2C), 119.17 (2C), 118.98 (2C), 117.21 (2C), 78.19, 52.80, 30.87, 30.27 (3C);

IR (film) 3038, 2953, 2866, 1589, 1486, 1231, 1165, 1051, 989, 821, 752, 691, 665 cm^{-1};

HRMS (DART) calcd for $C_{24}H_{25}ClO_2$ $[M-H]^-$ m/z = 379.1464; found = 379.1480.



***trans*-2-([1,1'-biphenyl]-4-yl)-3-(perfluoroheptyl)tetrahydro-2H-pyran (32):** Compound **32** was synthesized following the general procedure 1 (standard-scale), using 1-bromo-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoroheptane (89.7 mg, 0.2 mmol), 3,4-dihydro-2H-pyran (67.2 mg, 0.8 mmol) and 4-biphenylmagnesium bromide (0.6 mL, 0.5 M solution in THF, 0.3 mmol). The product **32** was obtained as a brown solid (38 mg, 31% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (24:1) to hexane/CH_2Cl_2 (47:3).

mp: 84-85 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.61-7.58 (m, 4H), 7.45-7.41 (m, 4H), 7.36-7.32 (m, 1H), 4.55 (d, *J* = 9.6 Hz, 1H), 4.13-4.09 (m, 1H), 3.63-3.57 (m, 1H), 2.78-2.71 (m, 1H), 2.29-2.26 (m, 1H), 1.87-1.79 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 141.27, 140.99, 139.68 (d, *J* = 1.5 Hz), 128.85 (3C), 127.80 (d, *J* = 1.8 Hz), 127.43, 127.28 (4C), 121.58-107.67 (7C), 79.52, 68.51, 45.03 (t, *J* = 18.6 Hz), 24.83, 23.71;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -104.64 to -105.53 (m, 1F), -116.41 to -123.85 (m, 14F);

IR (film) 3062, 2959, 2860, 1990, 1971, 1684, 1558, 1456, 1219, 772, 684, 659 cm^{-1};

HRMS (DART) calcd for $C_{24}H_{17}F_{15}O$ $[M+NH_4]^+$ m/z = 624.1383; found: 624.1398.

The stereochemistry of compound **32** was studied by 2D NOESY Spectrum (spectral data, compound 32). The absence of ^{1}H-^{1}H interaction between CH proton “a” and CH proton “b” indicates that both vicinal protons are in the *trans* diastereomer.

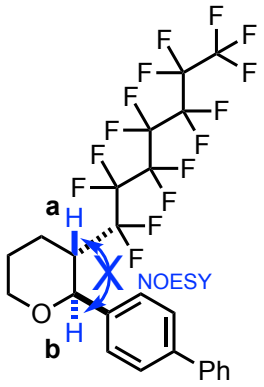
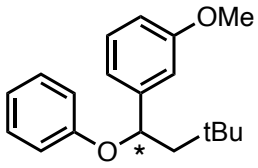
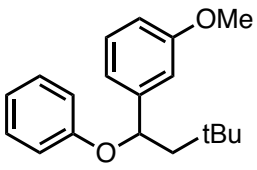


Figure A7.1 Confirmed the structure of 32 as *trans* based on NOESY NMR.



1-(3,3-dimethyl-1-phenoxybutyl)-3-methoxybenzene (4a): Compound **4a** was synthesized following the general procedure 2, using *tert*-butyl bromide (27.4 mg, 0.2 mmol), phenyl vinyl ether (96.1 mg, 0.8 mmol) and 3-methoxyphenylmagnesium bromide (0.3 mL, 1.0 M solution in THF, 0.3 mmol). The product **4a** was obtained as a colorless liquid (33 mg, 58% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (9:1) to hexane/CH_2Cl_2 (22:3)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.28-7.18 (m, 3H), 6.95-6.84 (m, 5H), 6.78 (dd, *J* = 8.0, 2.4 Hz, 1H), 5.19 (dd, *J* = 9.6, 2.0 Hz, 1H), 3.80 (s, 3H), 2.06 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.61 (dd, *J* = 14.8, 2.0 Hz, 1H), 1.05 (s, 9H); Spectral data matched compound **4**.



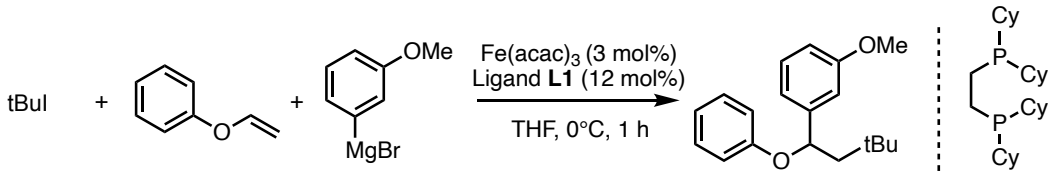
1-(3,3-dimethyl-1-phenoxybutyl)-3-methoxybenzene (4)-gram-scale: Compound **4** was synthesized following the general procedure 1, using *tert*-butyl iodide (1.0 g, 5.4 mmol), phenyl vinyl ether (2.6 g, 21.7 mmol) and 3-methoxyphenylmagnesium

bromide (8.1 mL, 1.0 M solution in THF, 8.1 mmol). The product **4** was obtained as a colorless liquid (1.02 g, 66% yield) after purification by column chromatography on silica gel with hexane/CH_2Cl_2 (9:1) to hexane/CH_2Cl_2 (22:3)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.27-7.17 (m, 3H), 6.95-6.83 (m, 5H), 6.77 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.18 (dd, *J* = 9.6, 2.0 Hz, 1H), 3.79 (s, 3H), 2.06 (dd, *J* = 14.8, 9.6 Hz, 1H), 1.60 (dd, *J* = 14.4, 2.4 Hz, 1H), 1.04 (s, 9H); Spectral data matched compound **4**.

A7.3 Supplementary Figures

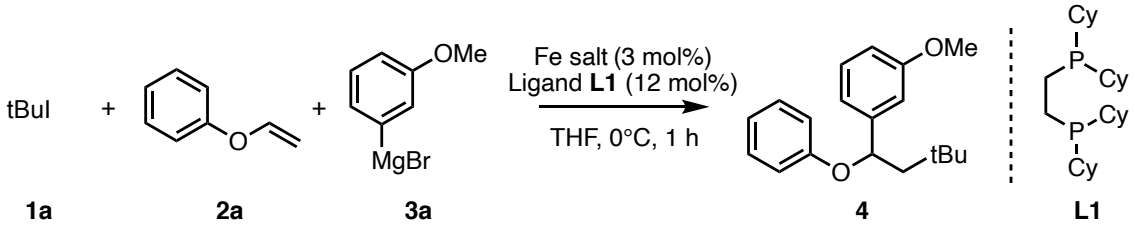
Figure A7.2 Screening of alkene loading



try	a (eq)	(eq)	(eq)	ield (%)	Recovered 2a (eq)
	1	14	1.5	89	12.4
	1	8	1.5	81	5.1
	1	4	1.5	75	2.4
	1	3	1.5	44	1.94
	1	2	1.5	44	0.68
	2	1	1.5	33	0.48

Reactions were performed with a 0.10 mmol scale, THF (0.1 mL) and Grignard addition for 1 h at 0 ºC. Reactions were then stirred additional 10 min after Grignard addition. Yield and recovered **2a** were determined by crude ^{1}H NMR with CH_2Br_2 as internal standard.

Figure A7.3 Screening of iron salts

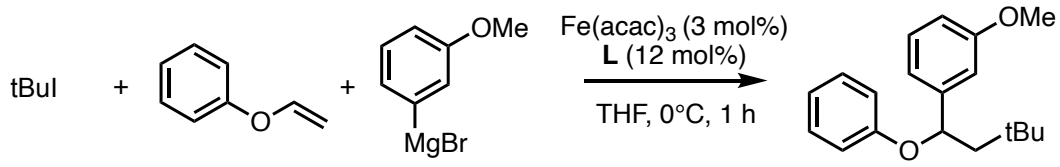


1a **2a** **3a** **4** **L1**

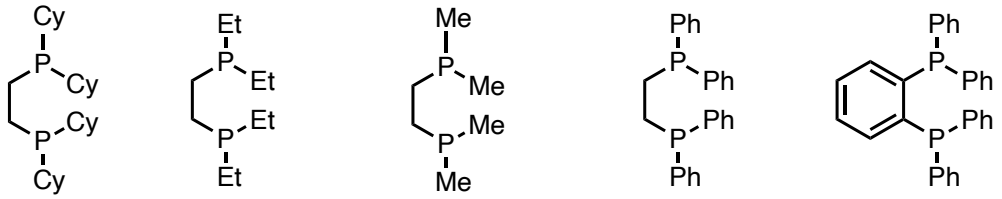
try	(eq)	(eq)	(eq)	Fe salt	eld (%)	ecovered 2a (eq)
	1	4	1.5	e(acac)$_3$	75	2.40
	1	4	1.5	$FeCl_2$	69	2.36
	1	4	1.5	$FeBr_2$	63	2.20
	1	4	1.5	$FeCl_3$	60	2.80
	1	4	1.5	e(OTf)$_2$	63	0.28

Reactions were performed with a 0.10 mmol scale, THF (0.1 mL) and Grignard addition for 1 h at 0 ºC. Reactions were then stirred additional 10 min after Grignard addition. Yield and recovered **2a** were determined by crude ^{1}H NMR with CH_2Br_2 as internal standard.

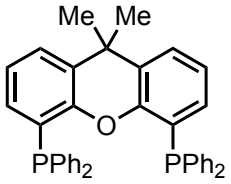
Figure A7.4 Screening of ligands



1a **2a** **3a** **4**



L1 **L2** **L3** **L4** **L5**



$P(Tol)_3$ PPh_3 $P(Cy)_3$

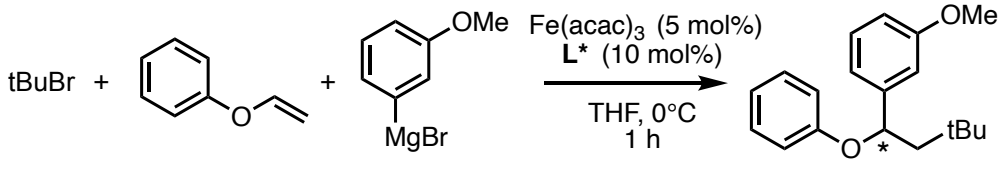
L6 **L7** **L8** **L9**

try	Ligand (L)	Yield (%)	Recovered 2a (eq)
	L1	75	2.4
	L2	0	--
	L3	0	--
	L4	45	3.1
	L5	0	--
	L6	0	--
	L7	0	--

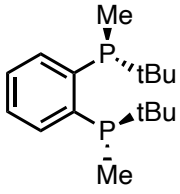
8	**L8**	0	--
9	**L9**	0	--
10	No **L**	0	--
11	No Fe, No **L**	0	--
12	neat	67	2.7

Reactions were performed with a 0.10 mmol scale of *tert*-butyl iodide, 4 eq of alkene, 1.5 eq of Grignard reagent, THF (0.1 mL) and Grignard addition for 1 h at 0 ºC. Reactions were then stirred additional 10 min after Grignard addition. Yield and recovered **2a** were determined by crude ^{1}H NMR with CH_2Br_2 as internal standard.

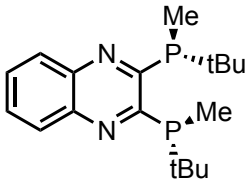
Figure A7.5 Screening of chiral ligands



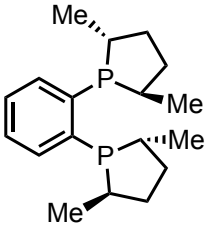
1b **2a** **3a** **4a**



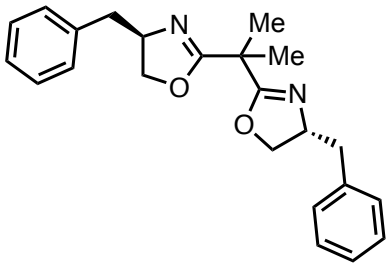
L10



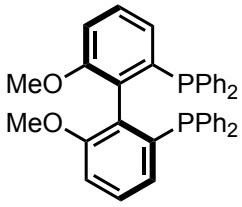
L11



L12



L13



L14

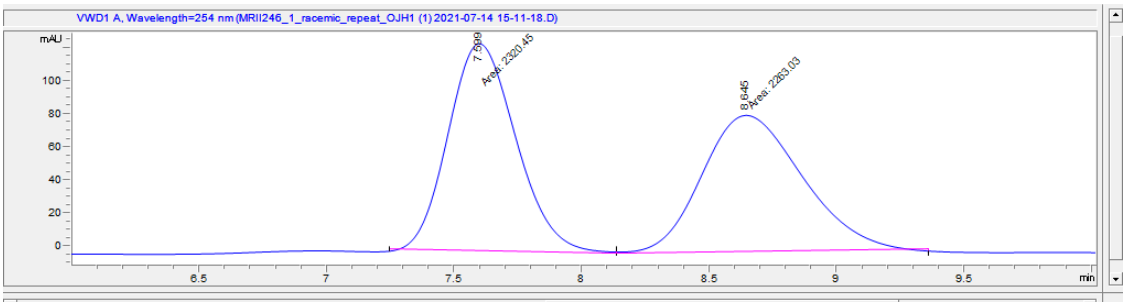
try	igand (L)	ield (%)	Enantiomeric Ratio (er)
	L10	58	75:25
	L11	22	28:72
	L12	18	73:27
	L13	0	--
	L14	0	--

Reactions were performed with a 0.20 mmol scale of *tert*-butyl bromide, 4 equiv of alkene, 1.5 equiv of Grignard reagent, THF (0.2 mL) and Grignard addition for 1 h at

0 ºC. Reactions were then stirred additional 10 min after Grignard addition. Yield determined by crude ^{1}H NMR with CH_2Br_2 as internal standard for all entries except entry 1 (isolated yield as an average of 4 trials). Enantiomeric ratio determined by chiral HPLC. Enantiomeric ratio of entry 2 determined as an average of 4 trials. Enantiomeric ratio of entries 3 and 4 determined as an average of 2 trials. Enantiomeric ratio (er) values were determined by HPLC with the Daicel Chiralcel OJ-H column (Hexane/*i*-PrOH 99.5:0.5, 0.7 mL/min, 214 nm).

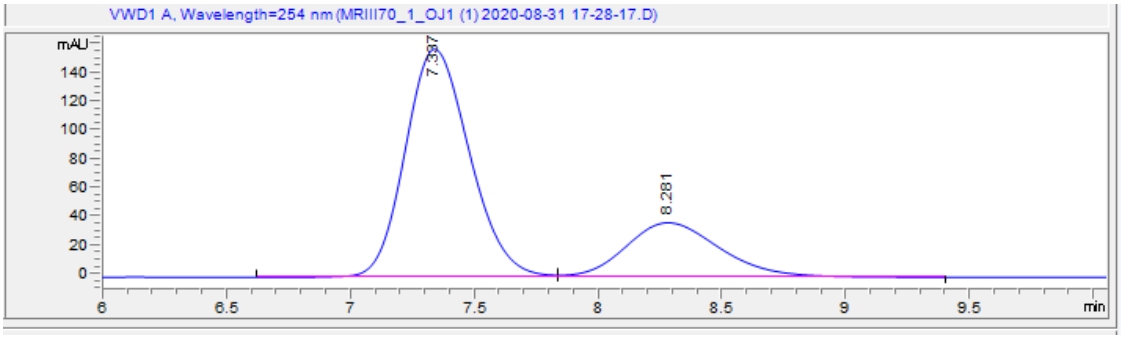
A7.4 HPLC Traces

Figure A7.6 HPLC Trace 1 (racemic)



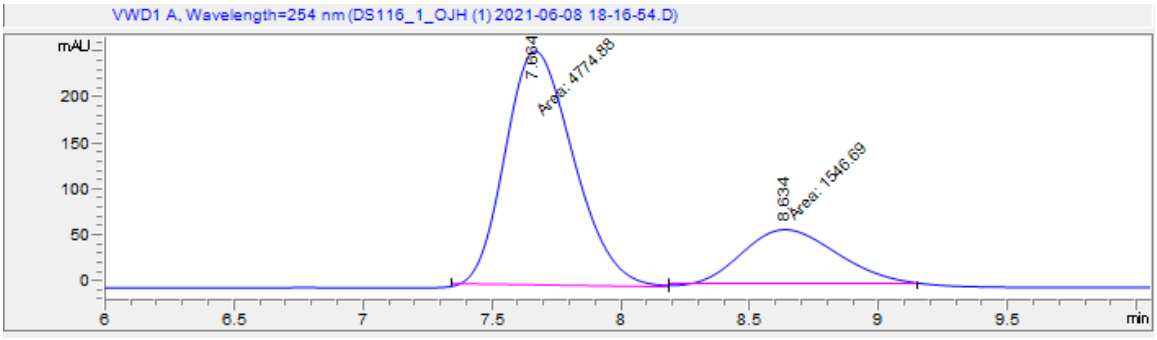
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.599	MM	2320.4	125.5	0.3083	50.626	0.825
2	8.645	MM	2263	82.6	0.4567	49.374	0.781

Figure A7.7 HPLC Trace 2 (entry 1, **L10**, run 1)



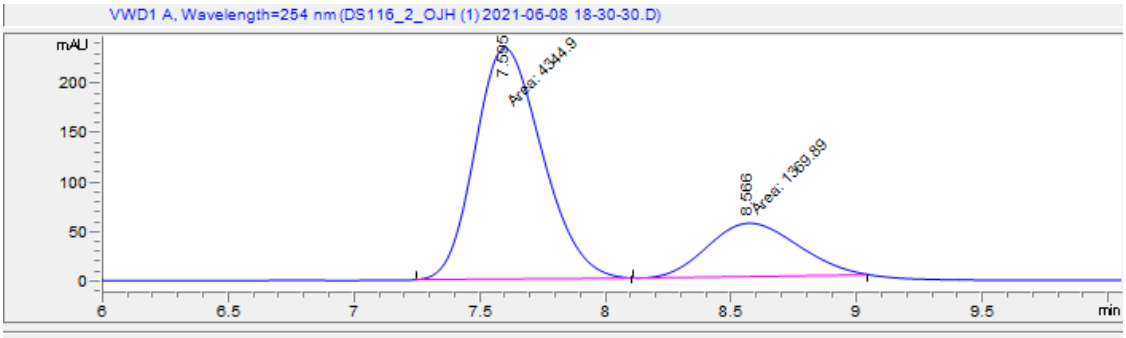
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.337	MM	2875.6	159.3	0.3008	74.118	0.821
2	8.281	MM	1004.2	38	0.4409	25.882	0.803

Figure A7.8 HPLC Trace 3 (entry 1, **L10**, run 2)



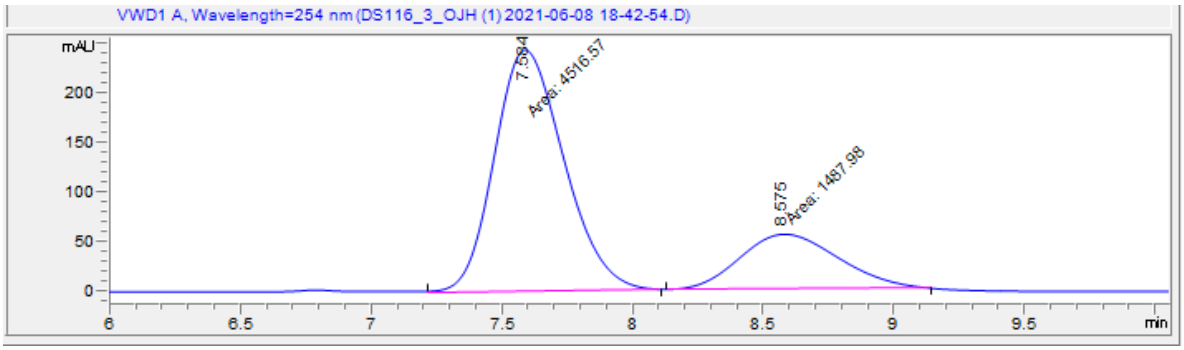
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.664	MM	4774.9	257.6	0.3089	75.533	0.757
2	8.634	MM	1546.7	60.2	0.4284	24.467	0.801

Figure A7.9 HPLC Trace 4 (entry 1, **L10**, run 3)



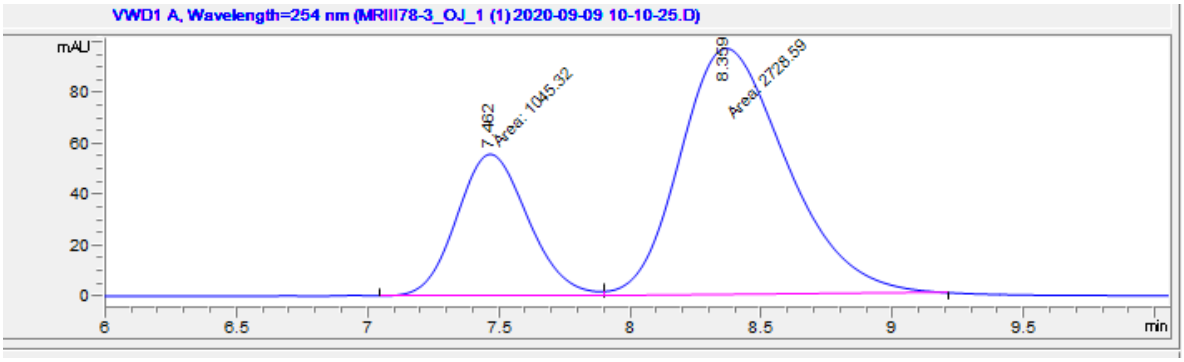
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.595	MM	4344.9	233.9	0.3097	76.029	0.777
2	8.566	MM	1369.9	54.3	0.4201	23.971	0.859

Figure A7.10 HPLC Trace 5 (entry 1, **L10**, run 4)



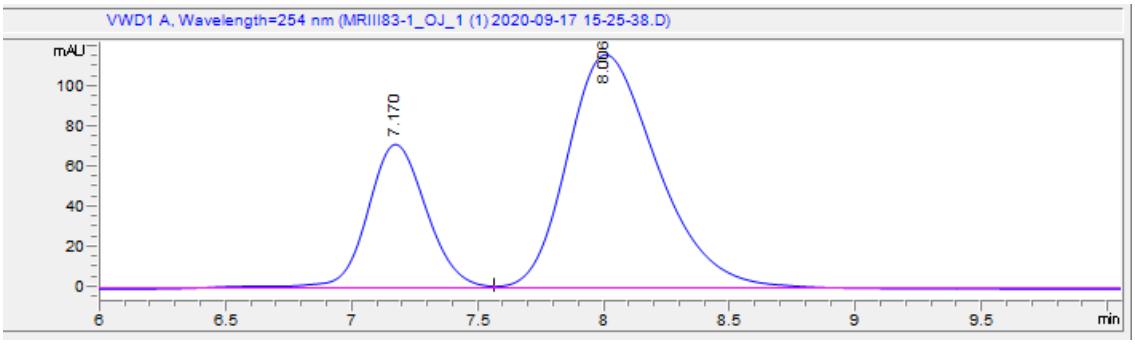
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.584	MM	4516.6	243.9	0.3087	75.219	0.778
2	8.575	MM	1488	55.9	0.4439	24.781	0.808

Figure A7.11 HPLC Trace 6 (entry 2, **L11**, run 1)



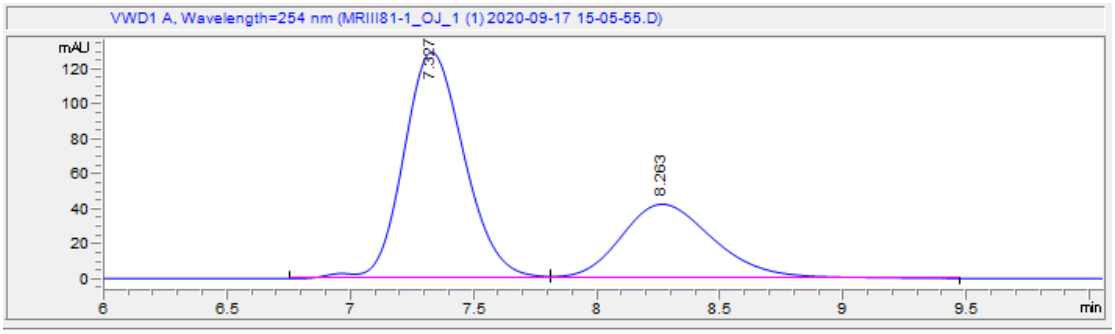
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.462	MM	1045.3	55.3	0.3152	27.699	0.86
2	8.359	MM	2728.6	96.2	0.4727	72.301	0.735

Figure A7.12 HPLC Trace 7 (entry 2, **L11**, run 2)



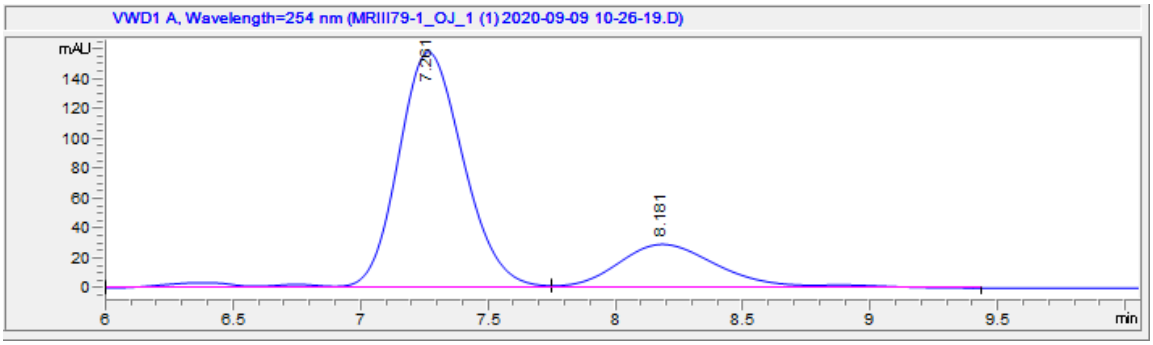
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.17	BV	1217.7	72.2	0.2606	29.202	0.943
2	8.006	VB	2952.3	117.1	0.3882	70.798	0.697

Figure A7.13 HPLC Trace 8 (entry 3, **L12**, run 1)



#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.327	VV R	2231.2	130	0.2644	66.425	0.851
2	8.263	VB	1127.8	42.6	0.4085	33.575	0.759

Figure A7.14 HPLC Trace 9 (entry 3, **L12**, run 2)



#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.261	MM	2699.1	155.8	0.2887	78.868	0.825
2	8.181	MM	723.2	28	0.4303	21.132	0.789

A7.5 NMR Spectra

Figure A7.15 Compound 4. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

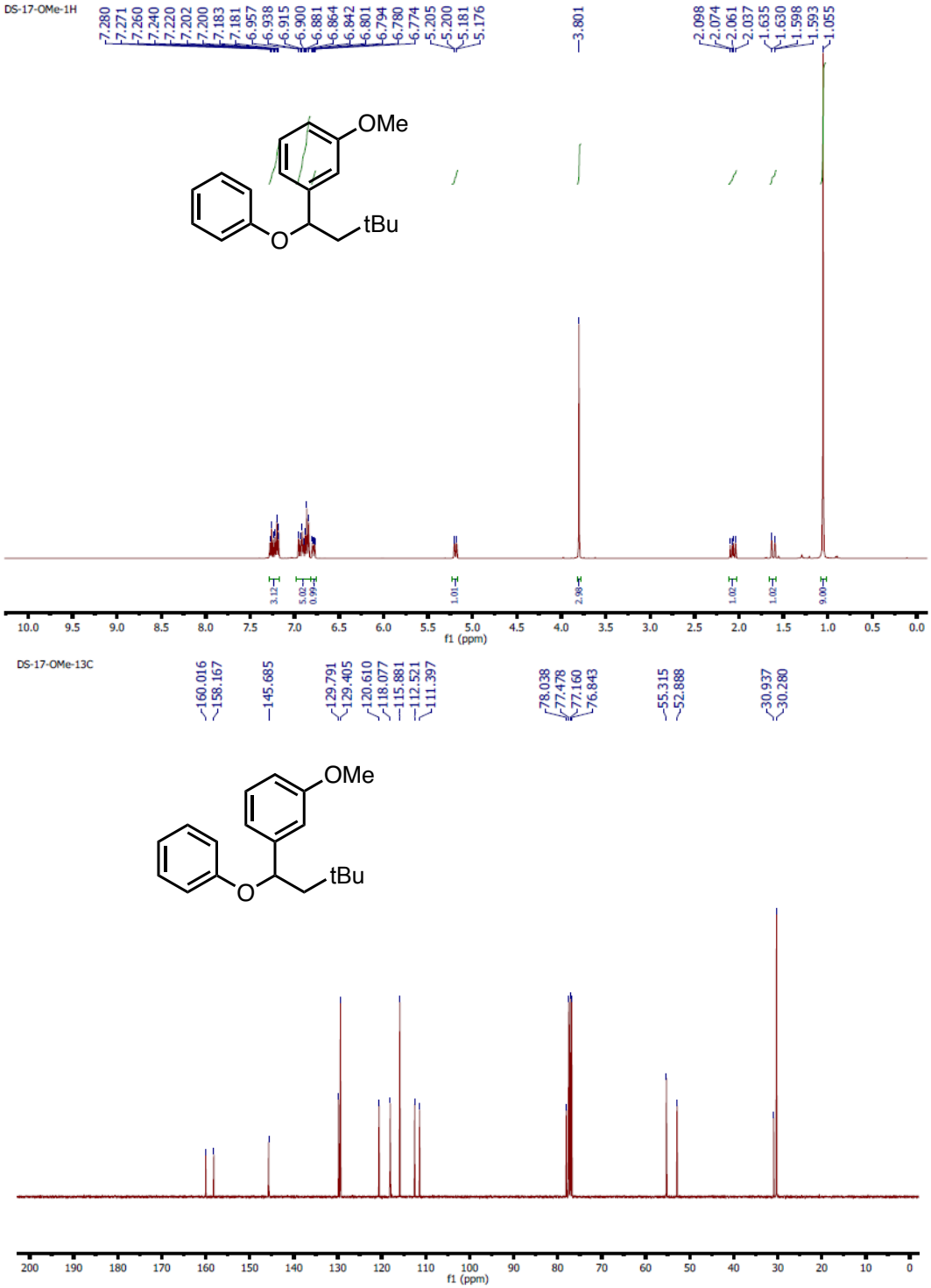


Figure A7.16 Compound 5. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

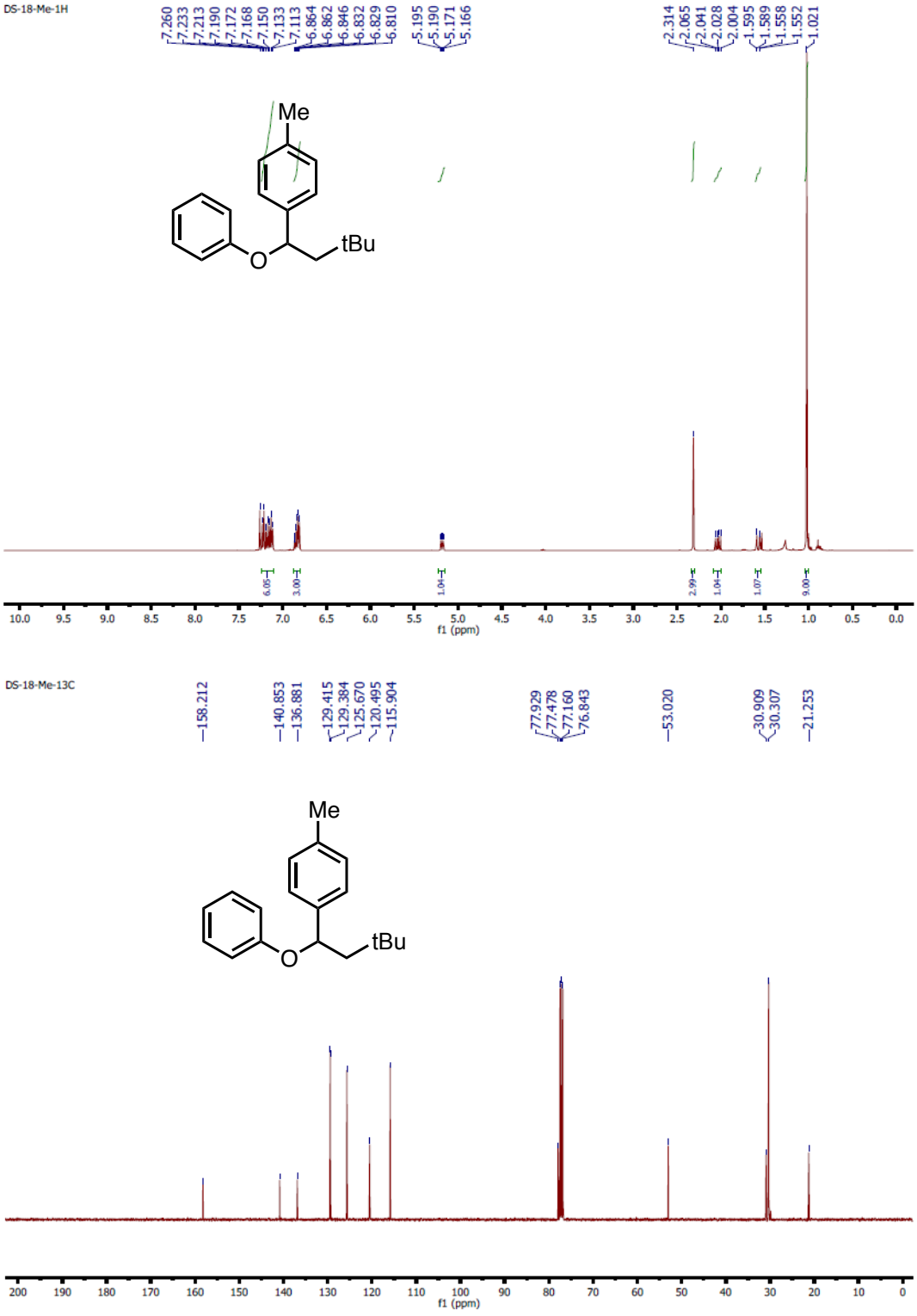
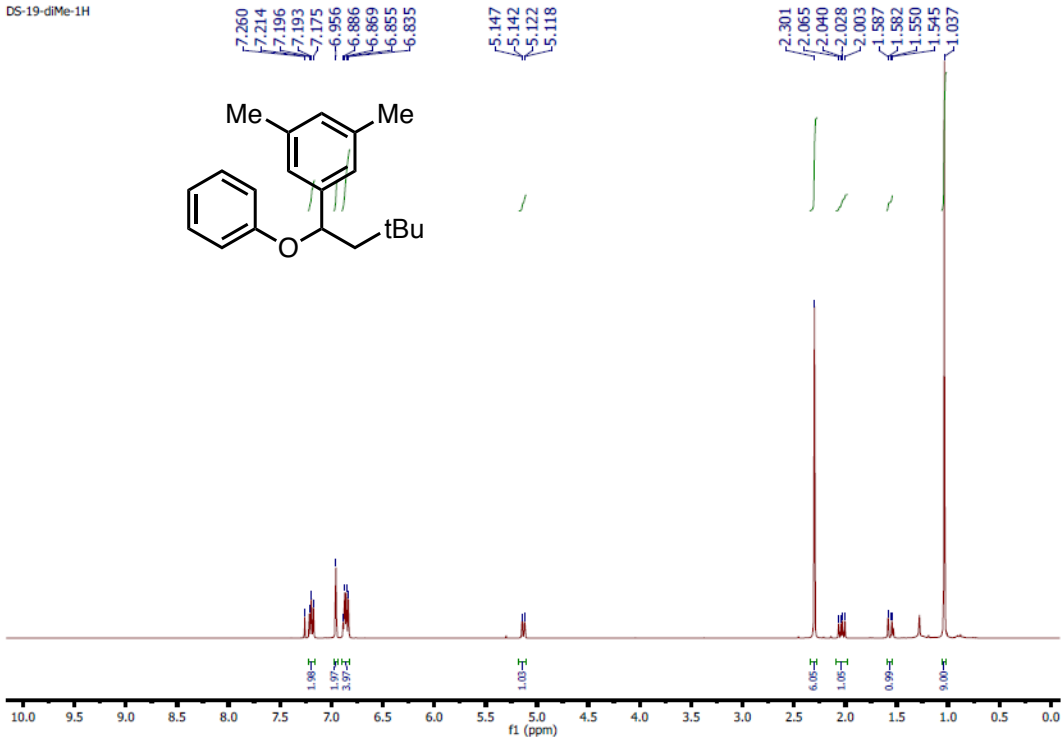


Figure A7.17 Compound 6. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



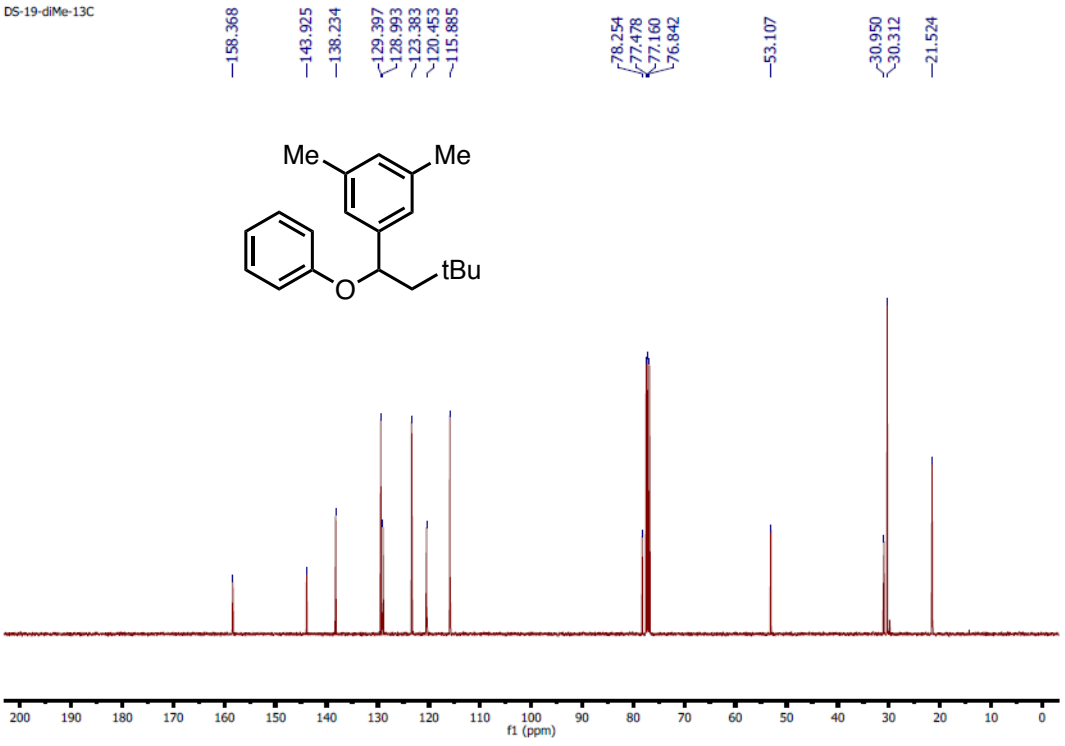


Figure A7.18 Compound 7. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

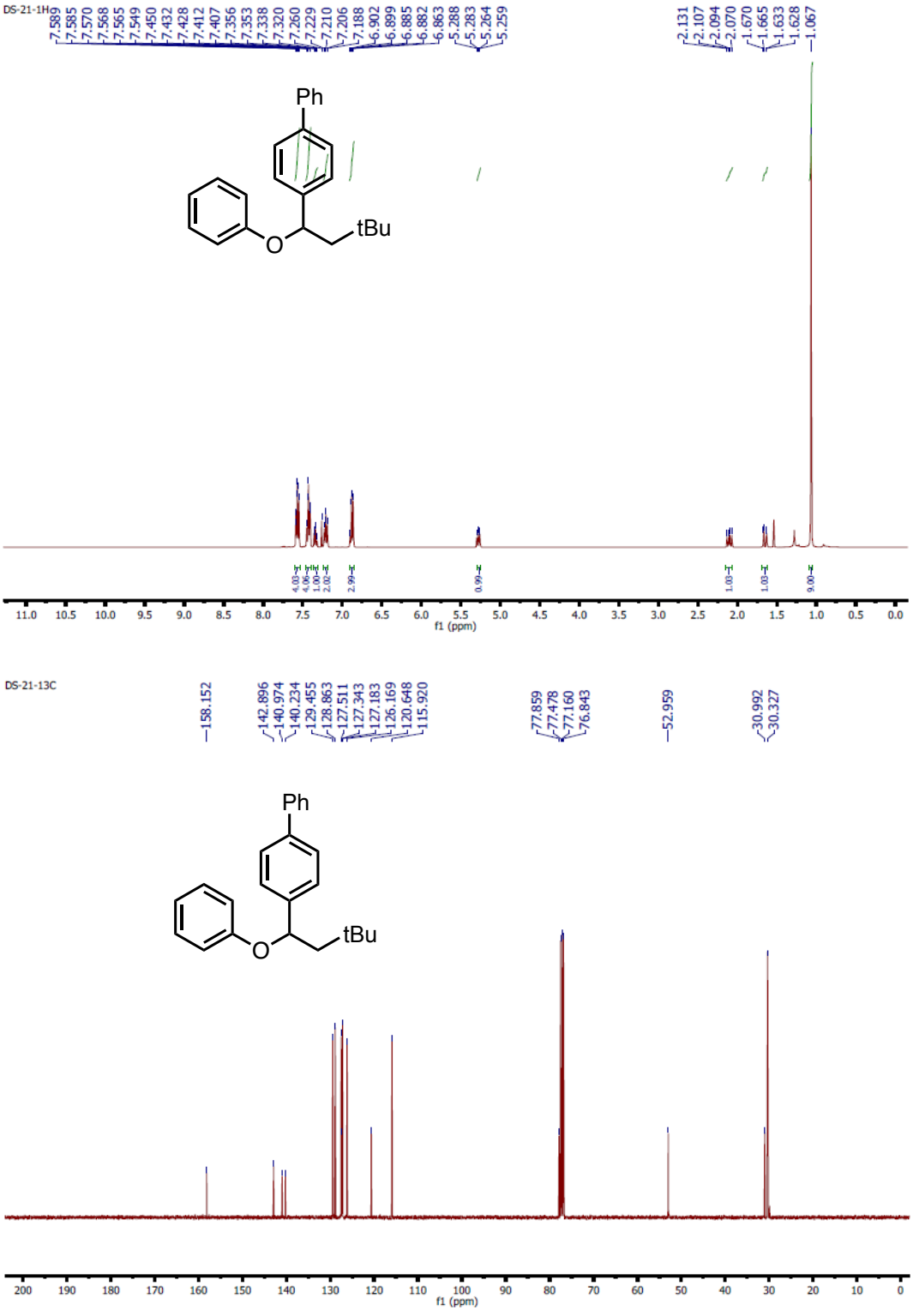


Figure A7.19 Compound 8. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

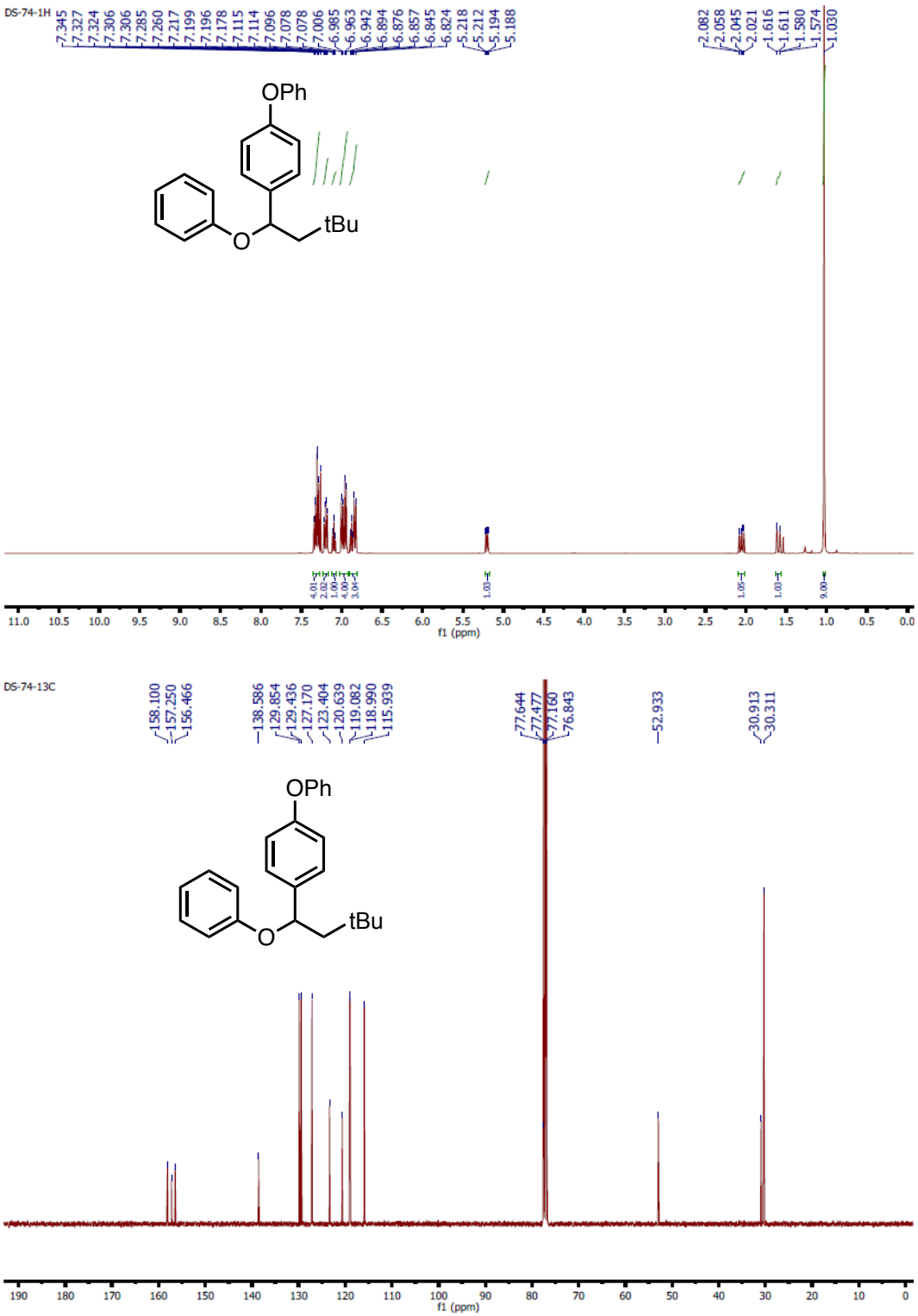


Figure A7.20 Compound 9. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

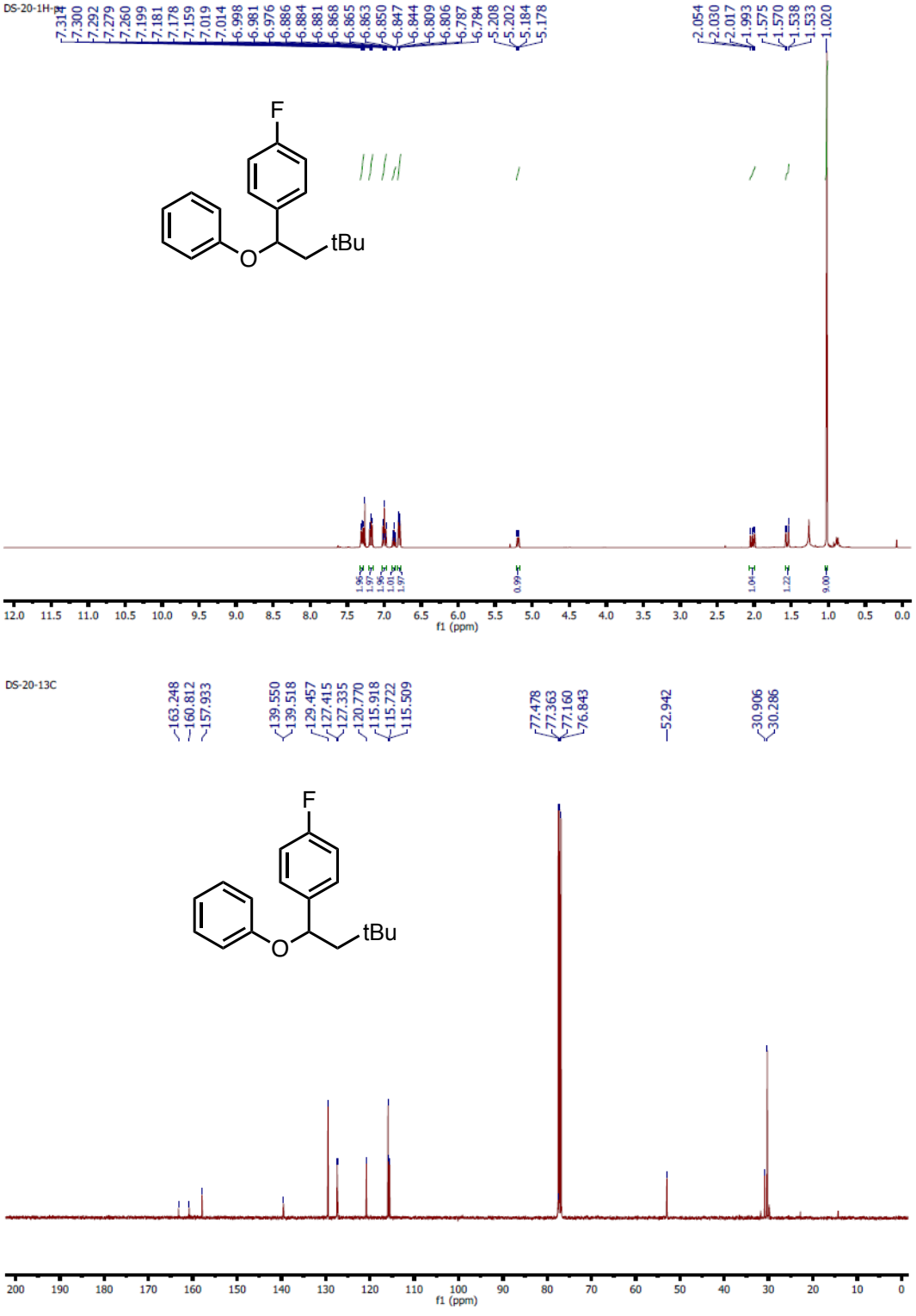


Figure A7.21 Compound 9. ^{19}F NMR ($CDCl_3$, 376 MHz)

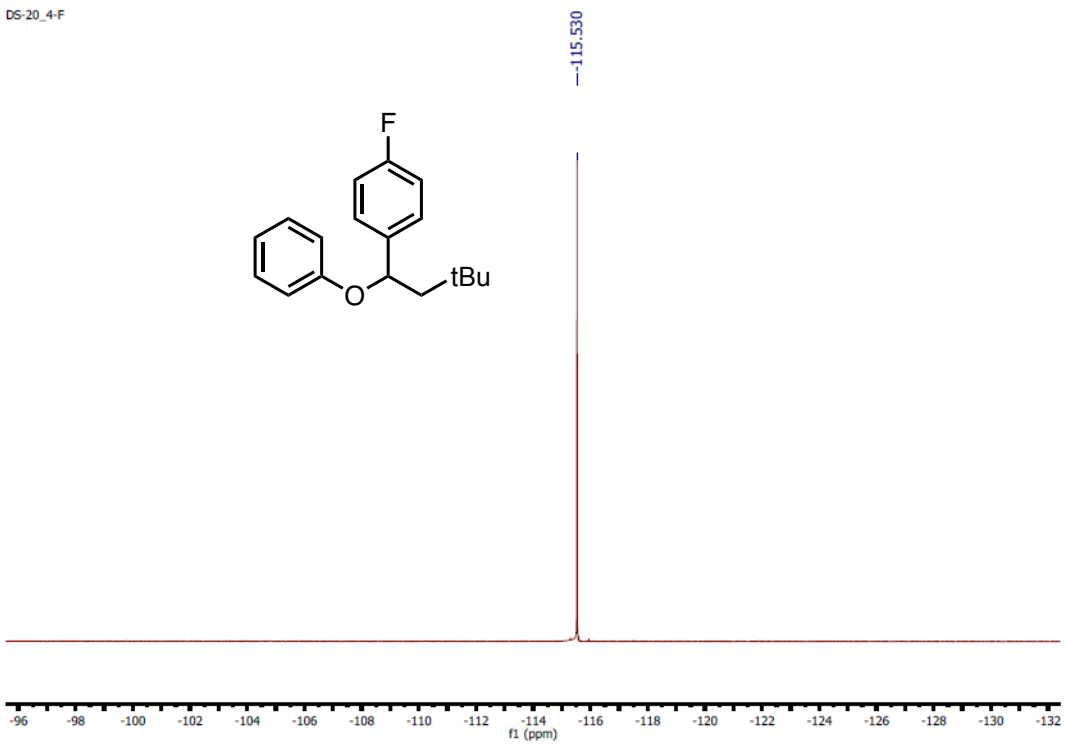


Figure A7.22 Compound 10. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

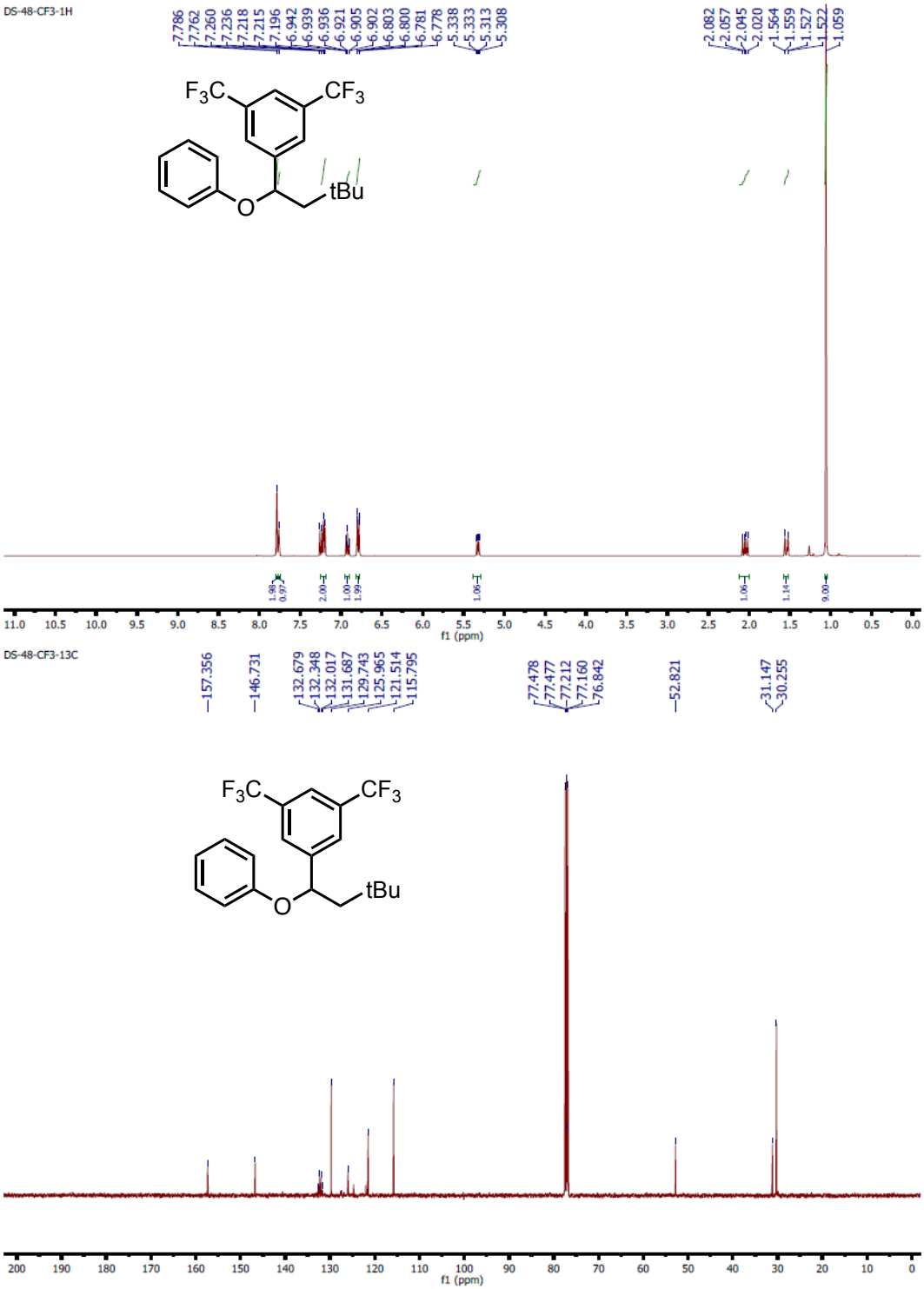


Figure A7.23 Compound 10. ^{19}F NMR ($CDCl_3$, 376 MHz)

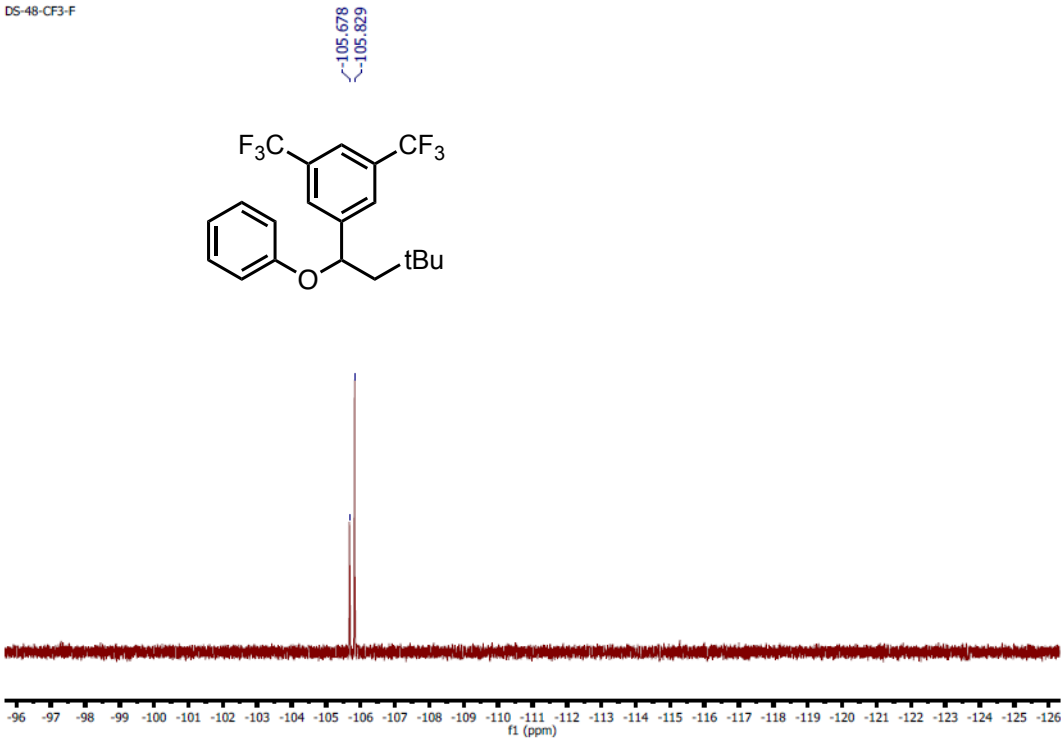
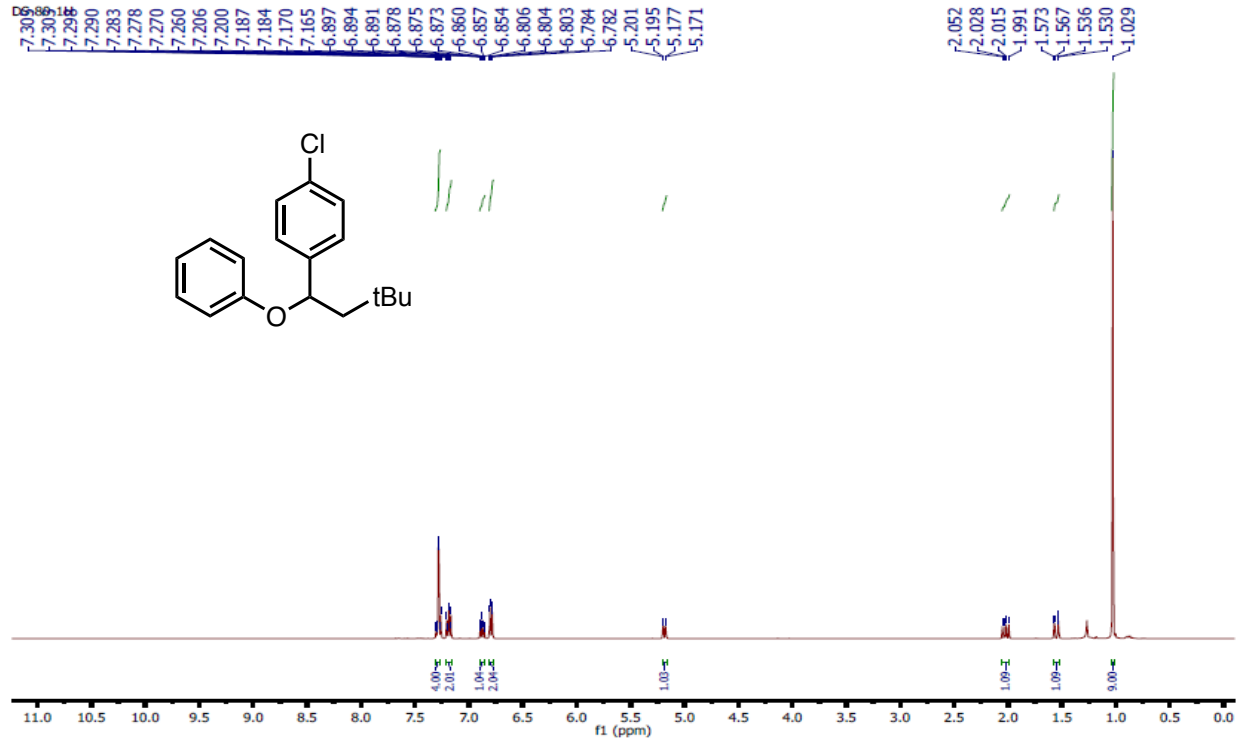


Figure A7.24 Compound 11. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



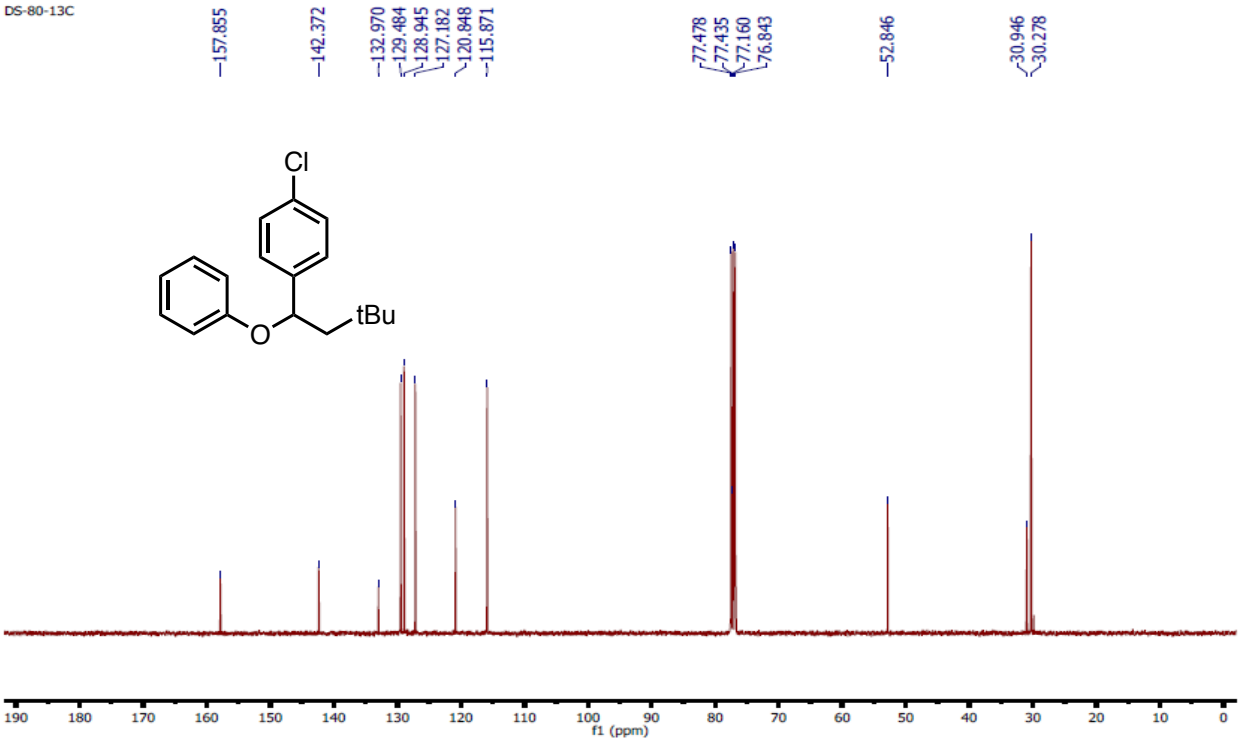


Figure A7.25 Compound 12. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

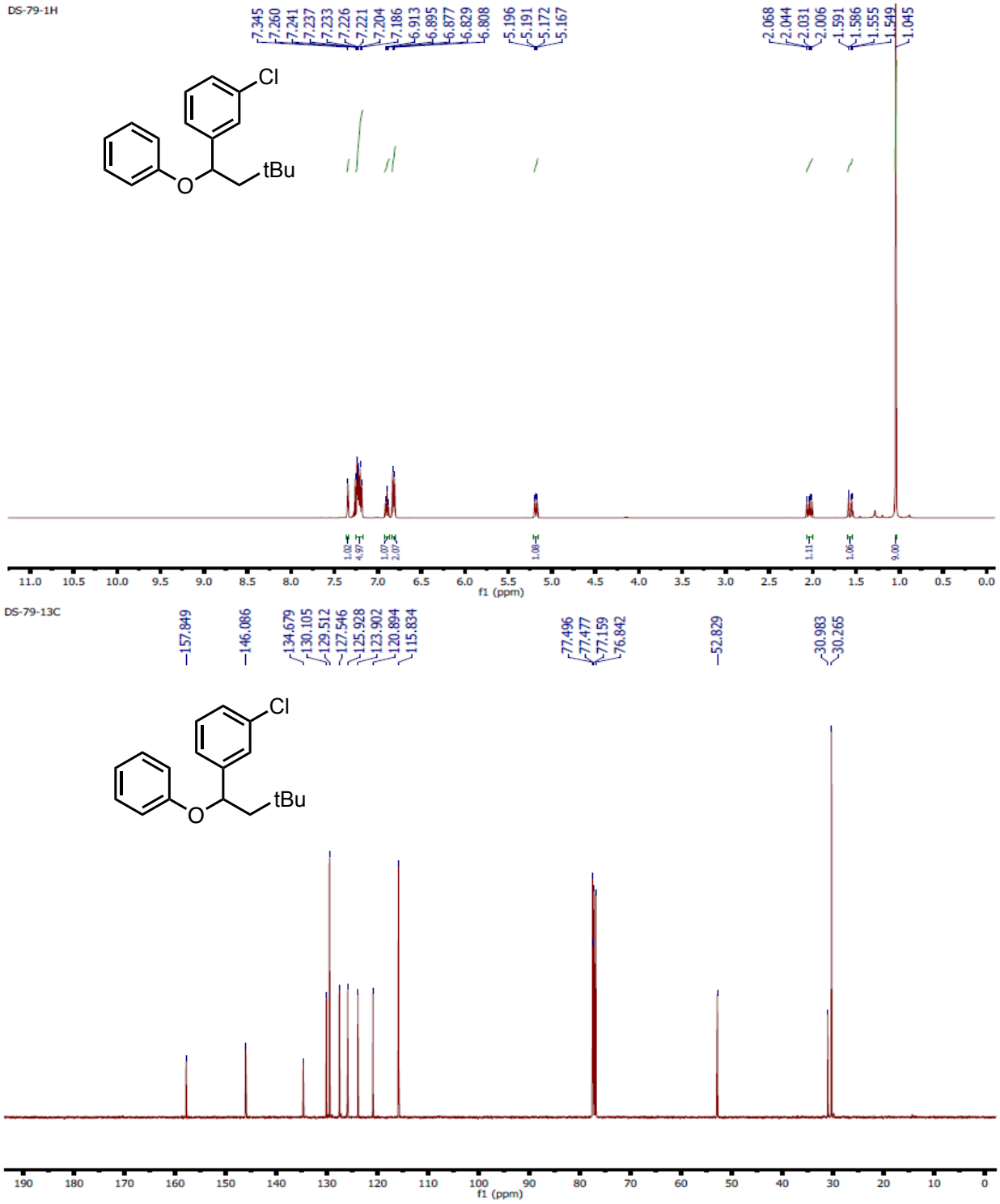


Figure A7.26 Compound 13. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

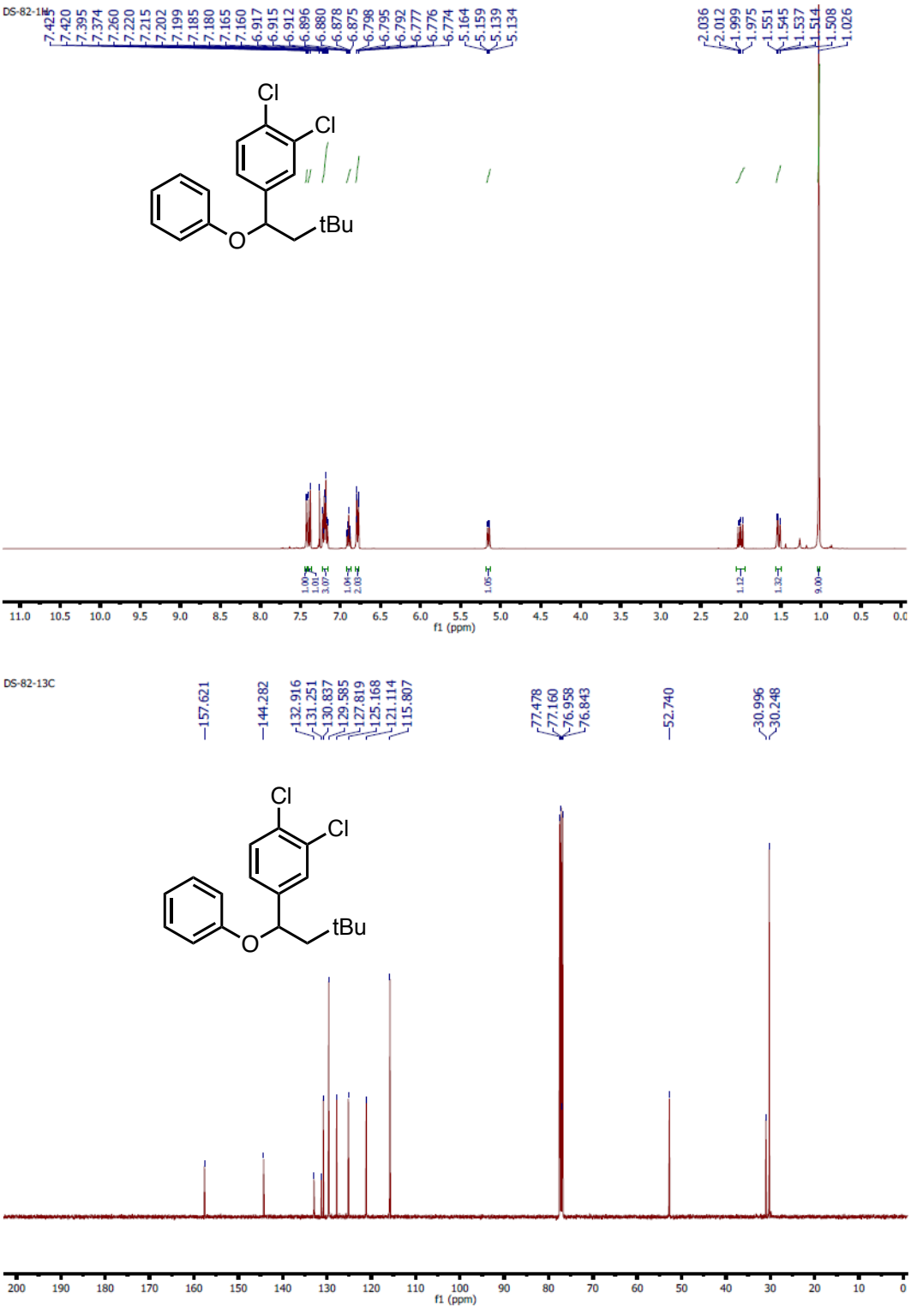


Figure A7.27 Compound 14. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

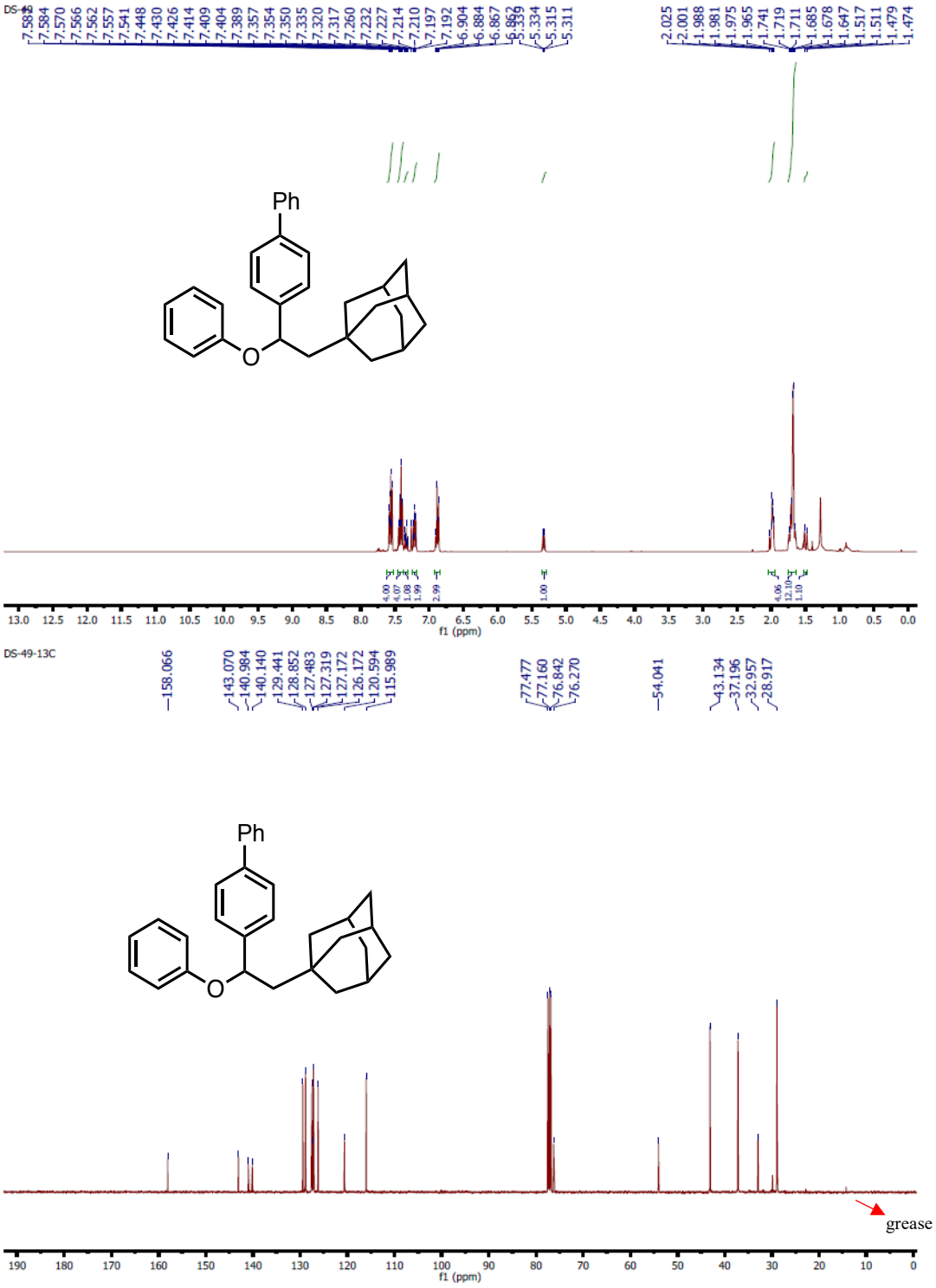


Figure A7.28 Compound 16. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

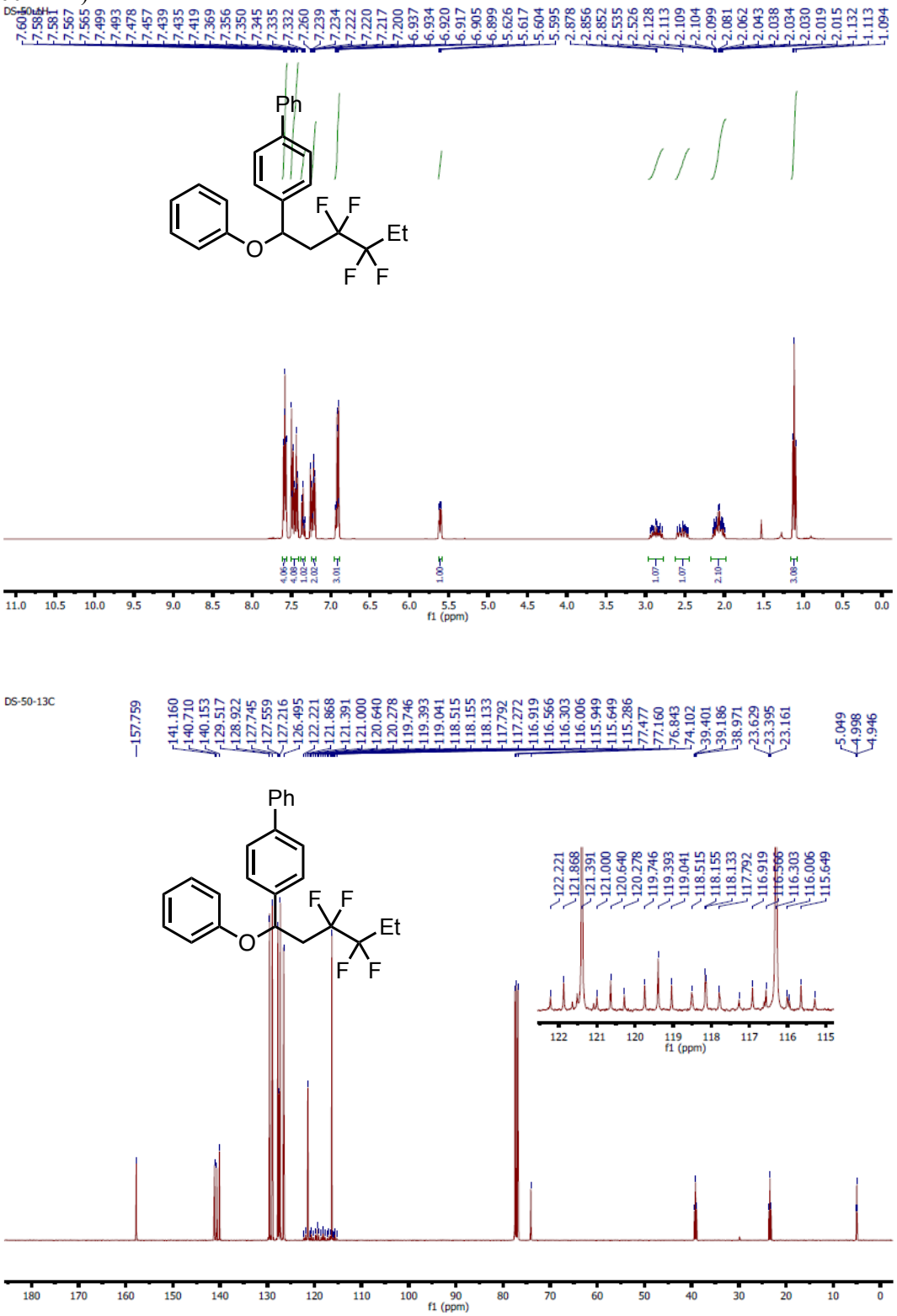


Figure A7.29 Compound 16. ^{19}F NMR ($CDCl_3$, 376 MHz)

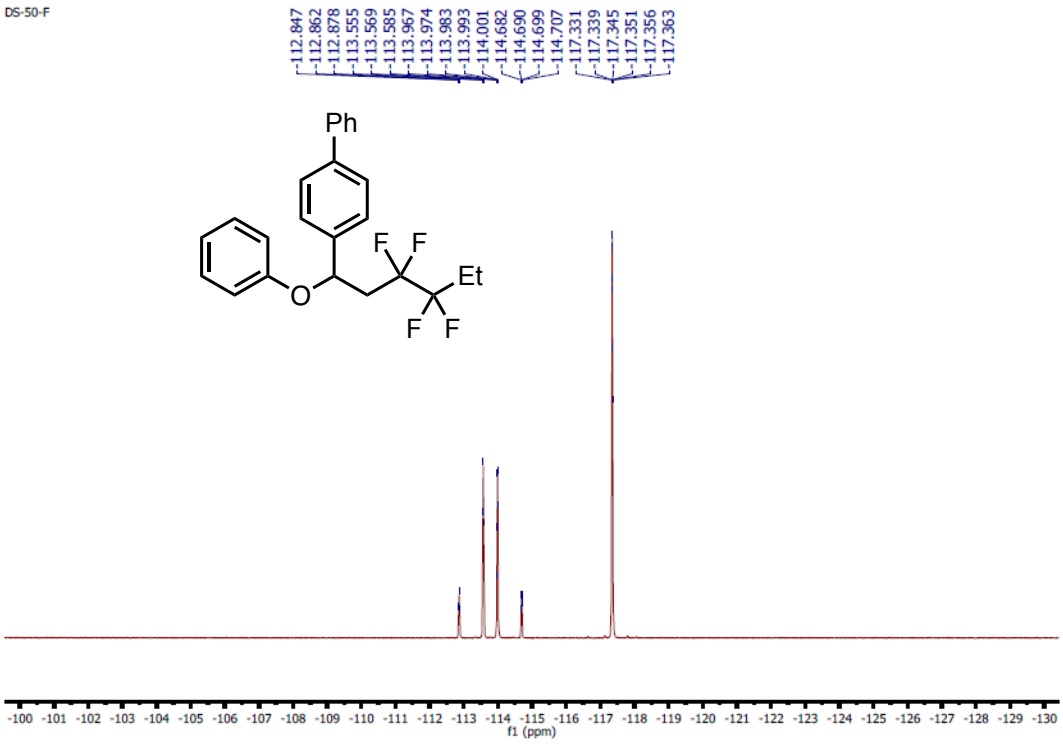


Figure A7.30 Compound 17. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

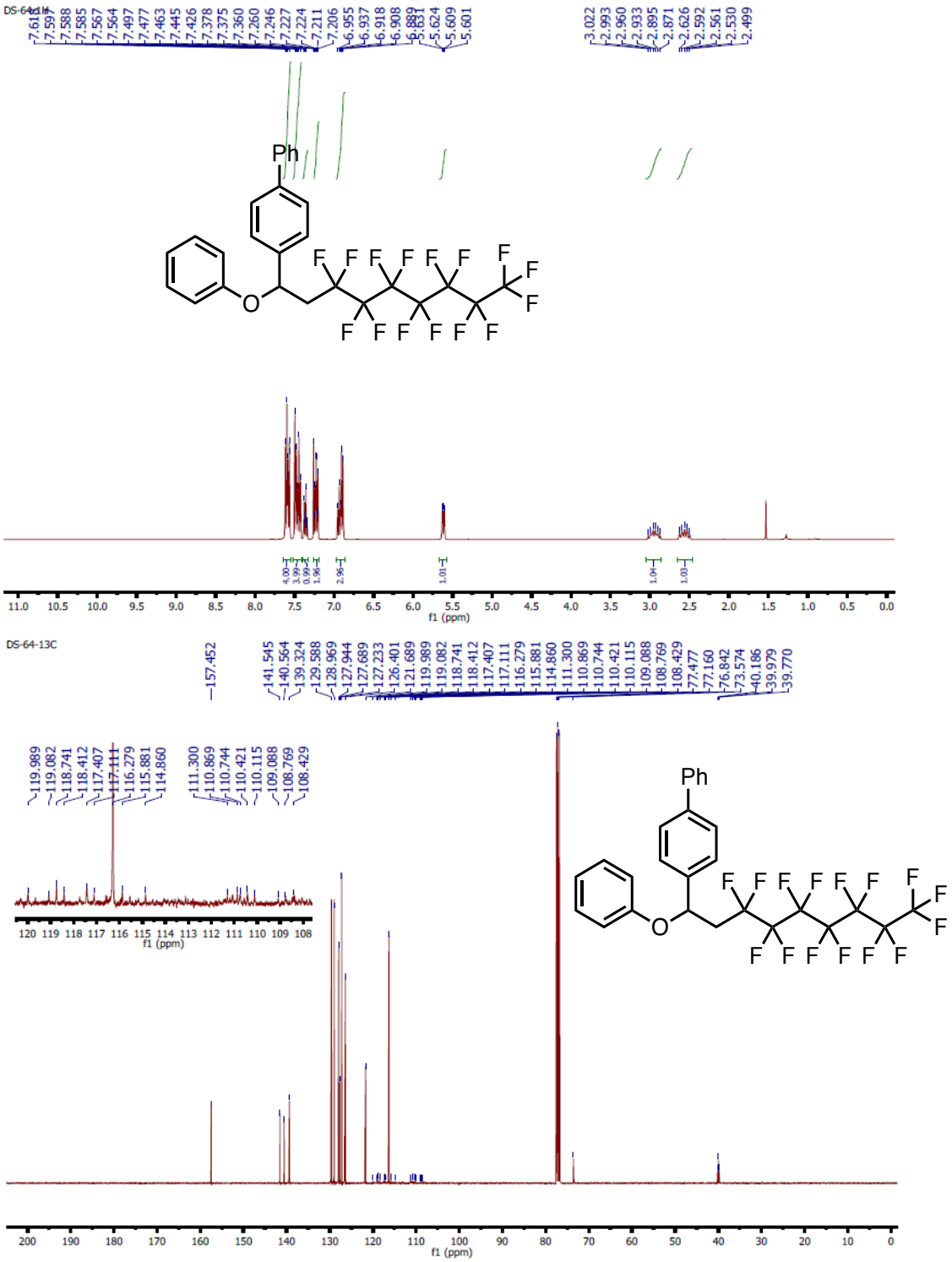


Figure A7.31 Compound 17. ^{19}F NMR ($CDCl_3$, 376 MHz)

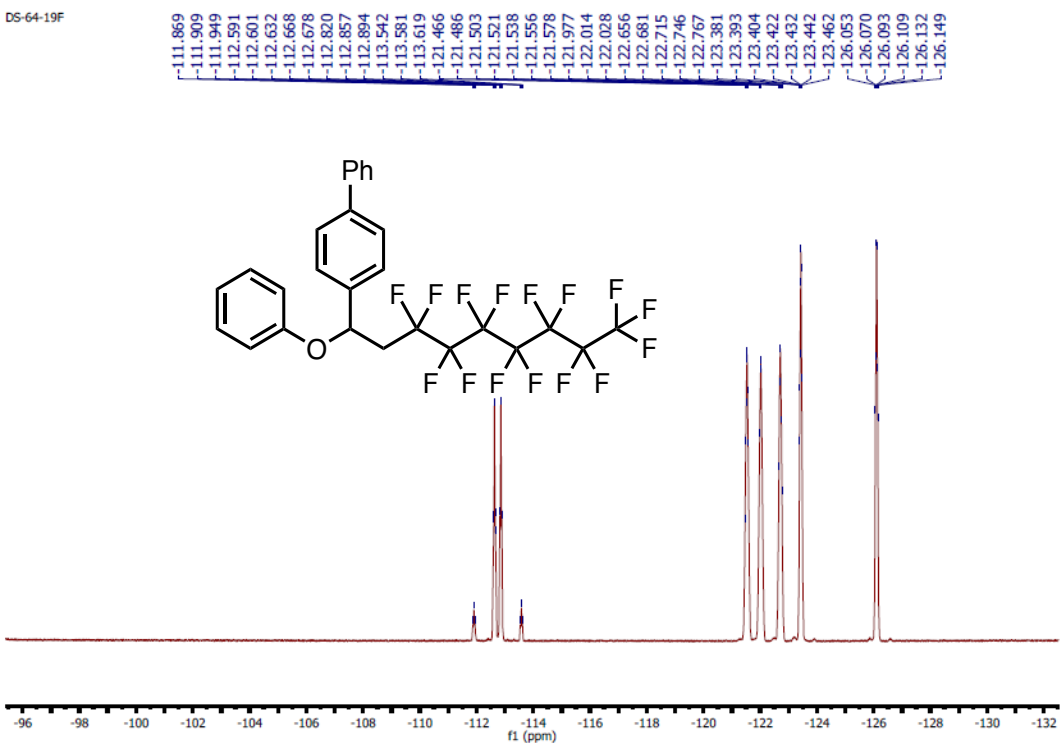


Figure A7.32 Compound 18. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

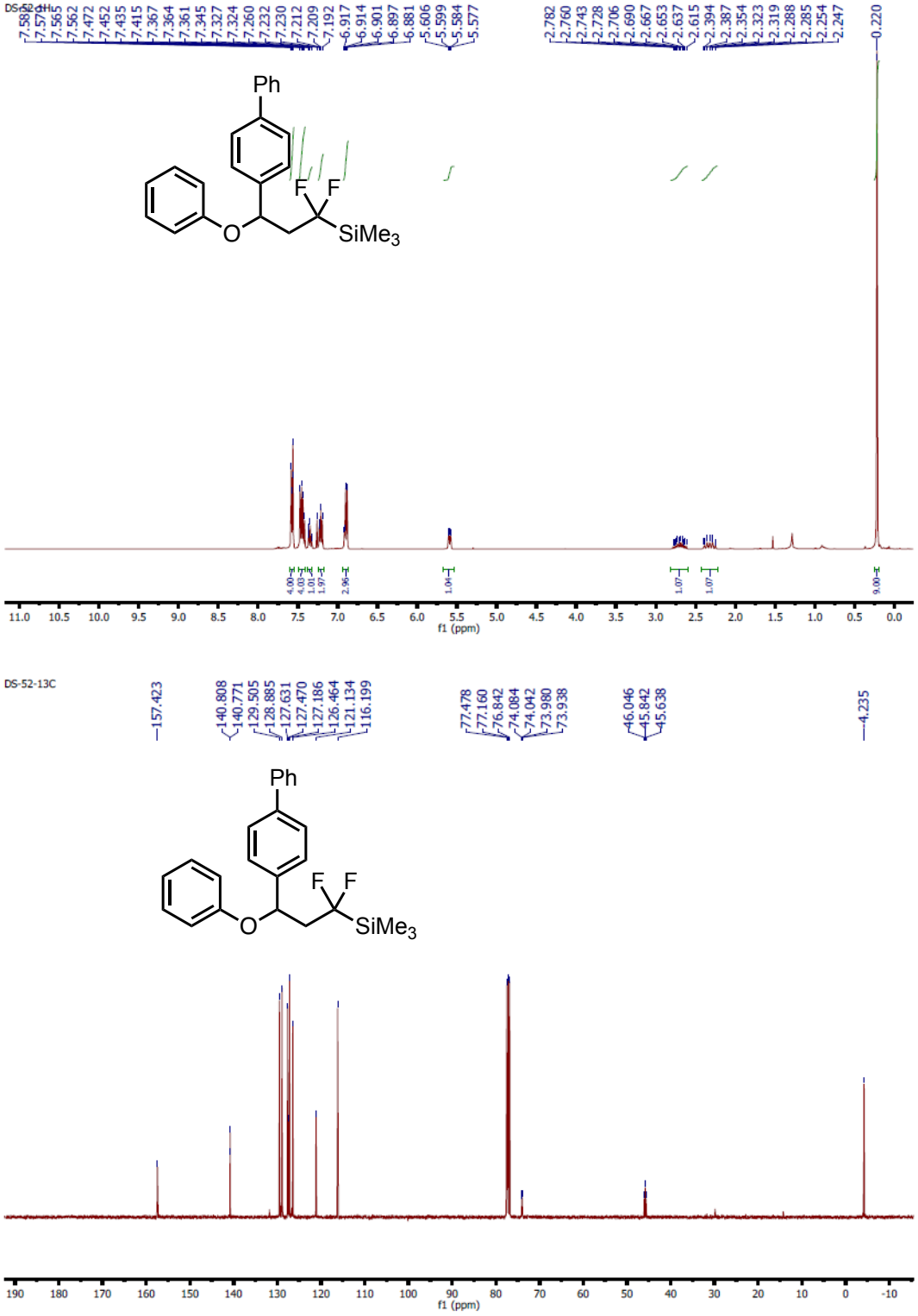


Figure A7.33 Compound 18. ^{19}F NMR ($CDCl_3$, 376 MHz)

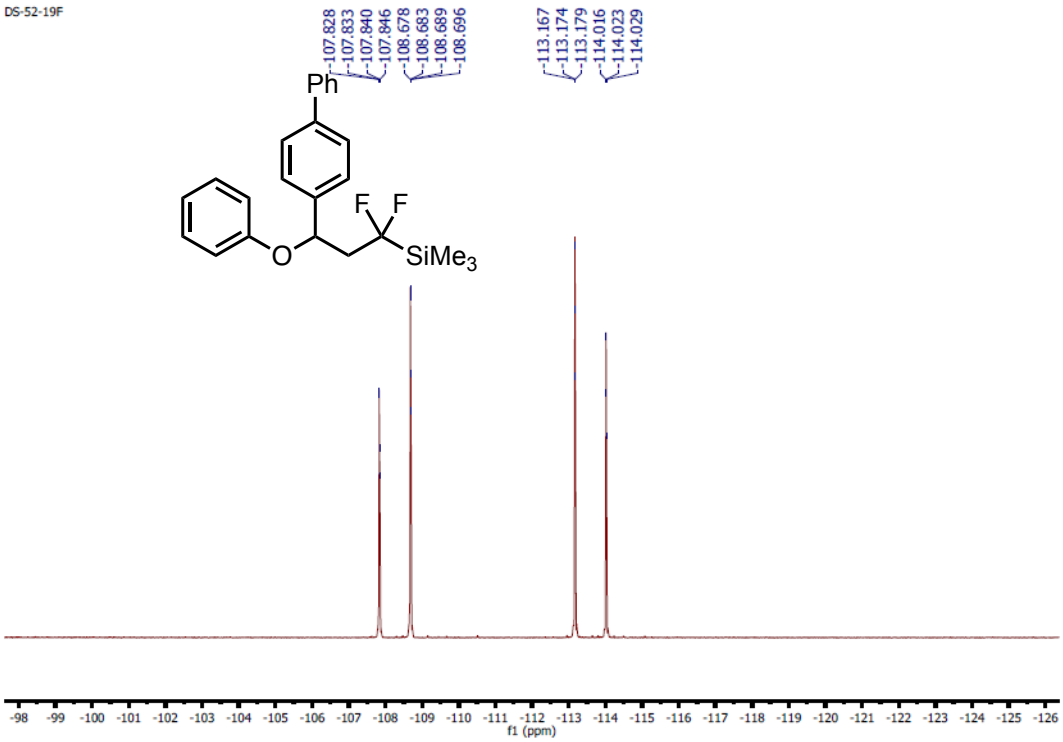


Figure A7.34 Compound 19. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

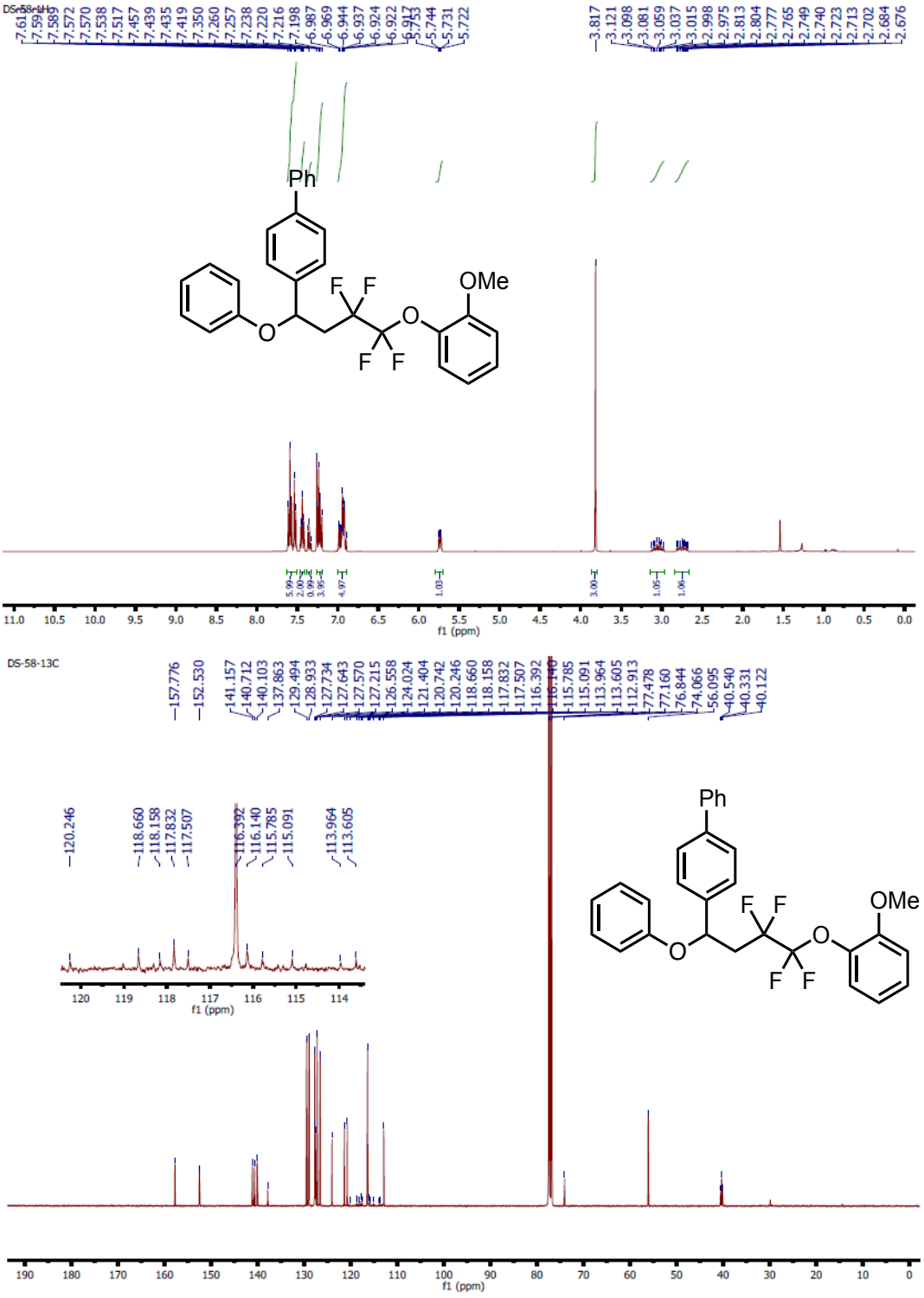


Figure A7.35 Compound 19. ^{19}F NMR ($CDCl_3$, 376 MHz)

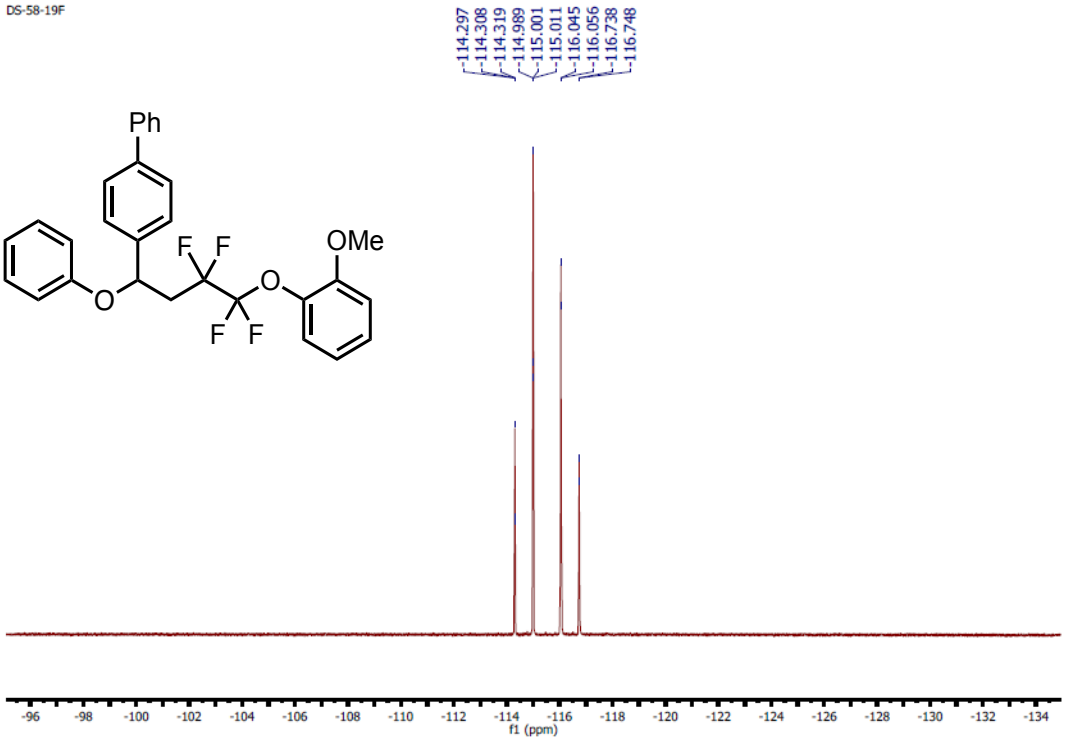


Figure A7.36 Compound 20. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

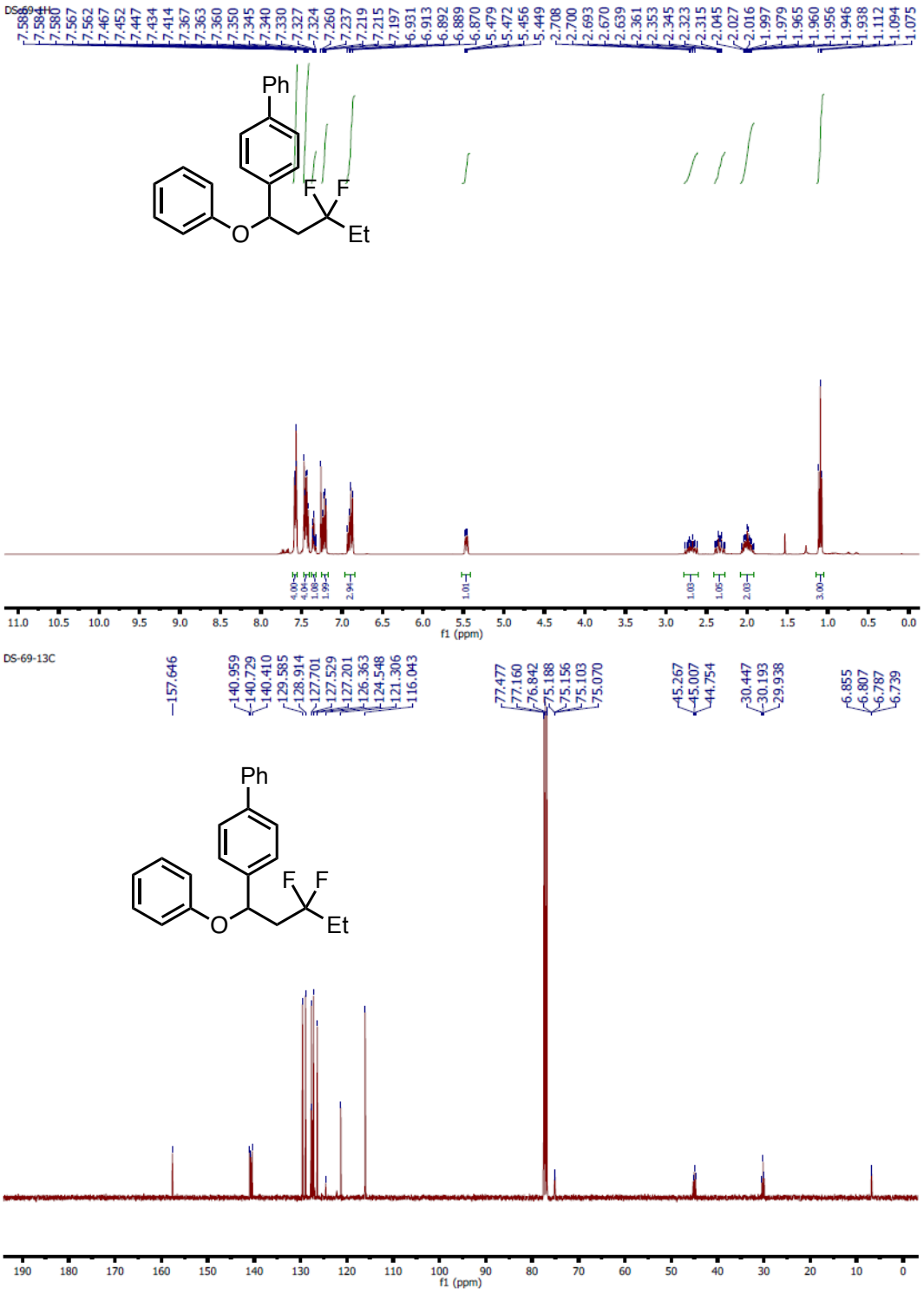


Figure A7.37 Compound 20. ^{19}F NMR ($CDCl_3$, 376 MHz)

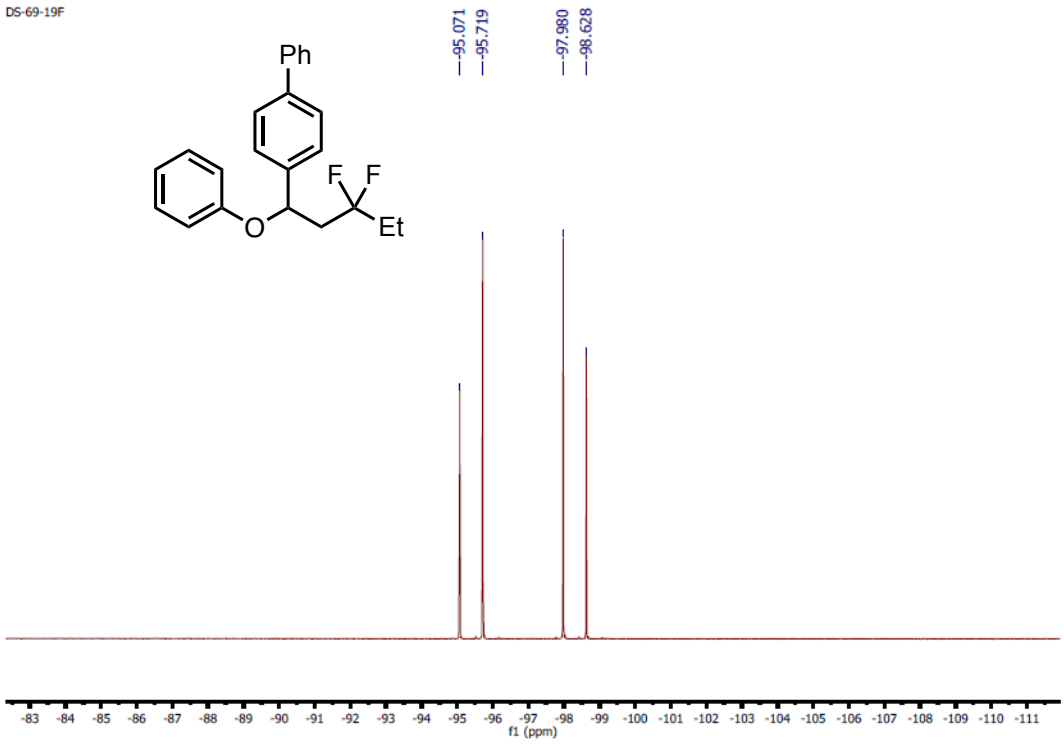
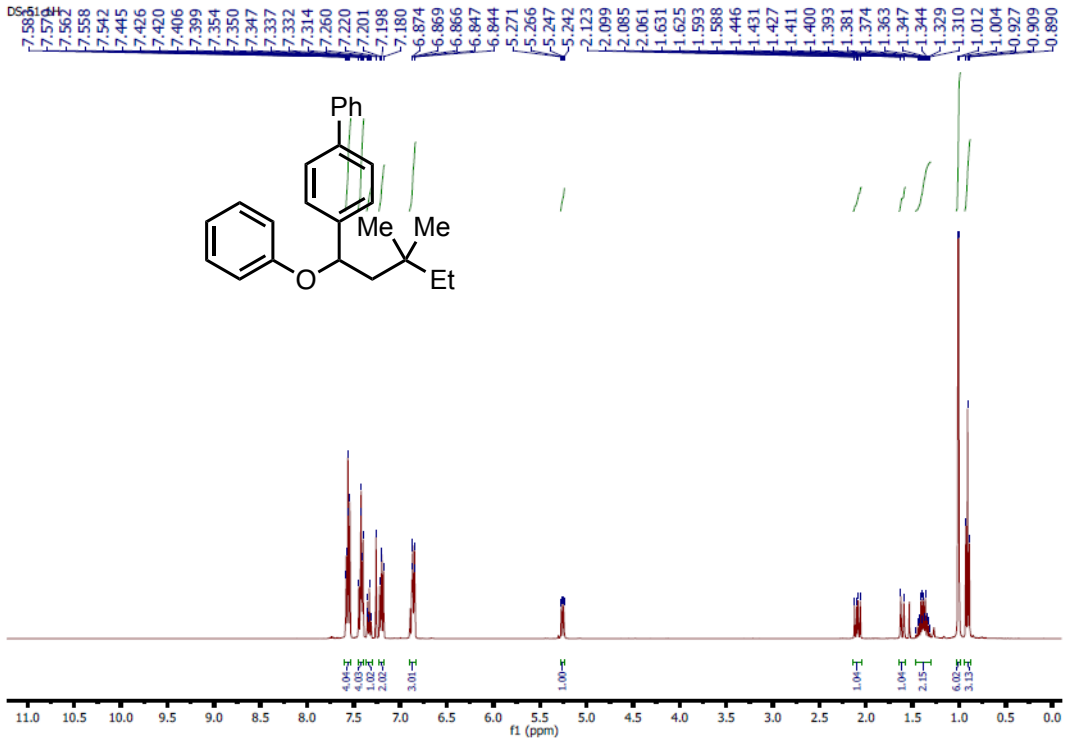


Figure A7.38 Compound 21. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



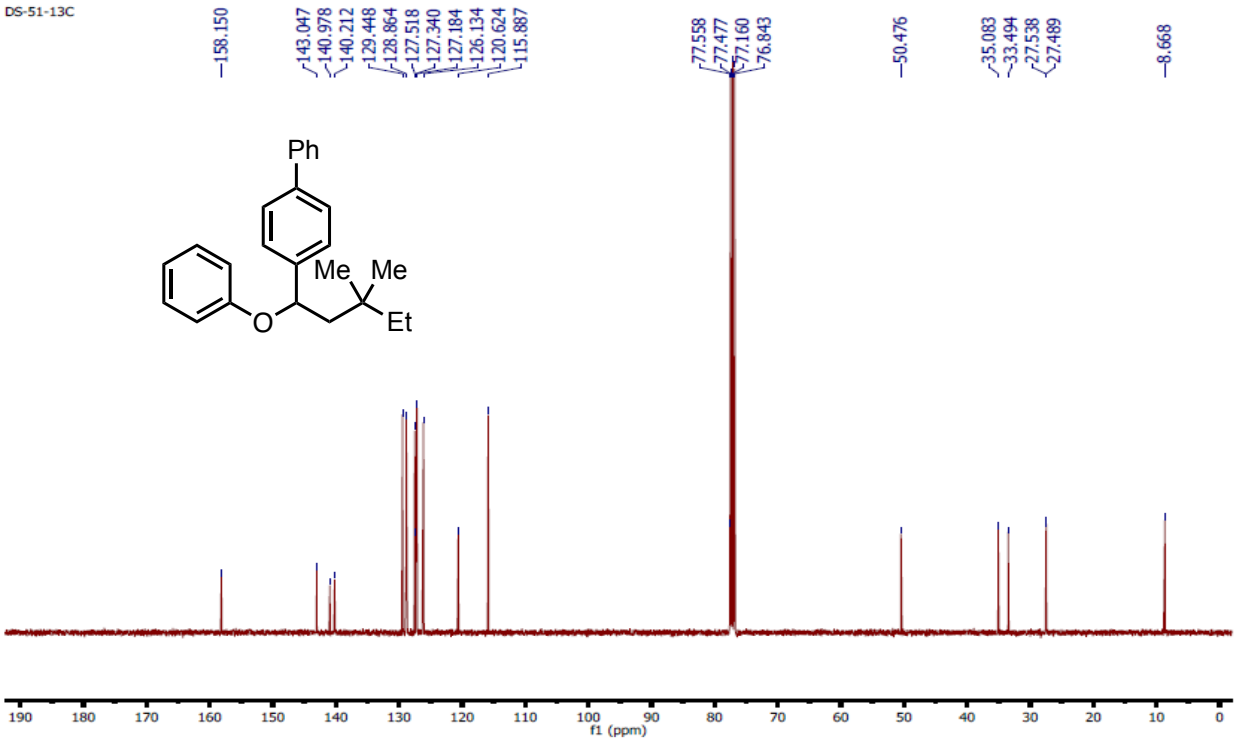


Figure A7.39 Compound 23. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

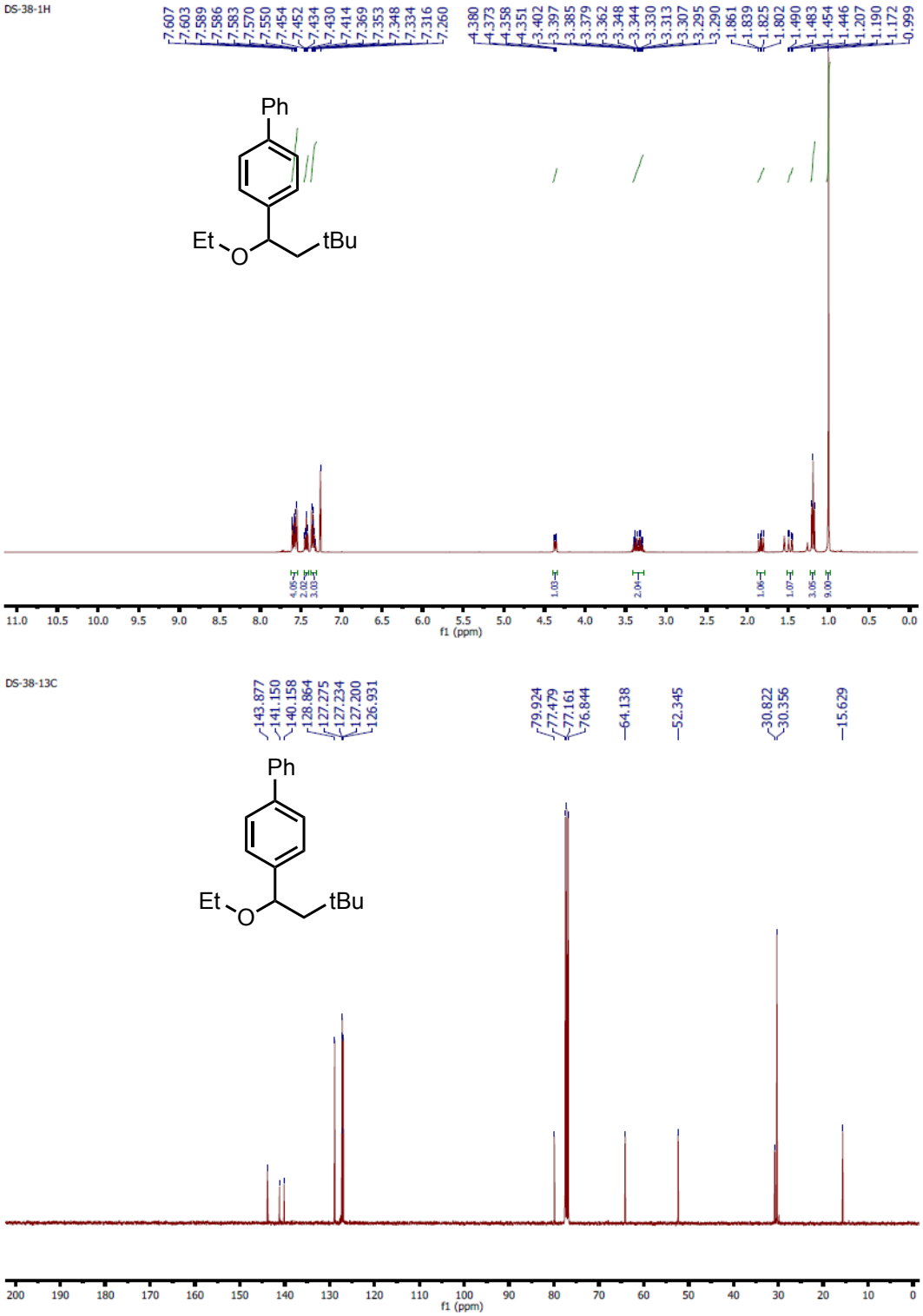


Figure A7.40 Compound 24. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

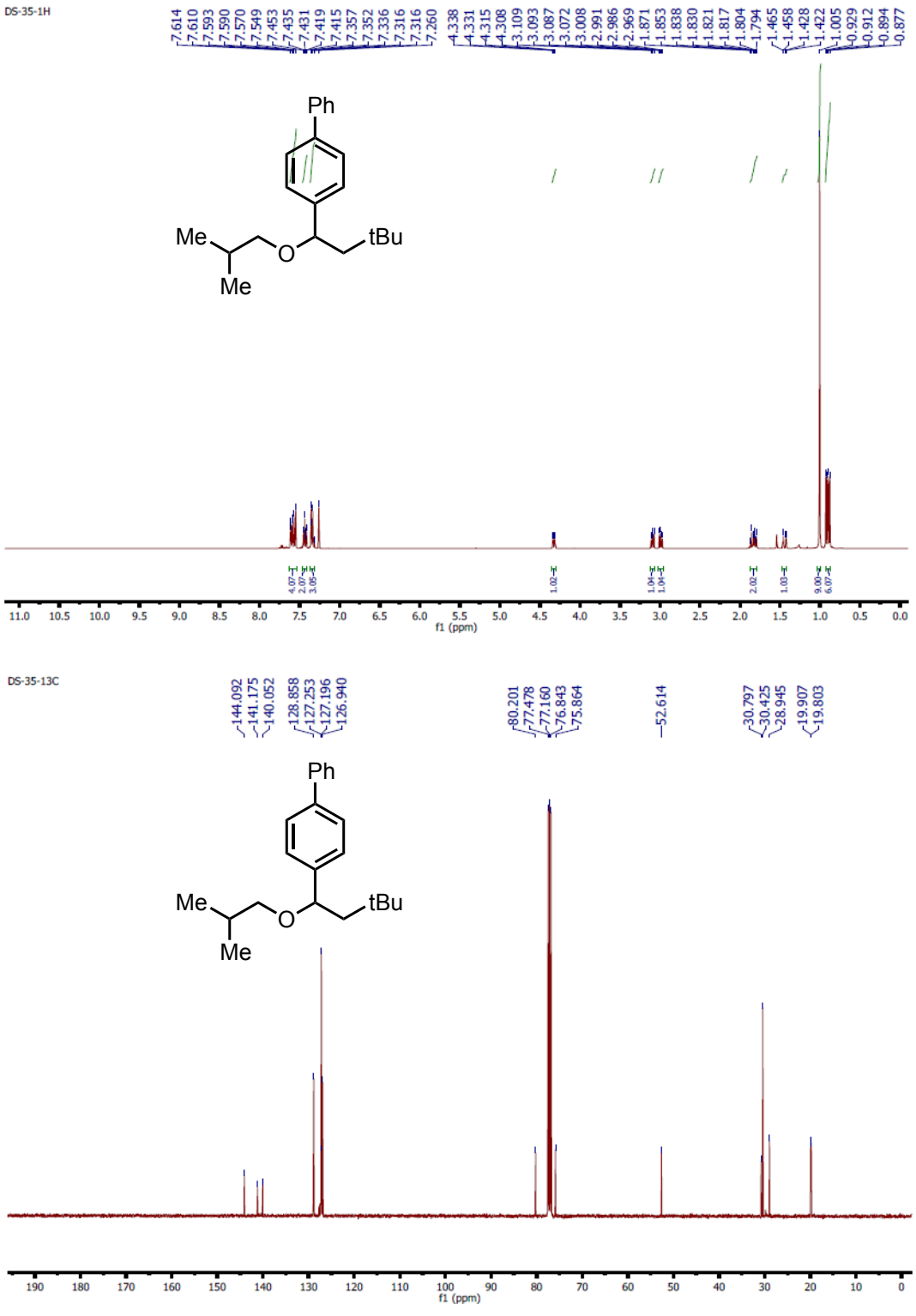


Figure A7.41 Compound 25. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

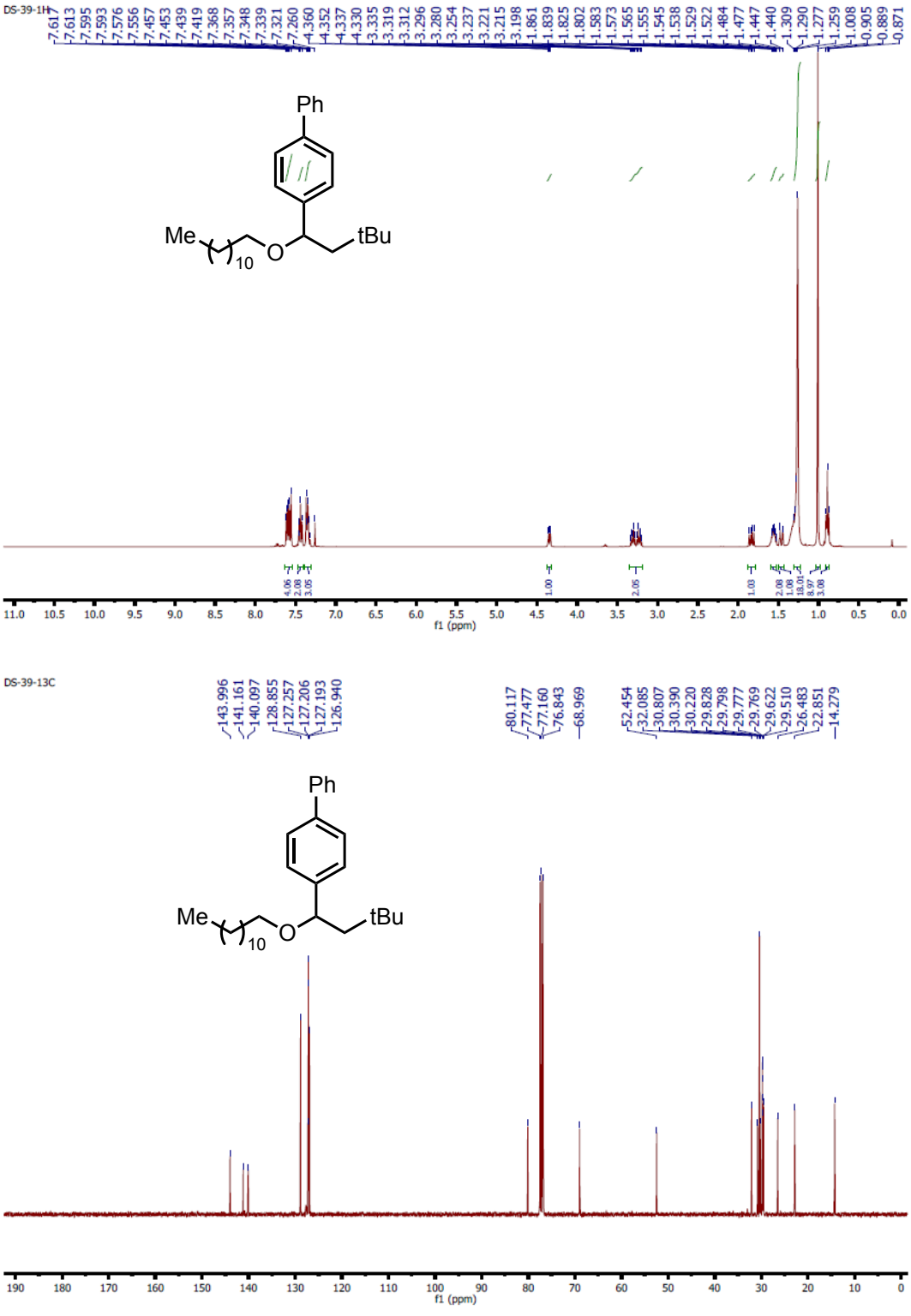


Figure A7.42 Compound 26. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

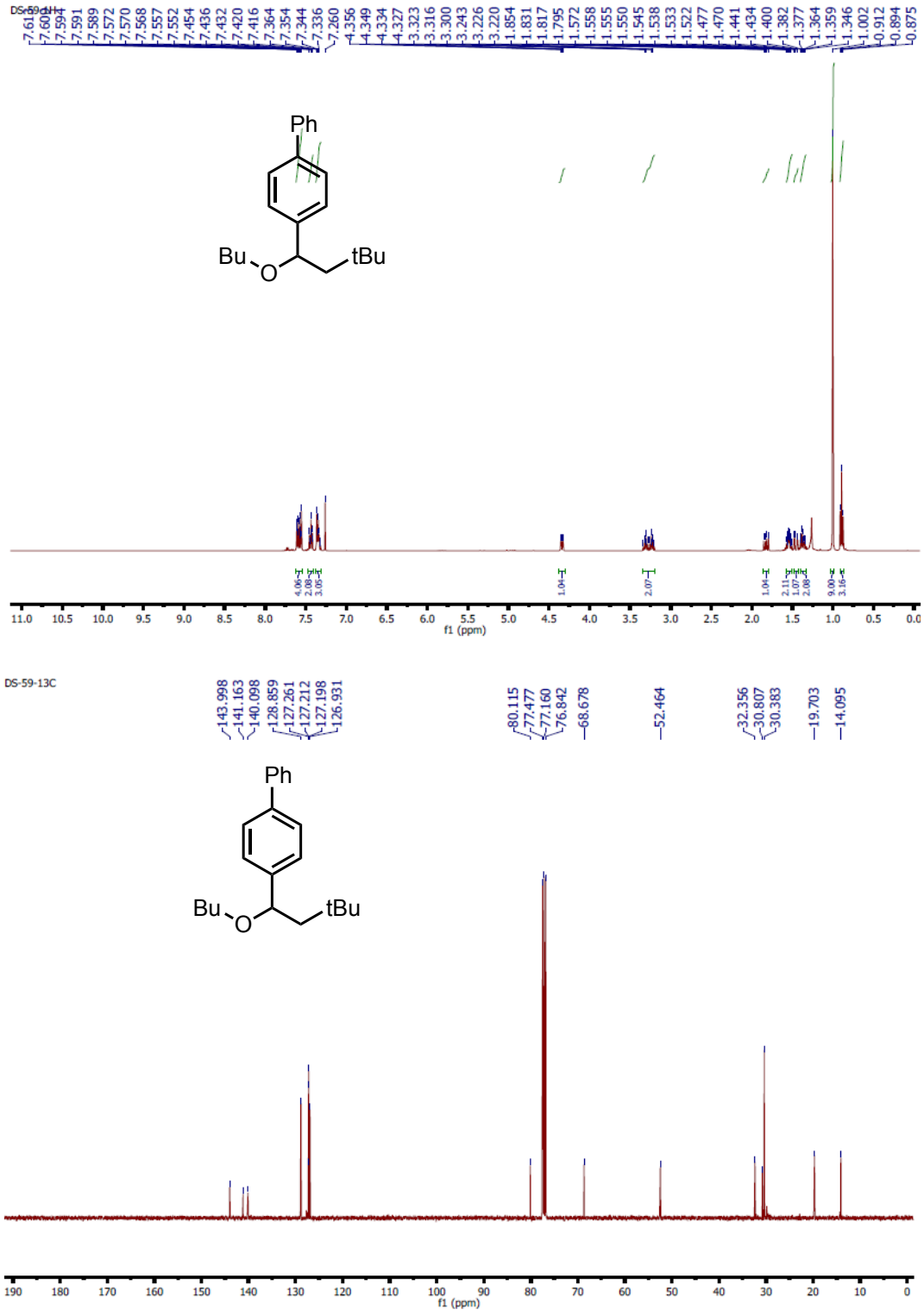
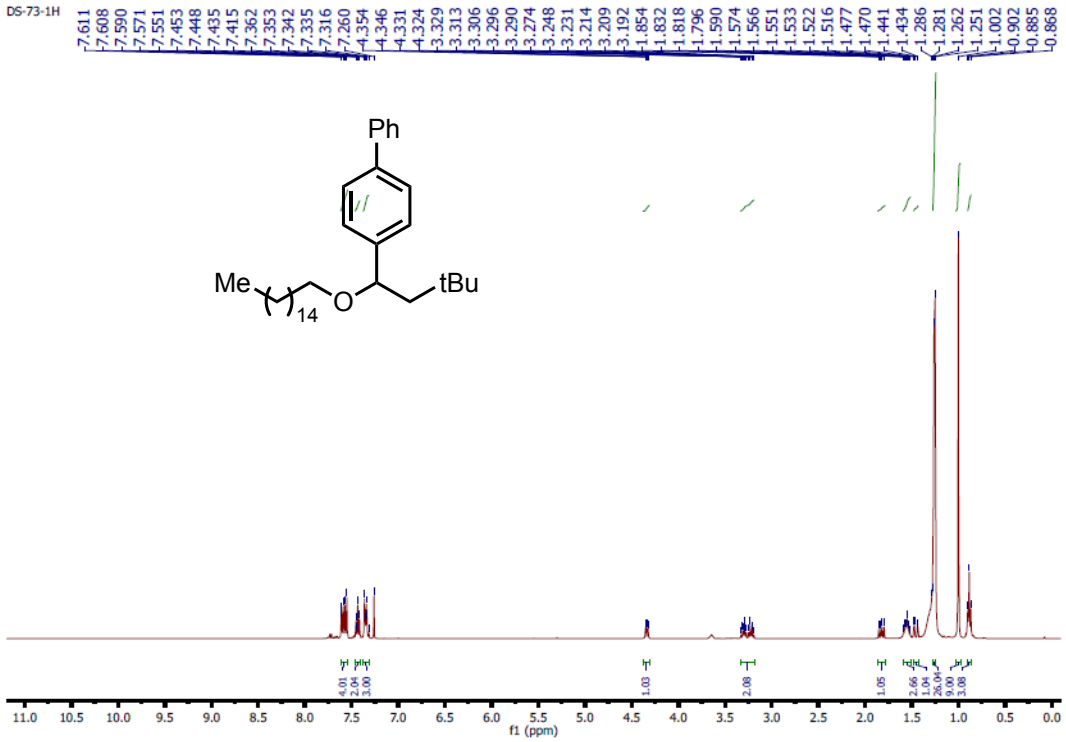


Figure A7.43 Compound 27. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



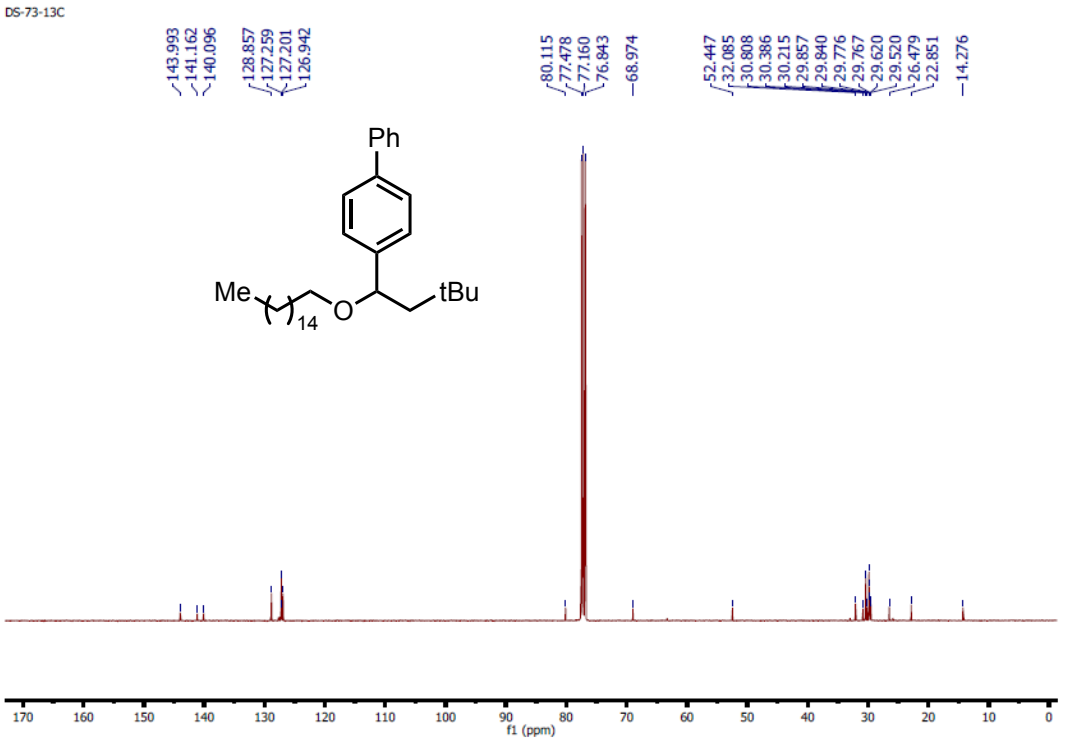


Figure A7.44 Compound 28. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

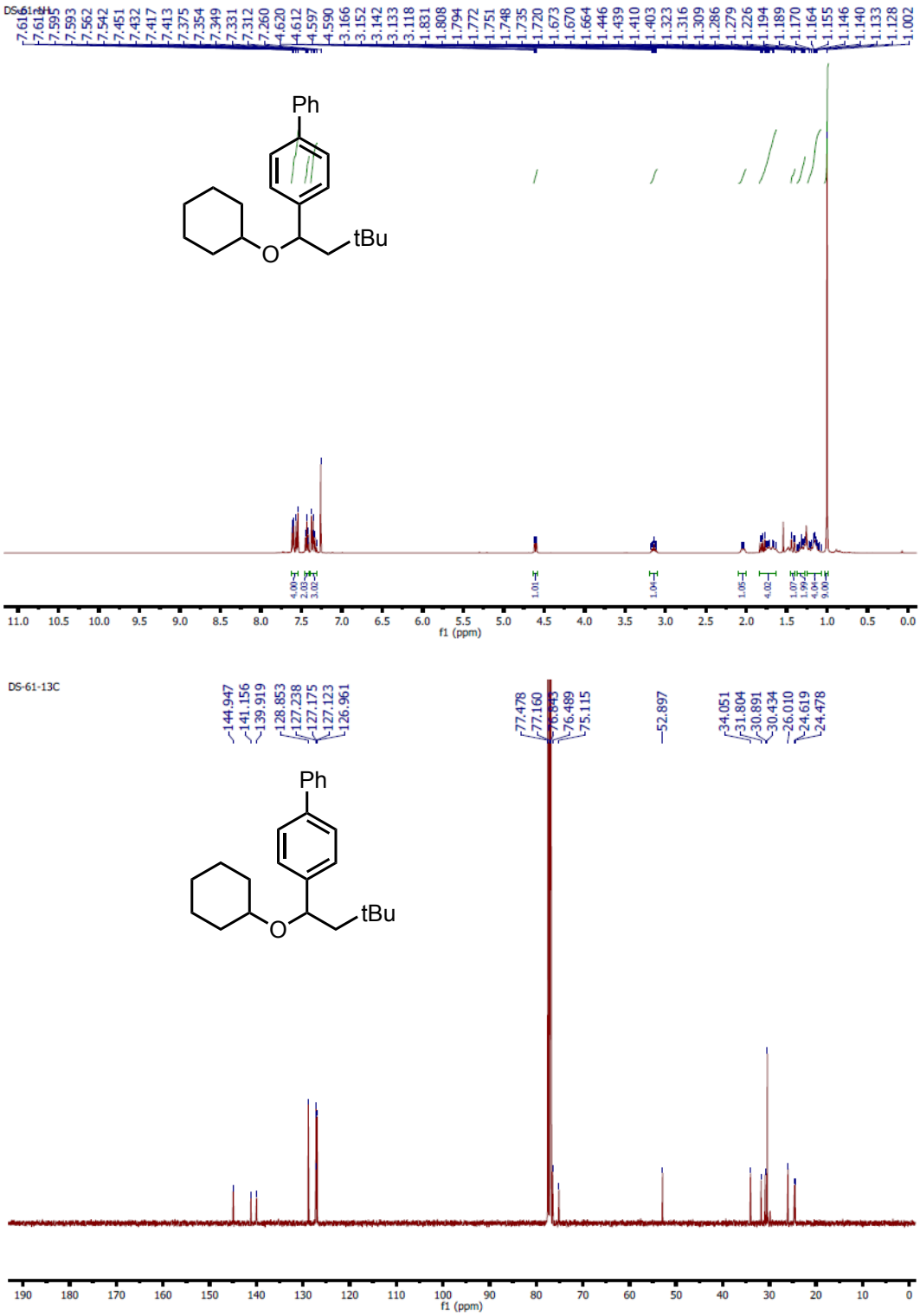


Figure A7.45 Compound 29. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

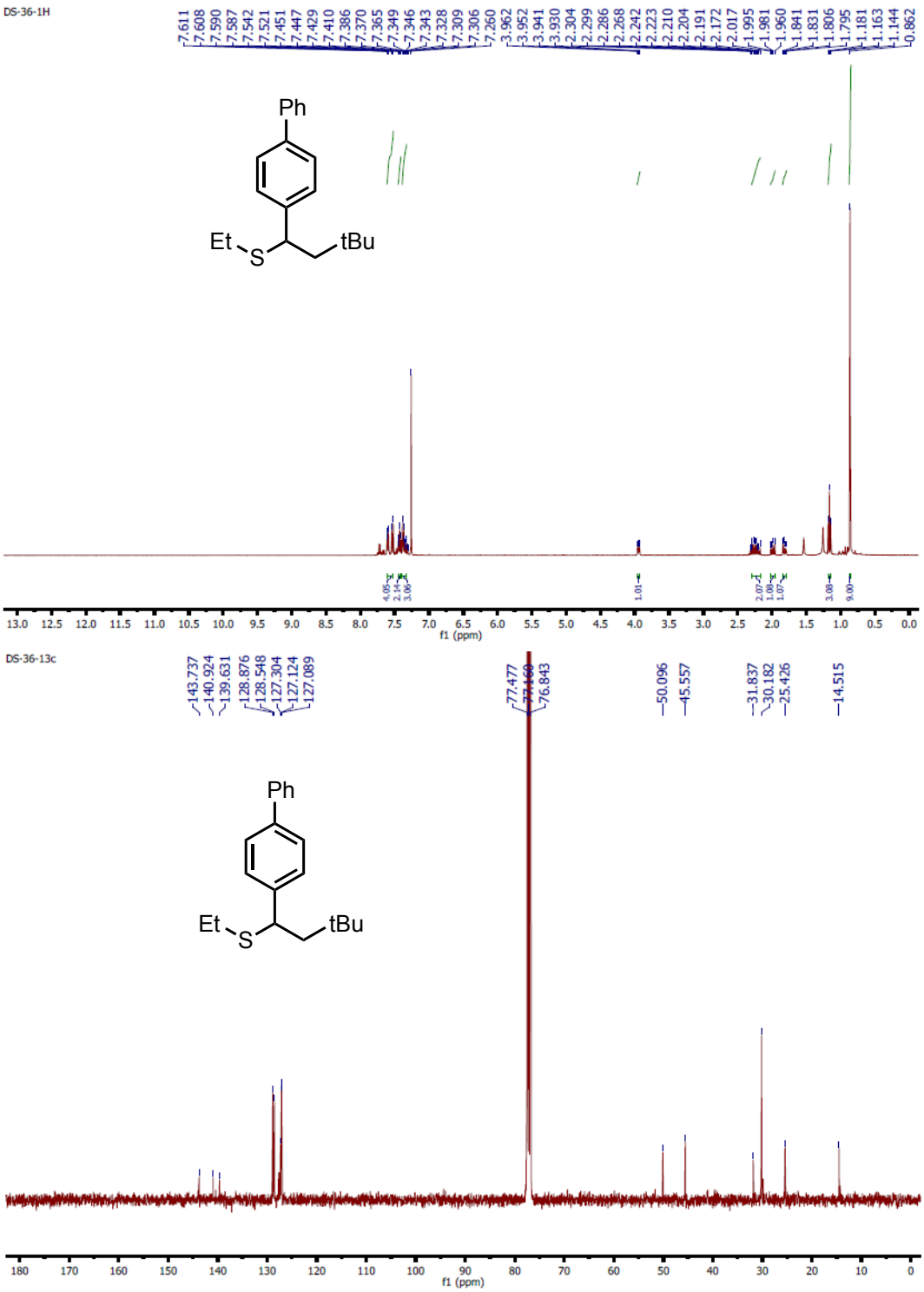


Figure A7.46 Compound 30. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

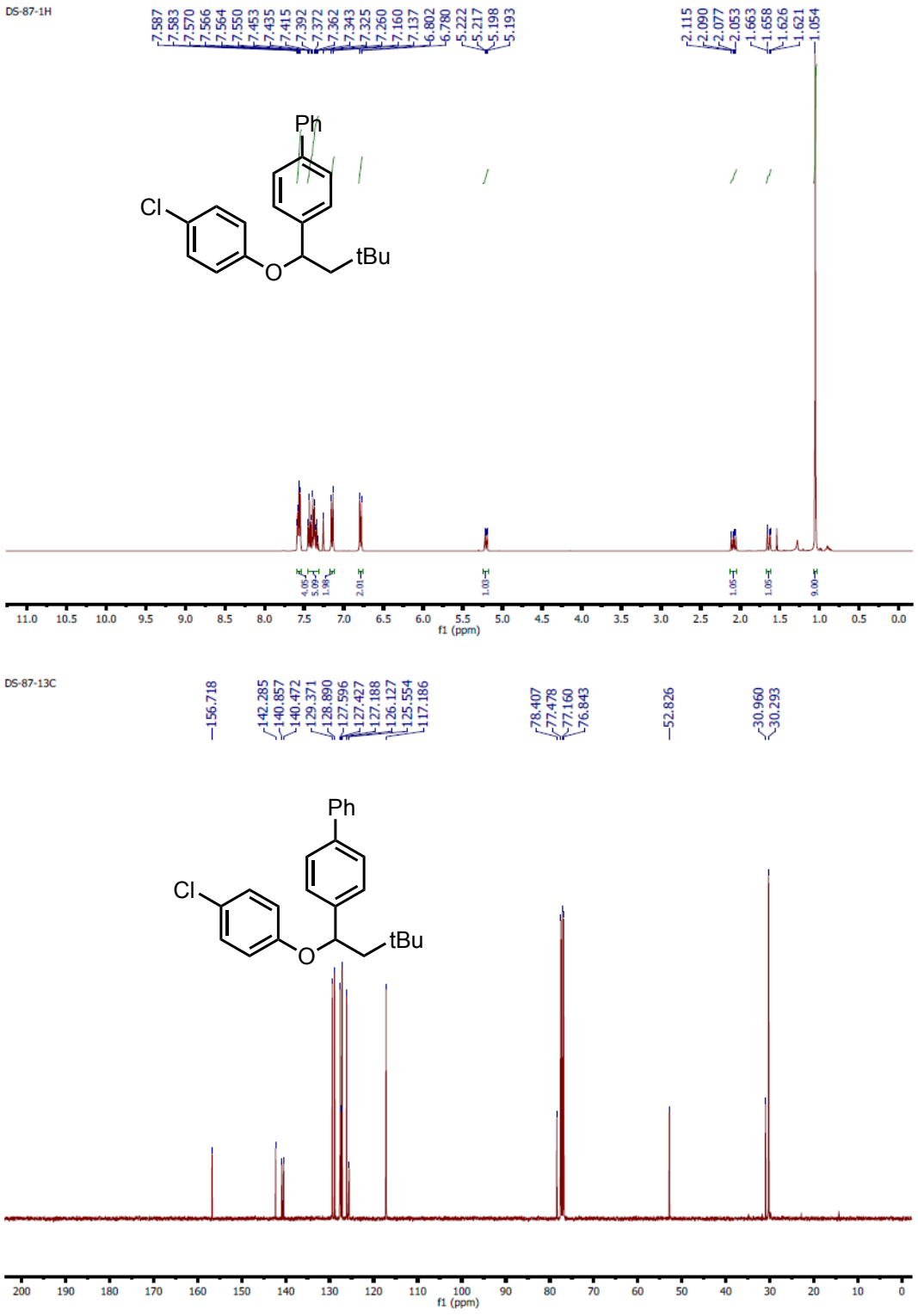


Figure A7.47 Compound 31. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

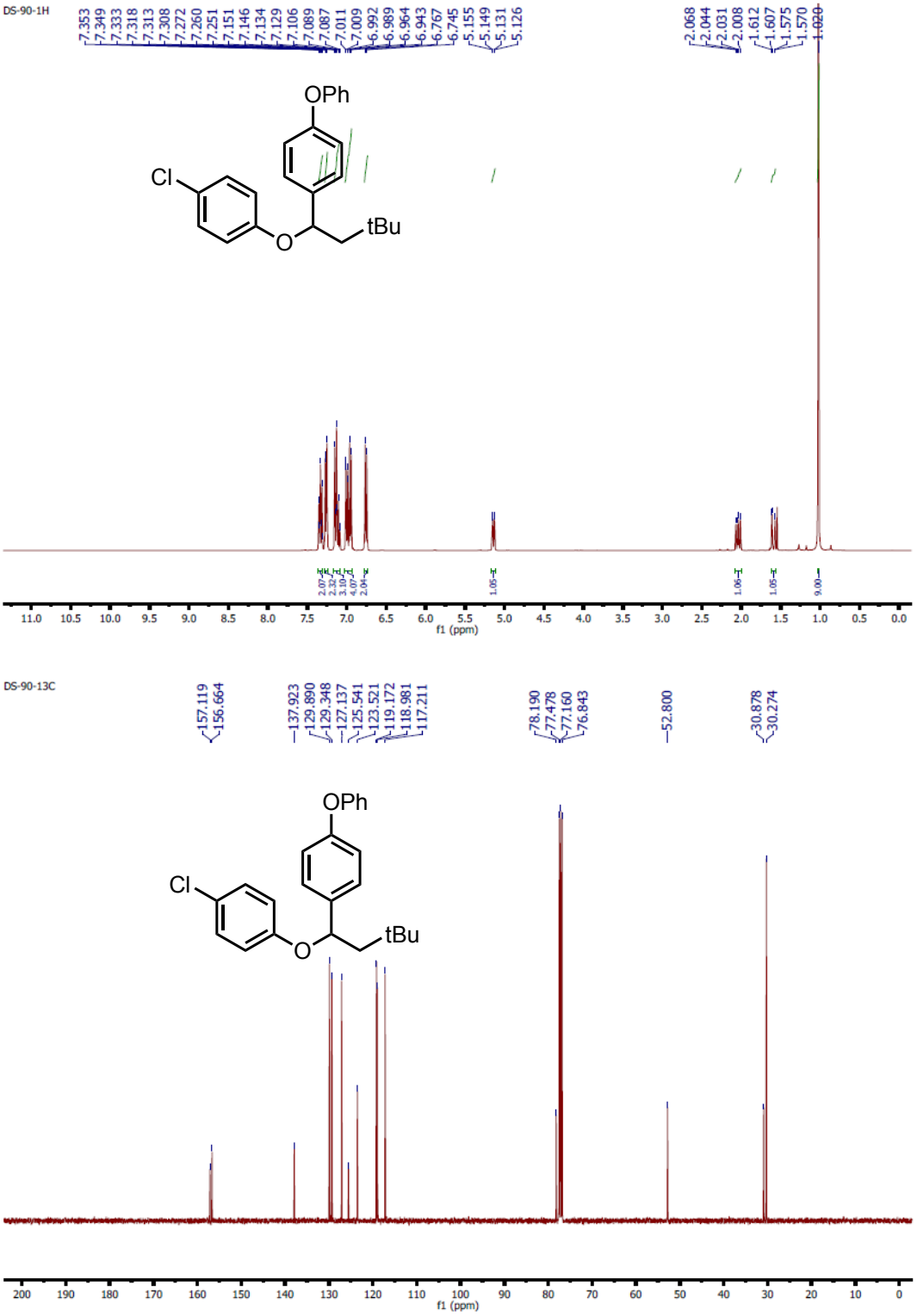


Figure A7.48 Compound 32. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

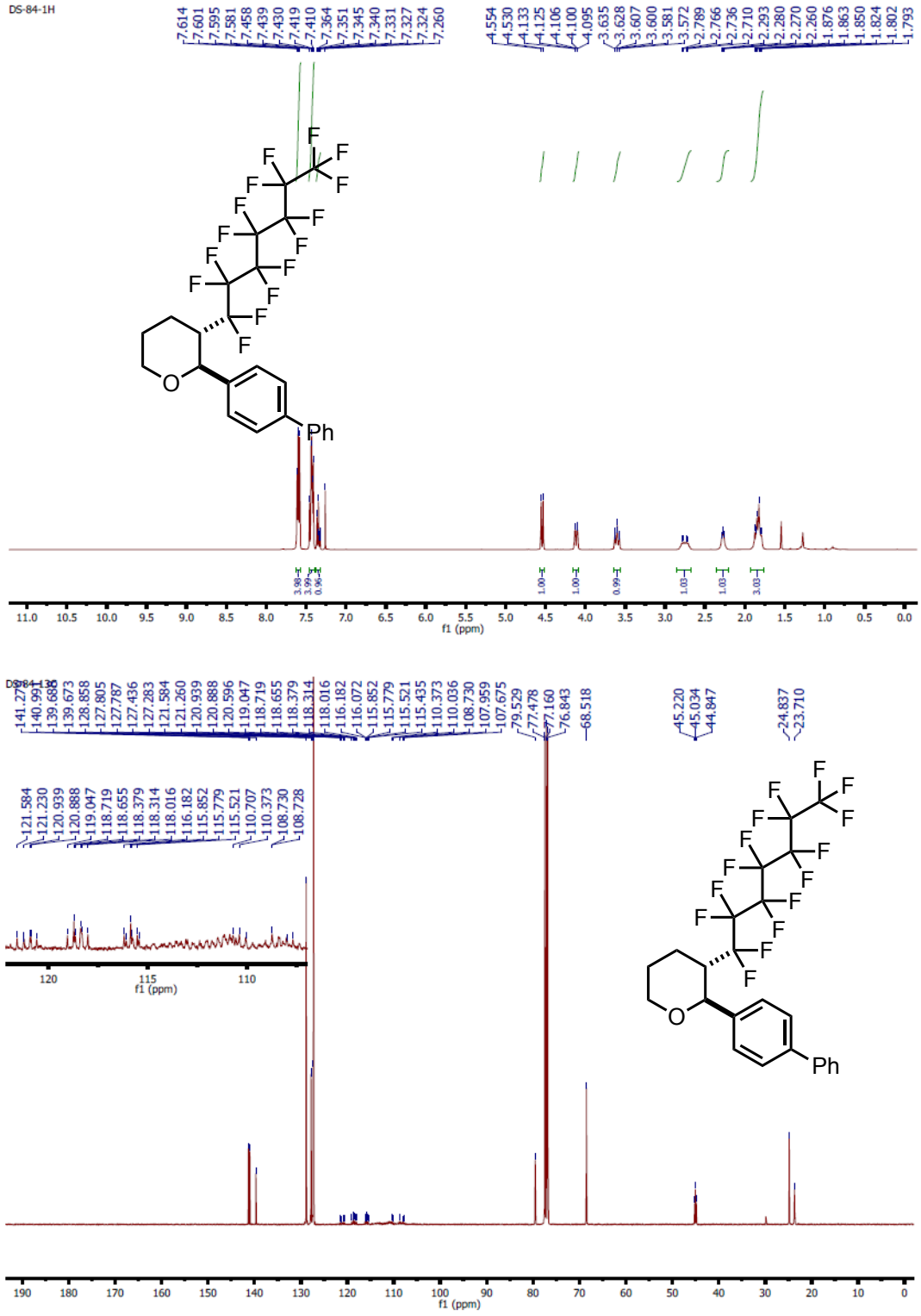
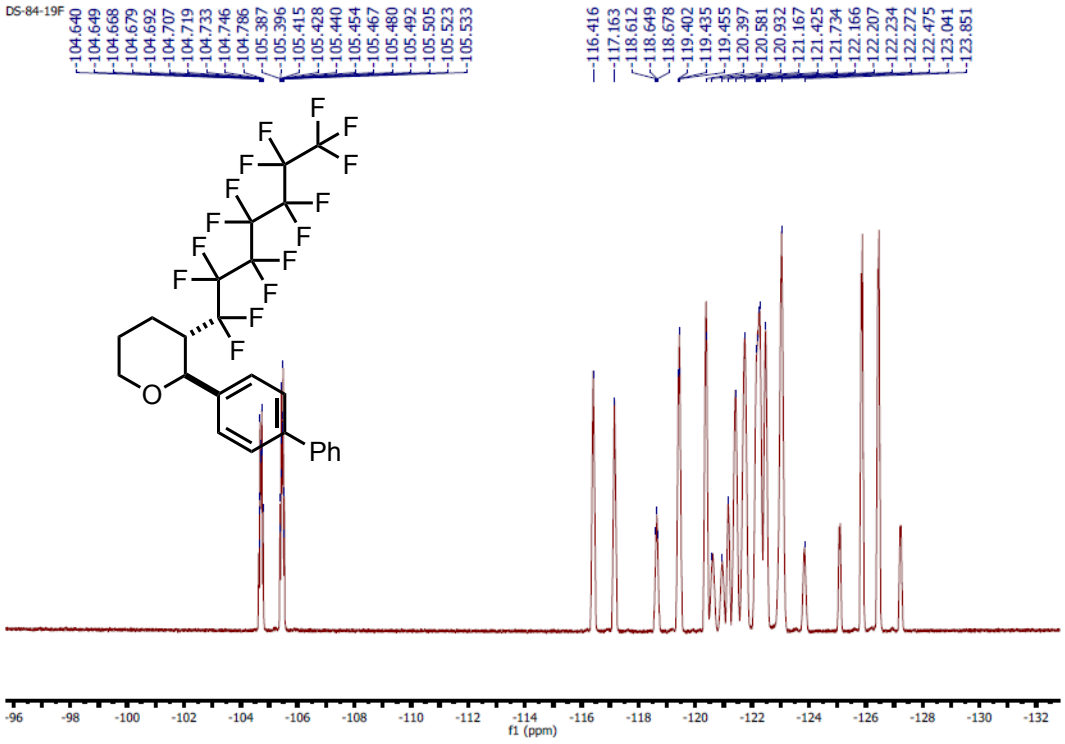
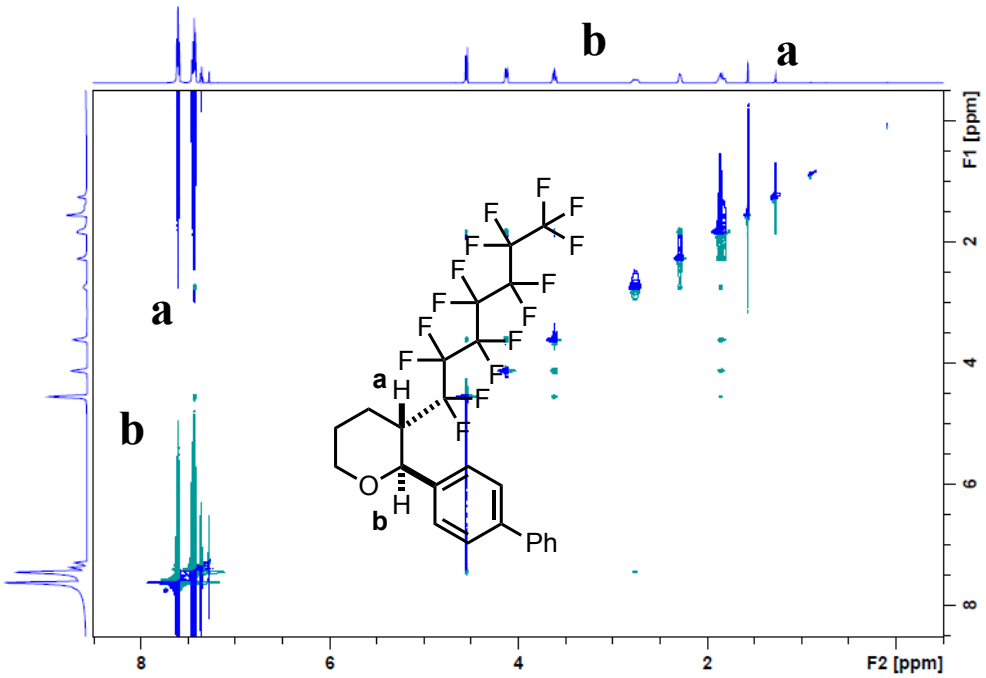


Figure A7.49 Compound 32. Top: ^{19}F NMR ($CDCl_3$, 376 MHz). Bottom: NOESY ($CDCl_3$, 600 MHz)




b
a
a
b
F1 [ppm]
2
4
6
8
8
6
4
2
F2 [ppm]
F
F
F
F
F
F
F
F
F
F
F
F
F
a
H
F
F
O
H
b
Ph

Bibliography

[1] Plietker, B., Ed.; *Iron Catalysis in Organic Chemistry*; Wiley-VCH: Weinheim, Germany 2008.

[2] Bauer, I.; Knölker, H. Iron Catalysis in Organic Synthesis. *Chem. Rev.* **2015**, *115*, 3170 – 3387.

[3] Plietker, B.; Dieskau, A. The Reincarnation of the Hieber Anion $[Fe(CO)3(NO)]^-$ – a New Venue in Nucleophilic Metal Catalysis *Eur. J. Org. Chem.* **2009**, 775.

[4] Bauer, E. B. Recent advances in iron catalysis in organic synthesis. *Curr. Org. Chem.* **2008**, *12*, 1341 – 1369.

[5] Dutch, S. Periodic Tables of Elemental Abundance *J. Chem. Educ.* **1999**, *76*, 356.

[6] a) Quintero-Duque, S.; Dyballa, K. M.; Fleischer, I. Metal-catalyzed carbonylation of alkynes: key aspects and recent development. *Tetrahedron Lett.* **2015**, *56*, 2634 – 2650. b) Millipore Sigma. https://www.sigmaaldrich.com (accessed Nov 29, 2018)

[7] Knölker, H.-J.; Reddy, K. R. Isolation and Synthesis of Biologically Active Carbazole Alkaloids. *Chem. Rev.* **2002**, *102*, 4303 – 4428.

[8] Mahy, J.-P.; Ciesielski, J.; Dauban, P. Catalytic C-H Amination: A Reaction Now Accessible to Engineered Natural Enzymes. *Angew. Chem., Int. Ed.* **2014**, *53*, 6862 – 6864.

[9] The Nobel Prize in Chemistry in 2018 was awarded to Frances Arnold, Greg Winter, and George Smith for their work in directed evolution of enzymes such as cytochrome P450 to catalyze commercially relevant reactions. Prize Announcement In *NobelPrize.org.* Nobel Media AB 2018. https://www.nobelprize.org/prizes/chemistry/2018/summary/ (accessed Dec 4, 2018)

[10] Britovsek, G. J. P.; England, J.; White, A. J. P. Iron(II), manganese(II) and cobalt(II) complexes containing tetradentate biphenyl-bridged ligands and their application in alkane oxidation catalysis. *Dalton Trans.* **2006**, 1399 – 1409.

[11] Fürstner, A. Iron Catalysis in Organic Synthesis: A Critical Assessment of What it Takes to Make this Base Metal a Multitasking Champion. *ACS Cent. Sci.* **2016**, *2*, 778 – 789.

[12] Jové, F. A.; Pariya, C.; Scoblete, M.; Yap, G. P. A; Theopold, K. H. A Family of Four-Coordinate Iron(II) Complexes Bearing the Sterically Hindered Tris(pyrazolyl)borato Ligand $Tp^{tBu,Me.}$ *Chem. Eur. J.* **2011**, *17*, 1310.

[13] Casitas, A.; Krause, H.; Goddard, R.; Fürstner, A. Elementary Steps of Iron Catalysis: Exploring the Links between Iron Alkyl and Iron Olefin Complexes for their Relevance in C-H Activation and C-C Bond Formation. *Angew. Chem., Int. Ed*. **2015**, *54*, 1521 – 1526.

[14] Holland, P. Distinctive Reaction Pathways at Base Metals in High-Spin Organometallic Catalysts. *Acc. Chem. Res.* **2015**, *48*, 1696 – 1702.

[15] White, C. M.; Zhao, J. Aliphatic C–H Oxidations for Late-Stage Functionalization. *J. Am. Chem. Soc.* **2018**, *140*, 13988 – 14009.

[16] a) Chen, M. S.; White, C. M. A Predictably Selective Aliphatic C–H Oxidation Reaction for Complex Molecule Synthesis. *Science* **2007**, *318*, 783 – 787. b) Suzuki. K.; Oldenburg, P. D.; Que, L. Iron-Catalyzed Asymmetric Olefin cis-Dihydroxylation with 97 % Enantiomeric Excess. *Angew. Chem., Int. Ed.* **2008**, *47*, 1887 – 1889.

[17] Gomez, L.; Garcia-Bosch, I.; Company, A.; Benet-Buchholz, J.; Polo, A.; Sala, X.; Ribas, X.; Costas, M. Stereospecific C-H Oxidation with H_2O_2 Catalyzed by a Chemically Robust Site-Isolated Iron Catalyst. *Angew. Chem., Int. Ed*. **2009**, *48*, 5720 – 5723.

[18] Cussó, O.; Cianfanelli, M.; Ribas, X.; Klein Gebbink, R. J. M.; Costas, M. Iron Catalyzed Highly Enantioselective Epoxidation of Cyclic Aliphatic Enones with Aqueous H_2O_2. *J. Am. Chem. Soc.* **2016**, *138*, 2732 – 2738.

[19] a) Brennan, Z. Top-Selling Drugs in 2018: Biosimilar Competition is FDA Approved but Not Marketed. *Regulatory Focus* [Online] 2018 https://www.raps.org/news-and-articles/news-articles/2018/2/top-selling-drugs-in-2018-biosimilar-competition (accessed Dec 23, 2018.) b) Rossiter, K. J. Structure−Odor Relationships. *Chem. Rev.* **1996**, *96*, 3201 – 3240.

[20] Chen, S.; Farina, V. Paclitaxel Structure—Activity Relationships and Core Skeletal Rearrangements. Georg, G. I., Chen, T. T., Ojima, I., Vyas, D. M., Eds.; ACS Symposium Series 583; American Chemical Society: Washington, DC, 1994; p 247 – 261.

[21] White, M. C.; Zhao, J. Aliphatic C−H Oxidations for Late-Stage Functionalization. *J. Am. Chem. Soc.* **2018**, *140*, 13988 – 14009.

[22] Genovino, J.; Lutz, S.; Sames, D.; Touré, B. B. Complementation of Biotransformations with Chemical C–H Oxidation: Copper-Catalyzed Oxidation of Tertiary Amines in Complex Pharmaceuticals *J. Am. Chem. Soc.* **2013**, *135*, 12346 – 12352.

[23] Bergman, R.G. C-H Activation. *Nature* **2007**, *446*, 391 – 393.

[24] Luo, Y.-R.; Cheng, J.-P. Bond Dissociation Energies. In *CRC Handbook of Chemistry and Physics, 99th ed.* (Internet Version 2018)

[25] Yosca, T. H.; Rittle, J.; Krest, C. M.; Onderko, E. L.; Silakov, A.; Calixto, J. C.; Behan, R. K.; Green, M. T. Iron (IV)hydroxide pKa and the Role of Thiolate Ligation in C–H Bond Activation by Cytochrome P450. *Science* **2013**, *342*, 825 – 829.

[26] Chen, K.; Baran, P.S. Total synthesis of eudesmane terpenes by site-selective C–H oxidations. *Nature* **2009**, *459*, 824 – 828.

[27] Gormisky, P. E.; White, C. M. Catalyst-Controlled Aliphatic C–H Oxidations with a Predictive Model for Site-Selectivity. *J. Am. Chem. Soc.* **2013**, *135*, 14052 – 14055.

[28] Feng, Y.; Ke, C.-y.; Xue, G.; Que, L., Jr. Bio-inspired Arene cis-Dihydroxylation by a Non-Heme Iron Catalyst Modeling the Action of Naphthalene Dioxygenase. *Chem. Commun*. **2009**, 50 – 52.

[29] Wackett, L. P. Mechanism and applications of Rieske non-heme iron dioxygenases. *Enzyme Microb. Technol*. **2002**, *31*, 577 – 587.

[30] Knight, P. D.; Scott, P. Predetermination of chirality at octahedral centres with tetradentate ligands: prospects for enantioselective catalysis *Coord. Chem. Rev.,* **2003**, *242*, 125 – 143.

[31] Britovsek, G. J. P.; England, J.; White, A. J. P. Iron(II), manganese(II) and cobalt(II) complexes containing tetradentate biphenyl-bridged ligands and their application in alkane oxidation catalysis. *Dalton Trans.* **2006**, 1399 – 1408.

[32] Hung, K.; Condakes, M. L.; Morikawa, T.; Maimone, T. J. Oxidative Entry into the Illicium Sesquiterpenes: Enantiospecific Synthesis of (+)-Pseudoanisatin. J. *Am. Chem. Soc.* **2016**, *138*, 16616 – 16619.

[33] Nakatsuka, H.; Yamamura, T.; Shuto, Y.; Tanaka, S.; Yoshimura, M.; Kitamura, M. Mechanism of Asymmetric Hydrogenation of Aromatic Ketones Catalyzed by a Combined System of $Ru(\pi\text{-}CH_2C(CH_3)CH_2)_2(cod)$ and the Chiral sp^2N/sp^3NH Hybrid Linear N_4 Ligand Ph-BINAN-H-Py *J. Am. Chem. Soc.* **2015**, *137*, 8138 – 8149.

[34] (a) Chen, M. S.; White, C. M. A Predictably Selective Aliphatic C–H Oxidation Reaction for Complex Molecule Synthesis. *Science* **2007**, *318*, 783 – 787. (b) Gormisky, P. E.; White, C. M. Catalyst-Controlled Aliphatic C–H Oxidations with a Predictive Model for Site-Selectivity. *J. Am. Chem. Soc.* **2013**, *135*, 14052 – 14055. (c) Font D; Canta M; Milan M; Cussó O; Ribas X; Klein Gebbink RJ; Costas M. Readily Accessible Bulky Iron Catalysts exhibiting Site Selectivity in the Oxidation of Steroidal Substrates. Angew. Chem. Int. Ed. **2016**, *55*, 5776 – 5779. (d) Britovsek, G. J. P.; England, J.; White, A. J. P. Iron(II), manganese(II) and cobalt(II) complexes containing tetradentate biphenyl-bridged ligands and their application in alkane oxidation catalysis. *Dalton Trans.* **2006**, 1399 – 1408. (e) Gomez, L.; Garcia-Bosch, I.; Company, A.; Benet-Buchholz, J.; Polo, A.; Sala, X.; Ribas, X.; Costas, M. Stereospecific C-H Oxidation with H_2O_2 Catalyzed by a Chemically Robust Site-Isolated Iron Catalyst. *Angew. Chem., Int. Ed*. **2009**, *48*, 5720 – 5723. (f) Cussó, O.; Garcia-Bosch, I.; Ribas, X.; Lloret-Fillol, J.; Costas, M. Asymmetric Epoxidation with H_2O_2 by Manipulating the Electronic Properties of Non-heme Iron Catalysts. *J. Am. Chem. Soc.* **2013**, *135*, 14871 – 14878. (g) Costas, M. ; Tipton, A. K. ; Chen, K. ; Jo, D. ; Que, L. Modeling Rieske Dioxygenases: The First Example of Iron-Catalyzed Asymmetric cis-Dihydroxylation of Olefins *J. Am. Chem. Soc.* **2001**, *123*, 6722 – 6723.

[35] Ryu, H.; Park, J.; Kim, H. K.; Park, J. Y.; Kim, S.; Baik, M. Pitfalls in Computational Modeling of Chemical Reactions and How to Avoid Them. *Organometallics*, **2018**, *37*, 3228 – 3239. Zhao, Y.; Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.* **2006**, *125*, 194101.

[36] Zhao, Y.; Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.* **2006**, *125*, 194101.

[37] Lawson Daku, L. M. Spin-state dependence of the structural and vibrational properties of solvated iron(II) polypyridyl complexes from AIMD simulations: aqueous [Fe(bpy)3]Cl2, a case study. *Phys. Chem. Chem. Phys*. **2018**, *20*, 6236 – 6253.

[38] Makhlynets, O. V.; Oloo, W. N.; Moroz, Y. S.; Belaya, I. S.; Palluccio, T. D.; Filatov, A. S.; Müller, P.; Cranswick, M. A.; Que, L.; Rybak-Akimova, E. V. H_2O_2 activation with biomimetic non-haem iron complexes and AcOH: connecting the g = 2.7 EPR signal with a visible chromophore. *Chem.Commun.* **2014**, *50*, 645 – 648.

[39] Nakatsuka, H.; Yamamura, T.; Shuto, Y.; Tanaka, S.; Yoshimura, M.; Kitamura, M Mechanism of Asymmetric Hydrogenation of Aromatic Ketones Catalyzed by a Combined System of Ru(π-$CH_2C(CH_3)CH_2)_2$(cod) and the Chiral sp^2N/sp^3NH Hybrid Linear N_4 Ligand Ph-BINAN-H-Py. *J. Am. Chem. Soc.* **2015**, *137*, 8138 – 8149.

[40] Sainna, M. A.; Sil, D.; Sahoo, D.; Martin, B.; Rath, S. P.; Comba, P.; de Visser, P. S. Spin-State Ordering in Hydroxo-Bridged Diiron(III)bisporphyrin Complexes. *Inorg. Chem.* **2015**, *54*, 1919 – 1930.

[41] Kejriwala, A.; Biswasa, S.; Biswasb, A. N.; Bandyopadhyay, P. *cis*-Dihydroxylation of electron deficient olefins catalysed by an oxo-bridged diiron(III) complex with H_2O_2. *J. Mol. Catal. A: Chem.* **2016**, *413*, 77 – 84.

[42] Goodson, P. A.; Oki, A. R.; Glerup, J.; Hodgson, D. J. Design, synthesis, and characterization of bis(μ-oxo)dimanganese(III,III) complexes. Steric and electronic control of redox potentials. *J. Am. Chem. Soc*. **1990**, *112*, 6248 – 6254.

[43] Evans, D. A. The determination of the paramagnetic susceptibility of substances in solution by nuclear magnetic resonance. *J. Chem. Soc.* **1959**, 2003 – 2005.

[44] Eckert, H. Structural Studies of Noncrystalline Solids Using Solid State NMR. New Experimental Approaches and Results. In *Solid-State NMR IV Methods and Applications of Solid-State NMR.* Blümich, B., Ed.; Springer, Berlin, Heidelberg,1994.

[45] Gómez, L.; Garcia-Bosch, I.; Company, A.; Benet-Buchholz, J.; Polo, A.; Sala, X.; Ribas, X.; Costas, M. Stereospecific C-H Oxidation with H_2O_2 Catalyzed by a Chemically Robust Site-Isolated Iron Catalyst. *Angew. Chem. Int. Ed.* **2009**, *48*, 5720 – 5723.

[46] Rotella, M. E.; Dyer, R. M. B.; Hilinski, M. K.; Gutierrez, O. Mechanism of Iminium Salt-Catalyzed C(sp^3)-H Amination: Factors Controlling Hydride Transfer versus H-atom Abstraction. *ACS Catal.* **2020**, *10,* 897 – 906.

[47] Vitaku, E.; Smith, D. T.; Njardarson, J. T. Analysis of the Structural Diversity, Substitution Patterns, and Frequency of Nitrogen Heterocycles Among U.S. FDA Approved Pharmaceuticals. *J. Med. Chem.* **2014**, *57*, 10257−10274.

[48] Blakemore, D. C.; Castro, L.; Churcher, I.; Rees, D. C.; Thomas, A. W.; Wilson, D. M.; Wood, A. Organic Synthesis Provides Opportunities to Transform Drug Discovery. *Nat. Chem.* **2018**, *10*, 383−394.

[49] Park, Y.; Kim, Y.; Chang, S. Transition Metal-Catalyzed C-H Amination: Scope, Mechanism, and Applications. *Chem. Rev.* **2017**, *117*, 9247−9301.

[50] For representative recent examples see: (a) Clark, J. R.; Feng, K.; Sookezian, A.; White, M. C. Manganese-Catalysed Benzylic C(sp^3)− H Amination for Late-Stage Functionalization. *Nat. Chem.* **2018**, *10*, 583−591. (b) Chiappini, N. D.; Mack, J. B. C.; Du Bois, J. Intermolecular C(sp^3)−H Amination of Complex Molecules. *Angew. Chem., Int. Ed.* **2018**, *130*, 5050−5053. (c) Prier, C. K.; Zhang, R. K.; Buller, A. R.; Brinkmann-Chen, S.; Arnold, F. H. Enantioselective, Intermolecular Benzylic C-H Amination Catalysed by an Engineered Iron-Haem Enzyme. *Nat. Chem.* **2017**, *9*, 629−634. (d) Dolan, N. S.; Scamp, R. J.; Yang, T.; Berry, J. F.; Schomaker, J. M. Catalyst- Controlled and Tunable, Chemoselective Silver-Catalyzed Intermo- lecular Nitrene Transfer: Experimental and Computational Studies. *J. Am. Chem. Soc.* **2016**, *138*, 14658−14667. (e) Bess, E. N.; DeLuca, R. J.; Tindall, D. J.; Oderinde, M. S.; Roizen, J. L.; Du Bois, J.; Sigman, M. S. Analyzing Site Selectivity in $Rh_2(esp)_2$-Catalyzed Intermolecular C−H Amination Reactions. *J. Am. Chem. Soc.* **2014**, *136*, 5783−5789. (f) Roizen, J. L.; Zalatan, D. N.; Du Bois, J. Selective Intermolecular Amination of C-H Bonds at Tertiary Carbon Centers. *Angew. Chem., Int. Ed.* **2013**, *52*, 11343−11346.

[51] Hazelard, D.; Nocquet, P.-A.; Compain, P. Catalytic C−H Amination at Its Limits: Challenges and Solutions. *Org. Chem. Front.* **2017**, *4,* 2500−2521.

[52] Johnson, S. L.; Combee, L. A.; Hilinski, M. K. Organocatalytic Atom-Transfer C(sp^3)−H Oxidation. *Synlett* **2018**, *29*, 2331−2336.

[53] Combee, L. A.; Raya, B.; Wang, D.; Hilinski, M. K. Organocatalytic Nitrenoid Transfer: Metal-Free Selective Intermolecular C(sp^3)−H Amination Catalyzed by an Iminium Salt. *Chem. Sci*. **2018**, *9*, 935−939.

[54] Johnson, S. L.; Hilinski, M. K. Organocatalytic Olefin Aziridination via Iminium-Catalyzed Nitrene Transfer: Scope, Limitations, and Mechanistic Insight. *J. Org. Chem.* **2019**, *84*, 8589−8595.

[55] Allen, J. M.; Lambert, T. H. Synthesis and Characterization of a Diaziridinium Ion. Conversion of 3,4-Dihydroisoquinolines to 4,5- Dihydro-3H-Benzo[2,3]Diazepines via a Formal N-Insertion Process. *Tetrahedron* **2014**, *70*, 4111−4117.

[56] (a) Lusinchi, X.; Hanquet, G. Oxygen transfer reactions from an Oxaziridinium tetrafluoroborate salt to Olefins. *Tetrahedron* **1997**, *53*, 13727−13738. (b) Hanquet, G.; Lusinchi, X.; Milliet, P. Transfert d'oxygene sur la double liaison ethylenique a partir d'un sel d'oxaziridinium. *Tetrahedron Lett.* **1988**, *29*, 3941−3944. (c) Bohe, L.; Hanquet, G.; Lusinchi, M.; Lusinchi, X. The stereospecific synthesis of a new chiral oxaziridinium salt. *Tetrahedron Lett.* **1993**, *34*, 7271−7274. Bohe, L.; Lusinchi, M.; Lusinchi, X. Oxygen atom transfer from a chiral oxaziridinium salt. Asymmetric epoxidation of unfunctionalized olefins. *Tetrahedron* **1999**, *55*, 141−154. (d) Aggarwal, V. K.; Wang, M. F. Catalytic asymmetric synthesis of epoxides mediated by chiral iminium salts. *Chem. Commun.* **1996**, 191−192. (e) Armstrong, A.; Ahmed, G.; Garnett, I.; Goacolou, K. Pyrrolidine- Derived Iminium Salts as Catalysts for Alkene Epoxidation by Oxone. *Synlett.* **1997**, 1075−1076. (f) Bulman Page, P. C.; Rassias, G. A.; Bethell, D.; Schilling, M. B. A New System for Catalytic Asymmetric Epoxidation Using Iminium Salt Catalysts. *J. Org. Chem.* **1998**, *63*, 2774−2777.

[57] Skyner, R. E.; McDonagh, J. L.; Groom, C. R.; van Mourik, T.; Mitchell, J. B. O. A review of methods for the calculation of solution free energies and the modelling of systems in solution. *Phys. Chem. Chem. Phys.,* **2015**, *17*, 6174-6191.

[58] (a) Lam, J. K.; Pham, H. V.; Houk, K. N.; Vanderwal, C. D. Computation and Experiment Reveal That the Ring-Rearrangement Metathesis of Himbert Cycloadducts Can Be Subject to Kinetic or Thermodynamic Control. *J. Am. Chem. Soc.* **2013**, *135*, 17585-17594. (b) Otsuka, M.; Tsuchida, N.; Ikeda, Y.; Kimura, Y.; Mutoh, Y.; Ishii, Y.; Takano, K. DFT Study of Internal Alkyne-to-Disubstituted Vinylidene Isomerization in [CpRu(PhC≡CAr)(dppe)]+ *J. Am. Chem. Soc.* **2012**, *134*, 17746-17756. (c) Haynes, M. T.; Liu, P.; Baxter, R. D.; Nett, A. J. Houk, K. N.; Montgomery, J. Dimer Involvement and Origin of Crossover in Nickel-Catalyzed Aldehyde–Alkyne Reductive Couplings. *J. Am. Chem. Soc.* **2014**, *136*, 17495-17504. (d) Gao, T.; Zhang, W.; Sun, X.; Lu, H.; Li, B. Stereodivergent Synthesis through Catalytic Asymmetric Reversed Hydroboration. *J. Am. Chem. Soc.* **2019**, *141*, 4670-4677.

(e) Wang, Z.; Li, B. Construction of Acyclic Quaternary Carbon Stereocenters by Catalytic Asymmetric Hydroalkynylation of Unactivated Alkenes. *J. Am. Chem. Soc.* **2019**, *141*, 9312-9320. (f) Wang, H.; Lu, G.; Sormunen, G. J.; Malik, H. A.; Liu, P.; Montgomery, J. NHC Ligands Tailored for Simultaneous Regio- and Enantiocontrol in Nickel-Catalyzed Reductive Couplings. *J. Am. Chem. Soc.* **2017**, *139*, 9317-9324. (g) Orlandi, M.; Hilton, M. J.; Yamamoto, E.; Toste, F. D.; Sigman, M. S. Mechanistic Investigations of the Pd(0)-Catalyzed Enantioselective 1,1- Diarylation of Benzyl Acrylates. *J. Am. Chem. Soc.* **2017**, *139*, 12688-12695.

[59] Vogiatzis, K. D.; Polynski, M. V.; Kirkland, J. K.; Townsend, J.; Hashemi, A.; Liu, C.; Pidko, E. A. Computational Approach to Molecular Catalysis by 3d Transition Metals: Challenges and Opportunities. *Chem. Rev.* **2019**, *119*, 2453-2523.

[60] Takano, Y.; Houk, K. N. Benchmarking the Conductor-like Polarizable Continuum Model (CPCM) for Aqueous Solvation Free Energies of Neutral and Ionic Organic Molecules. *J. Chem. Theory Comput.* **2005**, *1*, 70-77.

[61] (a) Al-Bataineh, N.; Houk, K. N.; Brewer, M.; Hong, X. (2+1)-Cycloaddition Reactions Give Further Evidence of the Nitrenium-like Character of 1-Aza-2-azoniaallene Salts. *J. Org. Chem.* **2017**, *82*, 4001−4005. (b) Cleary, S. E.; Li, X.; Yang, L.-C.; Houk, K. N.; Hong, X.; Brewer, M. Reactivity Profiles of Diazo Amides, Esters, and Ketones in Transition-Metal-Free C−H Insertion Reactions. *J. Am. Chem. Soc.* **2019**, *141*, 3558−3565. (c) Zhu, C.; Liang, Y.; Hong, X.; Sun, H.; Sun, W.-Y.; Houk, K. N.; Shi, Z. Iodoarene-Catalyzed Stereospecific Intramolecular sp^3 C−H Amination: Reaction Development and Mechanistic Insights. *J. Am. Chem. Soc.* **2015**, *137*, 7564− 7567.

[62] Issues do exist with single reference formalism in modeling these nitrenium species. However, for this study, multireference calculations (e.g., CASPT2/ CASSCF) were not used due to the prohibitively high computational cost associated with these types of calculations in such a complex mechanism. Furthermore, studies by Winter in which both DFT and CASPT2 were used to model open-shell species and the trends predicted by DFT methods agree with multireference methods although the calculated singlet-triplet energy gap differs by 2-4 kcal/mol depending on the method from experiment. For further discussion of this topic, refer to the following. (a) Winter, A. H.; Falvey, D. E.; Cramer, C. J.; Gherman, B. F. Benzylic Cations with Triplet Ground States: Computational Studies of Aryl Carbenium Ions, Silylenium Ions, Nitrenium Ions, and Oxenium Ions Substituted with Meta π Donors. *J. Am. Chem. Soc.* **2007**, *129*, 10113−10119.

(b) Albright, T. R.; Winter, A. H. A Fine Line Separates Carbocations from Diradical Ions in Donor-Unconjugated Cations. *J. Am. Chem. Soc.* **2015**, *137*, 3402− 3410. (c) Cramer, C. J.; Dulles, F. J.; Falvey, D. E. Ab Initio Characterization of Phenylnitrenium and Phenylcarbene: Remarkably Different Properties for Isoelectronic Species. *J. Am. Chem. Soc.* **1994**, *116*, 9787−9788. (d) Cramer, C. J.; Truhlar, D. G.; Falvey, D. E. Singlet−Triplet Splittings and 1,2-Hydrogen Shift Barriers for Methylphenylborenide, Methylphenylcarbene, and Methylphenylni- trenium in the Gas Phase and Solution. What a Difference a Charge Makes. *J. Am. Chem. Soc.* **1997**, *119*, 12338−12342. (e) Geise, C. M.; Hadad, C. M. Computational Study of the Electronic Structure of Substituted Phenylcarbene in the Gas Phase. *J. Org. Chem.* **2000**, *65*, 8348−8356. (f) McIlroy, S.; Cramer, C. J.; Falvey, D. E. Singlet− Triplet Energy Gaps in Highly Stabilized Nitrenium Ions: Experimental and Theoretical Study of 1,3-Dimethylbenzotriazolium Ion. *Org. Lett.* **2000**, *2*, 2451−2454. (g) Trindle, C. DFT Studies of Biarylcarbenes and the Carbene−Biradical Continuum. *Org. Chem.* **2003**, *68*, 9669−9677.

[63] Kuzmanich, G.; Spañig, F.; Tsai, C. K.; Um, J. M.; Hoekstra, R. M.; Houk, K. N.; Guldi, D. M.; Garcia-Garibay, M. A. Oxyallyl Exposed: An Open-Shell Singlet with Picosecond Lifetimes in Solution but Persistent in Crystals of a Cyclobutanedione Precursor. *J. Am. Chem. Soc*. **2011**, *133*, 2342−2345.

[64] Gassman, P. G. Nitrenium Ions. *Acc. Chem. Res.* **2002**, *3*, 26− 33.

[65] Hamlin, T. A.; Kelly, C. B.; Ovian, J. M.; Wiles, R. J.; Tilley, L. J.; Leadbeater, N. E. Toward a Unified Mechanism for Oxoammonium Salt-Mediated Oxidation Reactions: A Theoretical and Experimental Study Using a Hydride Transfer Model. *J. Org. Chem.* **2015**, *80*, 8150−8167.

[66] Singleton, D. A.; Wang, Z. Isotope Effects and the Nature of Enantioselectivity in the Shi Epoxidation. The Importance of Asynchronicity. *J. Am. Chem. Soc.* **2005**, *127*, 6679−6685.

[67] Shen, G.-B.; Xia, K.; Li, X.-T.; Li, J.-L.; Fu, Y.-H.; Yuan, L.; Zhu, X.-Q. Predicition of Kinetic Isotope Effects for Various Hydride Transfer Reactions Using a New Kinetic Model. *J. Phys. Chem. A* **2016**, *120*, 1779−1799.

[68] Braun, M.; Doyle, A. G. Palladium-Catalyzed C-H Allylic Fluorination. *J. Am. Chem. Soc.* **2013**, *135*, 12990−12993.

[69] Zhu, Y.; Han, J.; Wang, J.; Shibata, N.; Sodeoka, M.; Soloshonok, V. A.; Coelho, J. A. S.; Toste, F. D. Modern Approaches for Asymmetric Construction of Carbon-Fluorine Quaternary Stereogenic Centers: Synthetic Challenges and Pharmaceutical Needs. *Chem. Rev.* **2018**, *118*, 3887−3964.

[70] Braun, M.; Doyle, A. G. Palladium-Catalyzed Allylic C-H Fluorination. *J. Am. Chem. Soc.* **2013**, *135*, 12990 – 12993.

[71] (a) Hollingworth, C.; Hazari, A.; Hopkinson, M. N.; Tredwell, M.; Benedetto, E.; Huiban, M.; Gee, A. D.; Brown, J. M.; Gouverneur, V. Palladium-Catalyzed Allylic Fluorination. *Angew. Chem., Int. Ed.* **2011**, *50*, 2613−2617. (b) Benedetto, E.; Tredwell, M.; Hollingworth, C.; Khotavivattana, T.; Brown, J. M.; Gouverneur, V. *Chem. Sci.* **2013**, *4*, 89−96.

[72] Lauer, A. M.; Wu, J. Pd-Catalyzed Allylic Fluorination of Cinnamyl Phosphorothioate Esters. *Org. Lett.* **2012**, *14*, 5138−5141.

[73] Zhang, Z.; Wang, F.; Mu, X.; Chen, P.; Liu, G. Copper-Catalyzed Regioselective Fluorination of Allylic Halides. *Angew. Chem., Int. Ed.* **2013**, *52*, 7549−7553.

[74] Sorlin, A. M.; Fuad, U. O.; English, C. K.; Nguyen, H. M. Advances in Nucleophilic Allylic Fluorination. *ACS Catal.* **2020***, 10,* 11980-12010.

[75] Hollingworth, C.; Hazari, A.; Hopkinson, M. N.; Tredwell, M.; Benedetto, E.; Huiban, M.; Gee, A. D.; Brown, J. M.; Gouverneur, V. Palladium-Catalyzed Allylic Fluorination. *Angew. Chem., Int. Ed.* **2011**, *50*, 2613−2617.

[76] Benedetto, E.; Tredwell, M.; Hollingworth, C.; Khotavivattana, T.; Brown, J. M.; Gouverneur, V. Regio- and stereoretentive synthesis of branched, linear (E)- and (Z)-allyl fluorides from allyl carbonates under Ir-catalysis. *Chem. Sci.* **2013**, *4*, 89−96.

[77] Lauer, A. M.; Wu, J. Palladium-Catalyzed Allylic Fluorination of Cinnamyl Phosphorothioate Esters. *Org. Lett.* **2012**, *14*, 5138−5141.

[78] Braun, M. G.; Katcher, M. H.; Doyle, A. G. Carbofluorination via a palladium-catalyzed cascade reaction. *Chem. Sci.* **2013**, *4,* 1216−1220.

[79] Zhang, Q.; Nguyen, H. M. Rhodium-catalyzed regioselective opening of vinyl epoxides with Et3N·3HF reagent − formation of allylic fluorohydrins. *Chem. Sci*. **2014**, *5*, 291−296.

[80] Braun, M.-G.; Doyle, A. G. Palladium-Catalyzed Allylic C−H Fluorination. *J. Am. Chem. Soc.* **2013**, *135*, 12990−12993.

[81] Zhang, Z.; Wang, F.; Mu, X.; Chen, P.; Liu, G. Copper-Catalyzed Regioselective Fluorination of Allylic Halides. *Angew. Chem. Int. Ed.* **2013**, *52*, 7549−7553.

[82] Katcher, M. H.; Doyle, A. G. Palladium-Catalyzed Asymmetric Synthesis of Allylic Fluorides. *J. Am. Chem. Soc.* **2010**, *132*, 17402−17404.

[83] Katcher, M. H.; Sha, A.; Doyle, A. G. Palladium-Catalyzed Regio and Enantioselective Fluorination of Acyclic Allylic Halides. *J. Am. Chem. Soc*. **2011**, *133*, 15902−15905.

[84] Zhu, J.; Tsui, G. C.; Lautens, M. Rhodium-Catalyzed Enantioselective Nucleophilic Fluorination: Ring Opening of Oxabicyclic Alkenes. *Angew. Chem. Int. Ed.* **2012**, *51*, 12353−12356.

[85] Zhang, Q.; Stockdale, D. P.; Mixdorf, J. C.; Topczewski, J. J.; Nguyen, H. M. Iridium-Catalyzed Enantioselective Fluorination of Racemic, Secondary Allylic Trichloroacetimidates. *J. Am. Chem. Soc.* **2015**, *137*, 11912−11915.

[86] (a) Schmidt, R. R.; Michel, J. Facile Synthesis of α- and β-O-Glycosyl Imidates; Preparation of Glycosides and Disaccharides. *Angew. Chem. Int. Ed. Engl.* **1980**, *19*, 731−732. (b) Schmidt, R. R. New Methods for the Synthesis of Glycosides and Oligosaccharides - Are There Alternatives to the Koenigs-Knorr Method? [New Synthetic Methods (56)]. *Angew. Chem., Int. Ed. Engl.* **1986**, *25*, 212−235. (c) Schmidt, R. R.; Zhu, X. Glycosyl Trichloroacetimidates. In Glycoscience: Chemistry and Chemical Biology; Fraser-Reid, B. O., Tatsuta, K., Thiem, J., Eds.; Springer: Berlin, Heidelberg, 2008; pp 451−524.

[87] (a) Overman, L. E. Thermal and mercuric ion catalyzed [3,3]-sigmatropic rearrangement of allylic trichloroacetimidates. 1,3 Transposition of alcohol and amine functions. *J. Am. Chem. Soc.* **1974**, *96*, 597−599. (b) Anderson, C. E.; Overman, L. E. Catalytic Asymmetric Rearrangement of Allylic Trichloroacetimidates. A Practical Method for Preparing Allylic Amines and Congeners of High Enantiomeric Purity. *J. Am. Chem. Soc.* **2003**, *125*, 12412−12413.

[88] Mixdorf, J. C.; Sorlin, A. M.; Zhang, Q.; Nguyen, H. M. Asymmetric Synthesis of Allylic Fluorides via Fluorination of Racemic Allylic Trichloroacetimidates Catalyzed by a Chiral Diene-Iridium Complex. *ACS Catal.* **2018**, *8*, 790−801.

[89] Zhang, Q.; Stockdale, D. P.; Mixdorf, J. C.; Topczewski, J. J.; Nguyen, H. M. Iridium-Catalyzed Enantioselective Fluorination of Racemic, Secondary Allylic Trichloroacetimidates. *J. Am. Chem. Soc.* **2015**, *137*, 11912−11915.

[90] Sorlin, A. M., Mixdorf, J. C., Rotella, M. E., Martin, R. T., Gutierrez, O., Nguyen, H. T. The Role of Trichloroacetimidate to Enable Iridium-Catalyzed Regio and Enantioselective Allylic Fluorination: A Combined Experimental and Computational Study. *J. Am. Chem. Soc.* **2019**, *141*, 14843−14852.

[91] (a) Butt, N. A.; Zhang, W. Transition metal-catalyzed allylic substitution reactions with unactivated allylic substrates. *Chem. Soc. Rev.* **2015**, *44*, 7929−7967. (b) Trost, B. M.; Crawley, M. L. Asymmetric Transition-Metal-Catalyzed Allylic Alkylations: Applications in Total Synthesis. *Chem. Rev.* **2003**, *103*, 2921−2944. (c) Trost, B. M.; Van Vranken, D. L. Asymmetric Transition Metal-Catalyzed Allylic Alkylations. *Chem. Rev.* **1996**, *96*, 395−422. (d) Gansäuer, A.; Justicia, J.; Rosales, A.; Worgull, D.; Rinker, B.; Cuerva, J. M.; Oltra, J. E. Transition-Metal-Catalyzed Allylic Substitution and Titanocene-Catalyzed Epoxypolyene Cyclization as a Powerful Tool for the Preparation of Terpenoids. *Eur. J. Org. Chem.* **2006**, *2006*, 4115−4127. (e) Katcher, M. H.; Norrby, P. O.; Doyle, A. G. Mechanistic Investigations of Palladium-Catalyzed Allylic Fluorination. *Organometallics* **2014**, 33, 2121−2133. (f) Hayashi, T.; Kawatsura, M.; Uozumi, Y. Regio- and enantioselective allylic alkylation catalyzed by a chiral monophosphine−palladium complex. *Chem. Commun.* **1997**, *6*, 561−562. (g) Helmchen, G.; Pfaltz, A. Phosphinooxazolines: A New Class of Versatile, Modular P,N-Ligands for Asymmetric Catalysis. *Acc. Chem. Res.* **2000**, *33*, 336−345. (h) Aakermark, B.; Vitagliano, A. Reactivity and syn-anti isomerization of (.eta.3-geranyl)- and (.eta.3-neryl)palladium complexes. Evidence for electronic control of the regiochemistry of nucleophilic addition. *Organometallics* **1985**, *4*, 1275−1283. (i) Trost, B. M.; Dietsche, T. J.; Fullerton, T. J. New synthetic reactions. Chemospecificity of allylic alkylation. *J. Org. Chem.* **1974**, *39*, 737−738. (j) Madrahimov, S. T.; Hartwig, J. F. Origins of Enantioselectivity during Allylic Substitution Reactions Catalyzed by Metallacyclic Iridium Complexes. *J. Am. Chem. Soc*. **2012**, *134*, 8136−8147.

[92] Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. *J. Comput. Chem.* **2003**, *24*, 669−681.

[93] Takano, Y.; Houk, K. N. Benchmarking the Conductor-like Polarizable Continuum Model (CPCM) for Aqueous Solvation Free Energies of Neutral and Ionic Organic Molecules. *J. Chem. Theory Comput.* **2005**, *1*, 70−77.

[94] Hay, P. J.; Wadt, W. R. Ab initio effective core potentials for molecular calculations. Potentials for the transition metal atoms Sc to Hg. J. *Chem. Phys.* **1985**, *82*, 270−283.

[95] Wadt, W. R.; Hay, P. J. Ab initio effective core potentials for molecular calculations. Potentials for main group elements Na to Bi. *J. Chem. Phys.* **1985**, *82*, 284−298.

[96] Hay, P. J.; Wadt, W. R. Ab initio effective core potentials for molecular calculations. Potentials for K to Au including the outermost core orbitals. *J. Chem. Phys.* **1985**, *82*, 299−310.

[97] Sperger, T.; Sanhueza, I. A.; Kalvet, I.; Schoenebeck, F. Computational Studies of Synthetically Relevant Homogeneous Organometallic Catalysis Involving Ni, Pd, Ir, and Rh: An Overview of Commonly Employed DFT Methods and Mechanistic Insights. *Chem. Rev.* **2015**, *115*, 9532−9586.

[98] Similarly, a preference for bidentate coordination was also observed with use of both allylic (R)- and (S)-trichloroacetimidate substrates using chiral (S,S)-diene ligand **5** (see **Figure A3.1** in Appendix 3).

[99] Bhaskararao, B.; Sunoj, R. B. Origin of Stereodivergence in Cooperative Asymmetric Catalysis with Simultaneous Involvement of Two Chiral Catalysts. *J. Am. Chem. Soc.* **2015**, *137*, 15712−15722.

[100] Here, "E" in the labeling scheme stands for the trans isomer of the allylic moiety alkene.

[101] Faller, J. W.; Thomsen, M. E.; Mattina, M. J. Organometallic conformational equilibriums. X. Steric factors and their mechanistic implications in. pi.-allyl(amine)chloropalladium(II) complexes. *J. Am. Chem. Soc.* **1971**, *93*, 2642−2653.

[102] Tsutsui, M.; Courtney, A., σ-π Rearrangements of Organotransition Metal Compounds in Homogeneous Catalysis. In Fundamental Research in Homogeneous Catalysis; Ishii, Y., Tsutsui, M.,Eds.; Springer US: Boston, MA, 1978; Vol. 2, pp 125−158.

[103] Madrahimov, S. T.; Li, Q.; Sharma, A.; Hartwig, J. F. Origins of Regioselectivity in Iridium Catalyzed Allylic Substitution. *J. Am. Chem. Soc.* **2015**, *137*, 14968−14981.

[104] For information on the fluoride source used in the computational studies, see **Figures A3.10 – A3.11** in Appendix 3.

[105] See **Figure A3.12** in Appendix 3 for a distortion−interaction analysis of lowest energy diastereomeric transition states to gain insights into the energetic difference between them.

[106] Hughes, D. L.; Lloyd-Jones, G. C.; Krska, S. W.; Gouriou, L.; Bonnet, V. D.; Jack, K.; Sun, Y.; Mathre, D. J.; Reamer, R. A. Mechanistic studies of the molybdenum-catalyzed asymmetric alkylation reaction. *Proc. Natl. Acad. Sci. U. S. A.* **2004**, *101*, 5379−5384.

[107] Gouriou, L.; Lloyd-Jones, G. C.; Vyskočil, Š.; Kočovský, P. ^{2}H quadrupolar coupling-based analysis of stereochemical and regiochemical memory in the Pd-catalysed allylic alkylation of iso-cinnamyl type substrates employing the chiral monophosphine ligands 'MOP' and 'MAP'. *J. Organomet. Chem.* **2003**, *687*, 525−537.

[108] Skubi, K. L.; Blum, T. R.; Yoon, T. P. Dual Catalysis Strategies in Photochemical Synthesis. *Chem. Rev.* **2016**, *116*, 10035 – 10074.

[109] Trost, B. M. New Rules of Selectivity: Allylic Alkylations Catalyzed by Palladium. *Acc. Chem. Res.* **1980**, *13*, 385 – 393.

[110] Trost, B. M.; Machacek, M. R.; Aponick, A. Predicting the Stereochemistry of Diphenylphosphino Benzoic Acid (DPPBA)-Based Palladium-Catalyzed Asymmetric Allylic Alkylation Reactions: A Working Model. *Acc. Chem. Res.* **2006**, *39*, 747 – 760.

[111] Son, S.; Fu, G. C. Nickel-Catalyzed Asymmetric Negishi Cross-Couplings of Secondary Allylic Chlorides with Alkylzincs. *J. Am. Chem. Soc. 2008*, **130**, 2756–2757.

[112] a) Trost, B. M.; Self, C. R. On the Palladium-Catalyzed Alkylation of Silyl-Substituted Allyl Acetates with Enolates. *J. Org. Chem.* **1984**, *49*, 468–473; b) Trost, B. M.; Keinan, E. Enolstannanes as Electrofugal Groups in Allylic Alkylation. *Tetrahedron Lett.* **1980**, *21*, 2591 –2594.

[113]Negishi, E.; Matsushita, H.; Chatterjee, S.; John, R. A Selective carbon-carbon bond formation via transition metal catalysis. 29. A highly regio- and stereospecific palladium-catalyzed allylation of enolates derived from ketones. *J. Org. Chem.* **1982**, *47*, 3188–3190.

[114] Braun, M.; Meier, T. Tsuji-Trost Allylic Alkylation with Ketone Enolates. *Angew. Chem. Int. Ed.* **2006**, *45*, 6952–6955.

[115] Graening, T.; Hartwig, J. F. Iridium-Catalyzed Regio- and Enantioselective Allylation of Ketone Enolates. *J. Am. Chem. Soc.* **2005**, *127*, 17192 –17193.

[116] Trost, B. M.; Schroeder, G. M. Palladium-Catalyzed Asymmetric Alkylation of Ketone Enolates. *J. Am. Chem. Soc.* **1999**, *121*, 6759–6760.

[117]Lang, S. B.; O'Nele, K. M.; Tunge, J. A. Decarboxylative Allylation of Amino Alkanoic Acids and Esters via Dual Catalysis. *J. Am. Chem. Soc.* **2014**, *136*, 13606–13609.

[118] Tasker, S. Z.; Standley, E. A.; Jamison, T. F. Recent Advances in Homogeneous Nickel Catalysis. *Nature* **2014**, *509*, 299–309.

[119] Matsui, J. K.; Gutierrez-Bonet, A.; Rotella, M.; Alam, R.; Gutierrez, O.; Molander, G. A. Photoredox/Nickel-Catalyzed Single-Electron Tsuji-Trost Reaction: Development and Mechanistic Insights. *Angew. Chem. Int. Ed.* **2018**, *57*, 15947 – 15851.

[120] a) Tewari, N.; Dwivedi, N.; Tripathi, R. Tetrabutylammonium hydrogen sulfate catalyzed eco-friendly and efficient synthesis of glycosyl 1,4-dihydropyridines. *Tet. Lett.* **2004**, *45*, 9011–9014. b) Adibi, H.; Samimi, H. A.; Beygzadeh, M. Iron(III) trifluoroacetate and trifluoromethanesulfonate: Recyclable Lewis acid catalysts for one-pot synthesis of 3,4 dihydropyrimidinones or their sulfur analogues and 1,4-dihydropyridines via solvent-free Biginelli and Hantzsch condensation protocols. *Catal. Commun.* **2007**, *8,* 2119–2124. c) Heydari, A.; Khaksar, S.; Tajbakhsh, M.; Bijanzadeh, H. R. One-step, synthesis of Hantzsch esters and polyhydroquinoline derivatives in fluoro alcohols. *J. Fluorine Chem.* **2009**, *130*, 609 – 614. d) Zhang, D.; Wu, L. Z.; Zhou, L.; Han, X.; Yang, Q. Z.; Zhang, L. P.; Tung, C. H. Photocatalytic Hydrogen Production from Hantzsch 1,4-Dihydropyridines by Platinum(II) Terpyridyl Complexes in Homogeneous Solution. *J. Am. Chem. Soc.* **2004**, *126*, 3440–3441. e) Wei, X.; Wang, L.; Jia, W.; Du, S.; Wu, L.; Liu, Q. Metal-Free-Mediated Oxidation Aromatization of 1,4-

Dihydropyridines to Pyridines Using Visible Light and Air. *Chin. J. Chem.* **2014**, *32*, 1245–1250.
f) Fukuzumi, S.; Suenobu, T.; Patz, M.; Hirasaka, T.; Itoh, S.; Fujitsuka, M.; Ito, O. Selective One-Electron and Two-Electron Reduction of C_{60} with NADH and NAD Dimer Analogues via Photoinduced Electron Transfer. *J. Am. Chem. Soc.* **1998**, *120*, 8060–8068. g) Wang, D.; Liu, Q.; Chen, B.; Zhang, L.; Tung, C.; Wu, L. Photooxidation of Hantzsch 1,4-dihydropyridines by molecular oxygen. *Chin. Sci. Bull*. **2010**, *55*, 2855–2858.

[121] de Aguirre, A.; Funes-Ardoiz, I.; Maseras, F. Four Oxidation States in a Single Photoredox Nickel-Based Catalytic Cycle: A Computational Study. *Angew. Chem., Int. Ed.* **2019**, *58*, 3898−3902.

[122] Bickelhaupt, F. M.; Houk, K. N. Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. *Angew. Chem., Int. Ed.* **2017**, *56*, 10070−10086.

[123] Seeman, J. I. Effect of conformational change on reactivity in organic chemistry. Evaluations, applications, and extensions of Curtin-Hammett/Winstein-Holness kinetics. *Chem. Rev.* **1983**, *83*, 83−134.

[124] Gutierrez, O.; Tellis, J. C.; Primer, D. N.; Molander, G. A.; Kozlowski, M. C. Nickel-Catalyzed Cross-Coupling of Photoredox-Generated Radicals: Uncovering a General Manifold for Stereoconvergence in Nickel-Catalyzed Cross-Couplings. *J. Am. Chem. Soc.* **2015**, *137*, 4896–4899.

[125] Luo, Y.; Gutierrez-Bonet, A.; Matsui, J. K.; Rotella, M. E.; Dykstra, R.; Gutierrez, O.; Molander G. A. Oxa- and Azabenzonorbornadienes as Electrophilic Partners under Photoredox/Nickel Dual Catalysis. *ACS Catal*. **2019**, *9*, 8835 – 8842.

[126] (a) Rayabarapu, D. K.; Cheng, C.-H. New Catalytic Reactions of Oxa- and Azabicyclic Alkenes. *Acc. Chem. Res.* **2007**, *40*, 971−983. (b) Lautens, M.; Fagnou, K.; Hiebert, S. Transition Metal-Catalyzed Enantioselective Ring-Opening Reactions of Oxabicyclic Alkenes. *Acc. Chem. Res.* **2003**, *36*, 48−58.

[127] (a) Lovering, F.; Bikker, J.; Humblet, C. Escape From Flatland: Increasing Saturation as an Approach to Improving Clinical Success. *J. Med. Chem.* **2009**, *52*, 6752−6756. (b) Dandapani, S.; Marcaurelle, L. A. Accessing New Chemical Space for 'Undruggable' Targets. *Nat. Chem. Biol.* **2010**, *6,* 861−863.

[128] Caple, R.; Chen, G. M.-S.; Nelson, J. D. The Addition of Butyllithiums to Benzonorbornadiene and 1,4-Dihydronaphthalene 1,4-endo-Oxide. *J. Org. Chem.* **1971**, *36*, 2874−2876. (b) Brown, N.; Luo, D.; Velde, D. V.; Yang, S.; Brassfield, A.; Buszek, K. R. Regioselective Diels-Alder Cycloadditions and Other Reactions of 4,5- 5,6- and 6,7-Indole Arynes. *Tetrahedron Lett.* **2009**, *50*, 63−65. (c) Buszek, K. R.; Luo, D.; Kondrashov, M.; Brown, N.; VanderVelde, D. Indole-Derived Arynes and their Diels-Alder Reactivity with Furans. *Org. Lett.* **2007**, *9*, 4135−4137.

[129] For selected examples, see: (a) Lautens, M.; Renaud, J.-L.; Hiebert, S. Palladium-Catalyzed Enantioselective Alkylative Ring Opening. *J. Am. Chem. Soc.* **2000**, *122*, 1804−1805. (b) Lautens, M.; Hiebert, S.; Renaud, J.-L. Mechanistic Studies of the Palladium-Catalyzed Ring Opening of Oxabicyclic Alkenes with Dialkylzinc. *J. Am. Chem. Soc.* **2001**, *123*, 6834−6839. (c) Lautens, M.; Hiebert, S. Scope of Palladium-Catalyzed Alkylative Ring Opening. *J. Am. Chem. Soc.* **2004**, *126*, 1437−1447. (d) Cabrera, S.; Gomez Arrayas, R.; Carretero, J. C. Cationic Planar Chiral Palladium P,S Complexes as Highly Efficient Catalysts in the Enantioselective Ring Opening of Oxa- and Azabicyclic Alkenes. *Angew. Chem., Int. Ed.* **2004**, *43*, 3944−3947. (e) Li, M.; Yan, X.-Y.; Hong, W.; Zhu, X.-Z.; Cao, B.-X.; Sun, J.; Hou, X.-L. Palladium-Catalyzed Enantioselective Ring Opening of Oxabicyclic Alkenes with Organozinc Halides. *Org. Lett.* **2004**, *6*, 2833−2835. (f) Cabrera, S.; Arrayás, R. G.; Alonso, I.; Carretero, J. C. Fesulphos-Palladium(II) Complexes as Well-Defined Catalysts for Enantioselective Ring Opening of Meso Heterobicyclic Alkenes with Organozinc Reagents. *J. Am. Chem. Soc.* **2005**, *127*, 17938−17947.

[130] (a) Wu, M.-S.; Jeganmohan, M.; Cheng, C.-H. A Highly Regio and Stereoselective Nickel-Catalyzed Ring-Opening Reaction of Alkyl- and Allylzirconium Reagents to 7-Oxabenzonorbornadienes. *J. Org. Chem.* **2005**, *70*, 9545−9550. (b) Ladjel, C.; Fuchs, N.; Zhao, J.; Bernardinelli, G.; Alexakis, A. New Bifunctional Substrates for Copper-Catalyzed Asymmetric Conjugate Addition Reactions with Trialkylaluminum. *Eur. J. Org. Chem.* **2009**, *2009*, 4949−4955. (c) Huang, Y.; Ma, C.; Lee, Y. X.; Huang, R.-Z.; Zhao, Y. Cobalt-Catalyzed Allylation of Heterobicyclic Alkenes: Ligand-Induced Divergent Reactivities. *Angew. Chem., Int. Ed.* **2015**, *54*, 13696−13700.

[131] Shukla, P.; Sharma, A.; Pallavi, B.; Cheng, C.-C. Nickel-Catalyzed Reductive Heck Type Coupling of Saturated Alkyl Halides with Acrylates and Oxabenzonorbornadiene. *Tetrahedron* **2015**, *71*, 2260−2266.

[132]Youran, L.; Gutiérrez-Bonet, A.; Matsui, J.; Rotella, M. E.; Dykstra, R.; Gutierrez, O.; Molander, G. A. Oxa- and Azabenzonorbornadienes as

Electrophilic Partners under Photoredox/Nickel Dual Catalysis. *ACS Catal.* **2019**, *9,* 8835 – 8842.

[133] (a) Bertozzi, F.; Pineschi, M.; Macchia, F.; Arnold, L. A.; Minnaard, A. J.; Feringa, B. L. Copper Phosphoramidite Catalyzed Enantioselective Ring-Opening of Oxabicyclic Alkenes: Remarkable Reversal of Stereocontrol. *Org. Lett.* **2002**, *4*, 2703−2705. (b) Arrayás, R. G.; Cabrera, S.; Carretero, J. C. Copper-Catalyzed Anti-Stereocontrolled Ring Opening of Oxabicyclic Alkenes with Grignard Reagents. *Org. Lett.* **2003**, *5*, 1333−1336. (c) Zhang, W.; Wang, L.-X.; Shi, W.-J.; Zhou, Q.-L. Copper-Catalyzed Asymmetric Ring Opening of Oxabicyclic Alkenes with Grignard Reagents. *J. Org. Chem.* **2005**, *70*, 3734−3736. (d) Zhang, W.; Zhu, S.-F.; Qiao, X.-C.; Zhou, Q.-L. Highly Enantioselective Copper-Catalyzed Ring Opening of Oxabicyclic Alkenes with Grignard Reagents. *Chem. Asian J.* **2008**, *3*, 2105−2111. (e) Bos, P. H.; Rudolph, A.; Pérez, M.; Fañanás Mastral, M.; Harutyunyan, S. R.; Feringa, B. L. Copper-Catalyzed Asymmetric Ring Opening of Oxabicyclic Alkenes with Organolithium Reagents. *Chem. Commun.* **2012**, *48*, 1748−1750.

[134] (a) Chen, C.; Martin, S. F. Facile Synthesis of 2-Substituted 1,2-Dihydro-1-Naphthols and 2-Substituted 1-Napthols. *Org. Lett.* **2004***, 6*, 3581−3584. (b) Chen, C. L.; Martin, S. F. Pd-Catalyzed Ring Opening of Oxa- and Azabicylic Alkenes with Aryl and Vinyl Halides: Efficient Entry to 2-Substituted 1,2-Dihydro-1-Napthols and 2-Substituted 1-Naphthols. *J. Org. Chem.* **2006**, *71*, 4810−4817.

[135] (a) Kaelin, D. E., Jr.; Lopez, O. D.; Martin, S. F. General Strategies for the Synthesis of the Major Classes of C-Aryl Glycosides. *J. Am. Chem. Soc.* **2001**, *123*, 6937−6938. (b) Kitamura, K.; Ando, Y.; Matsumoto, T.; Suzuki, K. Total Synthesis of Aryl C-Glycoside Natural Products: Strategies and Tactics. *Chem. Rev.* **2018**, *118*, 1495−1598. (c) Martin, S. F. Unified Strategy for the Synthesis of C-Aryl Glycosides. *Pure Appl. Chem.* **2003**, *75*, 63−70.

[136] (a) Lautens, M.; Ma, S. Nickel-Catalyzed Addition of Grignard Reagents to Oxabicyclic Compounds. Ring-Opening Reactions with Previously Unreactive Substrates and Nucleophiles. *J. Org. Chem.* **1996**, *61*, 7246−7247. (b) Loh, C. C. J.; Fang, X.; Peters, B.; Lautens, M. Benzylic Functionalization of Anthrones via the Asymmetric Ring Opening of Oxabicyclic Utilizing a Fourth-Generation Rhodium Catalytic System. *Chem. Eur. J.* **2015**, *21*, 13883−13887.

[137] Kaur, R.; Vikas. Conflict in the Mechanism and Kinetics of the Barrierless Reaction between SH and NO_2 Radicals. *J. Phys. Chem. A* **2018**, *122*, 1926−1937.

[138] Wenthold, P. G.; Winter, A. H. Nucleophilic Addition to Singlet Diradicals: Homosymmetric Diradicals. *J. Org. Chem.* **2018**, *83*, 12390−12396.

[139] Breitenfeld, J.; Wodrich, M. D.; Hu, X. Bimetallic Oxidative Addition in Nickel-Catalyzed Alkyl−Aryl Kumada Coupling Reactions. *Organometallics* **2014**, *33*, 5708−5715.

[140] Bickelhaupt, F. M.; Houk, K. N. Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. *Angew. Chem., Int. Ed.* **2017**, *56*, 10070−10086.

[141] Seeman, J. I. Effect of conformational change on reactivity in organic chemistry. Evaluations, applications, and extensions of Curtin-Hammett/Winstein-Holness kinetics. *Chem. Rev.* **1983**, *83*, 83−134.

[142] For selected examples, see: (a) Lautens, M.; Renaud, J.-L.; Hiebert, S. Palladium-Catalyzed Enantioselective Alkylative Ring Opening. *J. Am. Chem. Soc.* **2000**, *122*, 1804−1805. (b) Lautens, M.; Hiebert, S.; Renaud, J.-L. Mechanistic Studies of the Palladium- Catalyzed Ring Opening of Oxabicyclic Alkenes with Dialkylzinc. *J. Am. Chem. Soc.* **2001**, *123*, 6834−6839. (c) Lautens, M.; Hiebert, S. Scope of Palladium-Catalyzed Alkylative Ring Opening. *J. Am. Chem. Soc.* **2004**, *126*, 1437−1447. (d) Cabrera, S.; Gomez Arrayas, R.; Carretero, J. C. Cationic Planar Chiral Palladium P,S Complexes as Highly Efficient Catalysts in the Enantioselective Ring Opening of Oxa- and Azabicyclic Alkenes. *Angew. Chem., Int. Ed.* **2004**, *43*, 3944− 3947. (e) Li, M.; Yan, X.-Y.; Hong, W.; Zhu, X.-Z.; Cao, B.-X.; Sun, J.; Hou, X.-L. Palladium-Catalyzed Enantioselective Ring Opening of Oxabicyclic Alkenes with Organozinc Halides. *Org. Lett.* **2004**, *6*, 2833−2835. (f)Cabrera,S.;Arrayaś,R.G.;Alonso,I.;Carretero,J.C. Fesulphos-Palladium(II) Complexes as Well-Defined Catalysts for Enantioselective Ring Opening of Meso Heterobicyclic Alkenes with Organozinc Reagents. *J. Am. Chem. Soc.* **2005**, *127*, 17938−17947.

[143] For representative reviews on reaction of alkenes, see: (a) Kolb, H. C.; Van Nieuwenhze, M. S.; Sharpless, K. B. Catalytic Asymmetric Dihydroxylation. *Chem. Rev.* **1994**, *94*, 2483−2547. (b) Hashimoto, T.; Maruoka, K. Recent Advances of Catalytic Asymmetric 1,3-Dipolar Cycloadditions. *Chem. Rev.* **2015**, *115*, 5366−5412. (c) Wu, W.; Lin, Z.; Jiang, H. Recent advances in the synthesis of cyclopropanes. *Org. Biomol. Chem.* **2018**, *16*, 7315−7329. (d) McDonald, R. I.; Liu, G.; Stahl, S. S. Palladium(II)-Catalyzed Alkene Functionalization via Nucleopalladation: Stereochemical Pathways and Enantioselective Catalytic Applications. *Chem. Rev.* **2011**, *111*, 2981−3019.

(e) Cresswell, A. J.; Eey, S. T.-C.; Denmark, S. E. Catalytic, Stereoselective Dihalogenation of Alkenes: Challenges and Opportunities. *Angew. Chem., Int. Ed.* **2015**, *54*, 15642−15682. (f) Heravi, M. M.; Lashaki, T. B.; Fattahi, B.; Zadsirjan, V. Application of asymmetric Sharpless aminohydroxylation in total synthesis of natural products and some synthetic complex bio-active molecules. *RSC Adv.* **2018**, *8*, 6634.

[144] (a) Kolb, H. C.; Van Nieuwenhze, M.S.; Sharpless, K. B. Catalytic Asymmetric Dihydroxylation. *Chem. Rev.* **1994**, *94*, 2483−2547. (b) Hashimoto, T.; Maruoka, K. Recent Advances of Catalytic Asymmetric 1,3-Dipolar Cycloadditions. *Chem. Rev.* **2015**, *115*, 5366−5412. (c) Wu, W.; Lin, Z.; Jiang, H. Recent advances in the synthesis of cyclopropanes. *Org. Biomol. Chem.* **2018**, *16*, 7315−7329. (d) McDonald, R. I.; Liu, G.; Stahl, S. S. Palladium (II)-Catalyzed Alkene Functionalization via Nucleopalladation: Stereochemical Pathways and Enantioselective Catalytic Applications. *Chem. Rev.* **2011**, *111*, 2981−3019. (e) Cresswell, A. J.; Eey, S. T.-C.; Denmark, S. E. Catalytic, Stereoselective Dihalogenation of Alkenes: Challenges and Opportunities. *Angew. Chem., Int. Ed.* **2015**, *54*, 15642−15682. (f) Heravi, M. M.; Lashaki, T. B.; Fattahi, B.; Zadsirjan, V. Application of asymmetric Sharpless aminohydroxylation in total synthesis of natural products and some synthetic complex bio-active molecules. *RSC Adv.* **2018**, *8*, 6634.

[145] (a) García-Domínguez, A.; Li, Z.; Nevado, C. Nickel-Catalyzed Reductive Dicarbofunctionalization of Alkenes. J. Am. Chem. Soc. 2017, 139, 6835 - 6838. (b) Terao, J.; Saito, K.; Nii, S.; Kambe, N.; Sonoda, N. J. Am. Chem. Soc. 1998, 120, 11822 – 11823.

[146] (a) Stadtmueller, H.; Lentz, R.; Tucker, C. E.; Stuedemann, T.; Doerner, W.; Knochel, P. Regioselective Double Alkylation of Styrenes with Alkyl Halides Using a Titanocene Catalyst. *J. Am. Chem. Soc.* **1993**, *115*, 7027 - 7028. (b) Wakabayashi, K.; Yorimitsu, H.; Oshima, K. Cobalt-catalyzed tandem radical cyclization and cross-coupling reaction: its application to benzyl-substituted heterocycles. *J. Am. Chem. Soc.* **2001**, *123*, 5374 - 5375. (c) Phapale, V. B.; Buñuel, E.; García-Iglesias, M.; Cárdenas, D. Ni-Catalyzed Cascade Formation of $C(sp^3)$-$C(sp^3)$ Bonds by Cyclization and Cross-Coupling Reactions of Iodoalkanes with Alkyl Zinc Halides. *Angew. Chem. Int. Ed.* **2007**, *46*, 8790 - 8795. (d) Cong, H.; Fu, G. C. Catalytic Enantioselective Cyclization/Cross-Coupling with Alkyl Electrophiles *J. Am. Chem. Soc.* **2014**, *136*, 3788 - 3791. (e) You, W.; Brown, M. K. Diarylation of Alkenes by a Cu-Catalyzed Migratory Insertion/Cross-Coupling Cascade. *J. Am. Chem. Soc.* **2014**, *136*, 14730 – 14733. (f) You, W.; Brown, M. K. Catalytic Enantioselective Diarylation of Alkenes. *J. Am. Chem. Soc.* **2015**, *137*, 14578 – 14581.

(g) McMahon, C. M.; Renn, M. S.; Alexanian, E. J. Manganese-Catalyzed Carboacylations of Alkenes with Alkyl Iodides. *Org. Lett.* **2016**, *18*, 4148 – 4150. (h) Dhungana, R. K.; Shrestha, B.; Thapa-Magar, R.; Basnet, P.; Giri, R. Pd-Catalyzed Regioselective 1,2-Dicarbofunctionalization of Unactivated Olefins by a Heck Reaction/Enolate Cyclization Cascade. *Org. Lett.* **2017**, *19*, 2154 – 2157. (i) Thapa, S.; Basnet, P.; Giri, R. Copper-Catalyzed Dicarbofunctionalization of Unactivated Olefins by Tandem Cyclization/Cross-Coupling. *J. Am. Chem. Soc.* **2017**, *139*, 5700 – 5703. (j) Xu, T.; Dong, G. Rhodium-Catalyzed Regioselective Carboacylation of Olefins: A C-C Bond Activation Approach for Accessing Fused-Ring Systems. *Angew. Chem. Int. Ed.* **2012**, *51*, 7567 – 7571. (k) Walker, J. A.; Vickerman, K. L.; Humke, J. N.; Stanley, L. M. Ni-Catalyzed Alkene Carboacylation via Amide C–N Bond Activation. *J. Am. Chem. Soc.* **2017**, *139*, 10228 – 10231.

[147] (a) Qin, T.; Cornella, J.; Li, C.; Malins, L. R.; Edwards, J. T.; Kawamura, S.; Maxwell, B. D.; Eastgate, M. D.; Baran, P. S. A general alkyl-alkyl cross-coupling enabled by redox-active esters and alkylzinc reagents. *Science* **2016**, *352*, 801 – 805. (b) Zhang, L.; Lovinger, G. J.; Edelstein, E. K.; Szymaniak, A. A.; Chierchia, M. P.; Morken, J. P. Catalytic Conjunctive Cross-Coupling Enabled by Metal-Induced Metallate Rearrangement. *Science* **2016**, *351*, 70 – 74.

[148] (a) Renata, H.; Zhou, Q.; Baran, P. S. Strategic Redox Relay Enables A Scalable Synthesis of Ouabagenin, A Bioactive Cardenolide. *Science* **2013**, *339*, 59 – 63. (b) Weinstein, A. B.; Stahl, S. S. Reconciling the Stereochemical Course of Nucleopalladation with the Development of Enantioselective Wacker-Type Cyclizations. *Angew. Chem. Int. Ed.* **2012**, *51*, 11505 – 11509. (c) Aspin, S.; Goutierre, A.-S.; Larini, P.; Jazzar, R.; Baudoin, O. Synthesis of Aromatic α-Aminoesters: Palladium-Catalyzed Long-Range Arylation of Primary C(sp^3)-H Bonds. *Angew. Chem. Int. Ed.* **2012**, *51*, 10808 – 10811. (d) Kohler, D. G.; Gockel, S. N.; Kennemur, J. L.; Waller, P. J.; Hull, K. L. Palladium-catalyzed anti-Markovnikov selective oxidative amination. *Nat. Chem.* **2018**, *10*, 333 – 340. (e) Park, J.-W.; Kou, K. G. M.; Kim, D. K.; Dong, V. M. Rh-catalyzed desymmetrization of α-quaternary centers by isomerization-hydroacylation. *Chem. Sci.* **2015**, *6*, 4479 – 4483. (e) Saini, V.; Sigman, M. S. Palladium-Catalyzed 1,1-Difunctionalization of Ethylene. *J. Am. Chem. Soc.* **2012**, *134*, 11372 – 11375. (f) Werner, E. W.; Urkalan, K. B.; Sigman, M. S. Pd^{II}-Catalyzed Oxidative 1,1-Diarylation of Terminal Olefins. *Org. Lett.* **2010**, *12*, 2848 – 2851.

[149] Werner, E. W.; Urkalan, K. B.; Sigman, M. S. Pd^{II}-Catalyzed Oxidative 1,1-Diarylation of Terminal Olefins. *Org. Lett.* **2010**, *12*, 2848 – 2851.

[150] (a) Shrestha, B.; Basnet, P.; Dhungana, R. K.; Kc, S.; Thapa, S.; Sears, J. M.; Giri, R. Ni-Catalyzed Regioselective 1,2-Dicarbofunctionalization of Olefins by Intercepting Heck Intermediates as Imine-Stabilized Transient Metallacycles. *J. Am. Chem. Soc.* **2017**, *139*, 10653 – 10656. (b) Thapa, S.; Dhungana, R. K.; Magar, R. T.; Shrestha, B.; Kc, S.; Giri, R. Ni-catalyzed regioselective 1,2-diarylation of unactivated olefins by stabilizing Heck intermediates as pyridylsilyl-coordinated transient metallacycles. *Chem. Sci.* **2018**, *9*, 904 – 909. (c) Basnet, P.; Dhungana, R. K.; Thapa, S.; Shrestha, B.; Kc, S.; Sears, J. M.; Giri, R. Ni-Catalyzed Regioselective β,δ-Diarylation of Unactivated Olefins in Ketimines via Ligand-Enabled Contraction of Transient Nickellacycles: Rapid Access to Remotely Diarylated Ketones. *J. Am. Chem. Soc.* **2018**, *140*, 7782 – 7786.

[151] (a) Gu, J. W.; Min, Q. Q.; Yu, L. C.; Zhang, X. Tandem Difluoroalkylation-Arylation of Enamides Catalyzed by Nickel. *Angew. Chem. Int. Ed.* **2016**, *55*, 12270 – 12274. (b) Li, W.; Boon, J. K.; Zhao, Y. Nickel-catalyzed difunctionalization of allyl moieties using organoboronic acids and halides with divergent regioselectivities. *Chem. Sci.* **2018**, *9*, 600 – 607. (c) Yahiaoui, S.; Fardost, A.; Trejos, A.; Larhed, M. Chelation-Mediated Palladium(II)-Catalyzed Domino Heck−Mizoroki/Suzuki−Miyaura Reactions Using Arylboronic Acids: Increasing Scope and Mechanistic Understanding. *J. Org. Chem.* **2011**, *76*, 2433 – 2438. (d) Derosa, J.; Tran, V. T.; Boulous, M. N.; Chen, J. S.; Engle, K. M. Nickel-Catalyzed β,γ-Dicarbofunctionalization of Alkenyl Carbonyl Compounds via Conjunctive Cross-Coupling. *J. Am. Chem. Soc.* **2017**, *139*, 10657 – 10660.

[152] Basnet, P.; Dhungana, R. K.; Thapa, S.; Shrestha, B.; KC, S.; Sears, J. M.; Giri, R. Ni-Catalyzed Regioselective β,δ-Diarylation of Unactivated Olefins in Ketimines via Ligand-Enabled Contraction of Transient Nickellacycles: Rapid Access to Remotely Diarylated Ketones. *J. Am. Chem. Soc.* **2018**, *140*, 7782 – 7786.

[153] Basnet, P.; KC, S.; Dhungana, R. K.; Shrestha, B.; Boyle, T. J.; Giri, R. Synergistic Bimetallic Ni/Ag and Ni/Cu Catalysis for Regioselective γ,δ-Diarylation of Alkenyl Ketimines: Addressing β-H Elimination by in Situ Generation of Cationic Ni(II) Catalysts. *J. Am. Chem. Soc.* **2018**, *140*, 15586 – 15590.

[154] (a) Bhattacharya, T.; Dutta, S.; Maiti, D. Deciphering the Role of Silver in Palladium-Catalyzed C–H Functionalizations. *ACS Catal.* **2021**,*11*, 9702 – 9714. (b) Anand, M.; Sunoj, R. B.; Schaefer, H. F. Palladium–Silver Cooperativity in an Aryl Amination Reaction through C–H Functionalization. *ACS Catal.* **2016,** *6*, 696-708.

(c) Yang, Y.; Cheng, G.; Liu, P.; Leow, D.; Sun, T.; Chen, P.; Zhang, X.; Yu, J.; Wu, Y.; Houk, K. N. Palladium-Catalyzed Meta-Selective C–H Bond Activation with a Nitrile-Containing Template: Computational Study on Mechanism and Origins of Selectivity. *J. Am. Chem. Soc.* **2014,** *136*, 344-355. (d) Bhaskararao, B.; Singh, S.; Anand, M.; Verma, P.; Prakash, P.; C, A.; Malakar, S.; Schaefer, H. F.; Sunoj, R. B. Is silver a mere terminal oxidant in palladium catalyzed C–H bond activation reactions? *Chem. Sci.* **2020**, *11*, 208 – 216. (e) Aufiero, M.; Proutiere, F.; Schoenebeck, F. Redox Reactions in Palladium Catalysis: On the Accelerating and/or Inhibiting Effects of Copper and Silver Salt Additives in Cross-Coupling Chemistry Involving Electron-rich Phosphine Ligands. *Angew. Chem. Int. Ed.* **2012**, *51*, 7226 –7230.

[155] (a) Honeycutt, A. P.; Hoover, J. M. Nickel-Catalyzed Oxidative Decarboxylative (Hetero)Arylation of Unactivated C–H Bonds: Ni and Ag Synergy. *ACS Catal.* **2017**, *7*, 4597-4601. (b) Gøgsig, T. M.; Kleimark, J.; Nilsson Lill, S. O.; Korsager, S.; Lindhardt, A. T.; Norrby, P.; Skrydstrup, T. Mild and Efficient Nickel-Catalyzed Heck Reactions with Electron-Rich Olefins. *J. Am. Chem. Soc*. **2012**, *134*, 443-452.

[156] (a) Fürstner, A. Alkyne metathesis on the rise. *Angew. Chem., Int. Ed.* **2013**, *52*, 2794−2819. (b) Ehrhorn, H.; Tamm, M. Well-Defined Alkyne Metathesis Catalysts: Developments and Recent Applications. *Chem. Eur. J.* **2018**, *25*, 3190−3208.

[157] (a) Fürstner, A.; Davies, P. W. Alkyne Metathesis. *Chem. Commun.* **2005**, 2307. (b) Zhang, W.; Moore, J. S. Alkyne Metathesis: Catalysts and Synthetic Applications. *Ad*v. *Synth. Catal.* **2007**, *349*, 93. (c) Schrock, R. R.; Czekelius, C. Recent Advances in the Syntheses and Applications of Molybdenum and Tungsten Alkylidene and Alkylidyne Catalysts for the Metathesis of Alkenes and Alkynes. *Ad*v. *Synth. Catal.* **2007**, *349*, 55.

[158] (a) Pennella, F.; Banks, R. L.; Bailey, G. C. Disproportionation of alkynes. *Chem. Commun.* **1968**, 1548−1549. (b) Mortreux, A.; Blanchard, M. Metathesis of alkynes by a molybdenum hexacarbonyl−resorcinol catalyst. *J. Chem. Soc., Chem. Commun.* **1974**, 786−787.

[159] Fürstner, A.; Seidel, G. Ring-Closing Metathesis of Functionalizaed Acetylene Derivatives: A New Entry into Cycloalkynes. *Angew. Chem., Int. Ed.* **1998**, *37*, 1734.

[160] (a) Bellone, D. E.; Bours, J.; Menke, E. H.; Fischer, F. R. Highly Selective Molybdenum ONO Pincer Complex Initiates the Living Ring-Opening Metathesis Polymerization of Strained Alkynes with Exceptionally Low Polydispersity Indices. *J. Am. Chem. Soc.* **2015**, *137*, 850−856. (b) Jeong, H.; von Kugelgen, S.; Bellone, D.; Fischer, F. R. Regioselective Termination Reagents for Ring-Opening Alkyne Metathesis Polymerization. *J. Am. Chem. Soc.* **2017**, *139*, 15509−15514. (c) von Kugelgen, S.; Bellone, D. E.; Cloke, R. R.; Perkins, W. S.; Fischer, F. R. Initiator Control of Conjugated Polymer Topology in Ring-Opening Alkyne Metathesis Polymerization. *J. Am. Chem. Soc.* **2016**, *138*, 6234−6239. (d) Bunz, U. H. F. Poly(p-phenyleneethynylene)s by Alkyne Metathesis. *Acc. Chem. Res.* **2001**, *34*, 998−1010.

[161] (a) Zhang, W.; Moore, J. S. Arylene Ethynylene Macrocycles Prepared by Precipitation-Driven Alkyne Metathesis. *J. Am. Chem. Soc.* **2004**, *126*, 12796. (b) Wang, Q.; Yu, C.; Zhang, C.; Long, H.; Azarnoush, S.; Jin, Y.; Zhang, W. Dynamic covalent synthesis of aryleneethynylene cages through alkyne metathesis: dimer, tetramer, or interlocked complex? *Chem. Sci.* **2016**, *7*, 3370−3376. (c) Wang, Q.; Yu, C.; Long, H.; Du, Y.; Jin, Y.; Zhang, W. Solution-Phase Dynamic Assembly of Permanently Interlocked Aryleneethynylene Cages through Alkyne Metathesis. *Angew. Chem., Int. Ed.* **2015**, *54*, 7550−7554. (d) Zhou, X.; Thompson, R. R.; Fronczek, F. R.; Lee, S. Size-Selective Synthesis of Large Cycloparaphenyleneacetylene Carbon Nanohoops Using Alkyne Metathesis. *Org. Lett.* **2019**, *21*, 4680−4683.

[162] (a) Meng, Z.; Fürstner, A. Total Synthesis of (−)-Sinulariadiolide. ATransannular Approach. *J. Am. Chem. Soc.* **2019**, *141*, 805−809. (b) Schaubach, S.; Gebauer, K.; Ungeheuer, F.; Hoffmeister, L.; Ilg, M. K.; Wirtz, C.; Fürstner, A. A Two-Component Alkyne Metathesis Catalyst System with an Improved Substrate Scope and Functional Group Tolerance: Development and Applications to Natural Product Synthesis. *Chem. Eur. J.* **2016**, *22*, 8494−8507. (c) Hötling, S.; Bittner, C.; Tamm, M.; Dähn, S.; Collatz, J.; Steidle, J. L. M.; Schulz, S. Identification of a Grain Beetle Macrolide Pheromone and Its Synthesis by Ring-Closing Metathesis Using a Terminal Alkyne. *Org. Lett.* **2015**, *17*, 5004−5007.

[163] Ehrhorn, H.; Bockfeld, D.; Freytag, M.; Bannenberg, T.; Kefalidis, C. E.; Maron, L.; Tamm, M. Studies on Molybdena- and Tungstenacyclobutadiene Complexes Supported by Fluoroalkoxy Ligands as Intermediates of Alkyne Metathesis. *Organometallics* **2019**, *38*, 1627−1639.

[164] Geyer, A. M.; Wiedner, E. S.; Gary, J. B.; Gdula, R. L.; Kuhlmann, N. C.; Johnson, M. J. A.; Dunietz, B. D.; Kampf, J. W. Highly Active Molybdenum-Alkylidyne Catalysts for Alkyne Metathesis: Synthesis from the Nitrides by Metathesis with Alkynes. *J. Am. Chem. Soc.* **2008**, *130*, 8984.

[165] Heppekausen, J.; Stade, R.; Goddard, R.; Fürstner, A. Practical New Silyloxy-Based Alkyne Metathesis Catalysts with Optimized Activity and Selectivity Profiles. *J. Am. Chem. Soc.* **2010**, *132*, 11045 – 11057.

[166] (a) Heppekausen, J.; Stade, R.; Kondoh, A.; Seidel, G.; Goddard, R.; Fürstner, A. Optimized Synthesis, Structural Investigations, Ligand Tuning and Synthetic Evaluation of Silyloxy-Based Alkyne Metathesis Catalysts. *Chem. Eur. J.* **2012**, *18*, 10281−10299. (b) Lhermet, R.; Fürstner, A. Cross-Metathesis of Terminal Alkynes. *Chem. Eur. J.* **2014**, *20*, 13188−13193.

[167] Thompson, R. R.; Rotella, M. E.; Du, P.; Zhou, X.; Fronczek, F. R.; Kumar, R.; Gutierrez, O.; Lee, S. Siloxide Podand Ligand as a Scaffold for Molybdenum-Catalyzed Alkyne Metathesis and Isolation of a Dynamic Metallatetrahedrane Intermediate. *Organometallics* **2019**, *38,* 4054 – 4059.

[168] Schrock, R. R. High-oxidation-state molybdenum and tungsten alkylidyne complexes. *Acc. Chem. Res.* **1986**, *19*, 342−348.

[169] Thompson, R. R.; Rotella, M. E.; Zhou, X.; Fronczek, F. R.; Gutierrez, O.; Lee, S. Impact of Ligands and Metals on the Formation of Metallacyclic Intermediates and a Non-traditional Mechanism for Group VI Alkyne Metathesis Catalysts. *J. Am. Chem. Soc.* **2021**, *143*, 9026 – 9039.

[170] Estes, D. P.; Gordon, C. P.; Fedorov, A.; Liao, W.-C.; Ehrhorn, H.; Bittner, C.; Zier, M. L.; Bockfeld, D.; Chan, K. W.; Eisenstein, O.; Raynaud, C.; Tamm, M.; Coperet, C. Molecular and Silica-Supported Molybdenum Alkyne Metathesis Catalysts: Influence of Electronics and Dynamics on Activity Revealed by Kinetics, Solid-State NMR, and Chemical Shift Analysis. *J. Am. Chem. Soc.* **2017**, *139*, 17597−17607.

[171] Becke, A. D., Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993,** *98*, 5648-5652.

[172] Grimme, S. A., J.; Ehrlich, S.; Krieg, H., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. . *J. Chem. Phys.* **2010,** *132*, 154104.

[173] Weigend, F.; Ahlrichs, R., Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005,** *7*, 3297-3305.

[174] Cossi, M.; Barone, V.; Cammi, R.; Tomasi, J., Ab initio study of solvated molecules: a new implementation of the polarizable continuum model. *Chem. Phys. Lett.* **1996,** *255*, 327-335.

[175] Fuentealba, P.; Preuss, H.; Stoll, H.; Von Szentpály, L., A proper account of core-polarization with pseudopotentials: single valence-electron alkali compounds. *Chem. Phys. Lett.* **1982,** *89*, 418-422.

[176] Vogiatzis, K. D.; Polynski, M. V.; Kirkland, J. K.; Townsend, J.; Hashemi, A.; Liu, C.; Pidko, E. A., Computational Approach to Molecular Catalysis by 3d Transition Metals: Challenges and Opportunities. *Chem. Rev.* **2019,** *119*, 2453-2523.

[177] Haack, A.; Hillenbrand, J.; Leutzsch, M.; van Gastel, M.; Neese, F.; Fürstner, A. Productive Alkyne Metathesis with "Canopy Catalysts" Mandates Pseudorotation. *J. Am. Chem. Soc.* **2021**, *143*, 5643 - 5648.

[178] Flook, M. M.; Börner, J.; Kilyanek, S. M.; Gerber, L. C. H.; Schrock, R. R., Five-Coordinate Rearrangements of Metallacyclobutane Intermediates during Ring-Opening Metathesis Polymerization of 2,3-Dicarboalkoxynorbornenes by Molybdenum and Tungsten Monoalkoxide Pyrrolide Initiators. *Organometallics* **2012,** *31*, 6231-6243.

[179] Flook, M. M.; Börner, J.; Kilyanek, S. M.; Gerber, L. C. H.; Schrock, R. R., Five-Coordinate Rearrangements of Metallacyclobutane Intermediates during Ring-Opening Metathesis Polymerization of 2,3-Dicarboalkoxynorbornenes by Molybdenum and Tungsten Monoalkoxide Pyrrolide Initiators. *Organometallics* **2012,** *31*, 6231-6243.

[180] Shao, Y.; Gan, Z.; Epifanovsky, E.; Gilbert, A. T. B.; Wormit, M.; Kussmann, J.; Lange, A. W.; Behn, A.; Deng, J.; Feng, X.; Ghosh, D.; Goldey, M.; Horn, P. R.; Jacobson, L. D.; Kaliman, I.; Khaliullin, R. Z.; Kus, T.; Landau, A.; Liu, J.; Proynov, E. I.; Rhee, Y. M.; Richard, R. M.; Rohrdanz, M. A.; Steele, R. P.; Sundstrom, E. J.; Woodcock, H. L.; Zimmerman, P. M.; Zuev, D.; Albrecht, B.; Alguire, E.; Austin, B.; Beran, G. J. O.; Bernard, Y. A.; Berquist, E.; Brandhorst, K.; Bravaya, K. B.; Brown, S. T.; Casanova, D.; Chang, C.-M.; Chen, Y.; Chien, S. H.; Closser, K. D.; Crittenden, D. L.; Diedenhofen, M.; DiStasio, R. A.; Do, H.; Dutoi, A. D.; Edgar, R. G.; Fatehi, S.; Fusti-Molnar, L.; Ghysels, A.; Golubeva-Zadorozhnaya, A.; Gomes, J.;

Hanson-Heine, M. W. D.; Harbach, P. H. P.; Hauser, A. W.; Hohenstein, E. G.; Holden, Z. C.; Jagau, T.-C.; Ji, H.; Kaduk, B.; Khistyaev, K.; Kim, J.; Kim, J.; King, R. A.; Klunzinger, P.; Kosenkov, D.; Kowalczyk, T.; Krauter, C. M.; Lao, K. U.; Laurent, A. D.; Lawler, K. V.; Levchenko, S. V.; Lin, C. Y.; Liu, F.; Livshits, E.; Lochan, R. C.; Luenser, A.; Manohar, P.; Manzer, S. F.; Mao, S.-P.; Mardirossian, N.; Marenich, A. V.; Maurer, S. A.; Mayhall, N. J.; Neuscamman, E.; Oana, C. M.; Olivares-Amaya, R.; O'Neill, D. P.; Parkhill, J. A.; Perrine, T. M.; Peverati, R.; Prociuk, A.; Rehn, D. R.; Rosta, E.; Russ, N. J.; Sharada, S. M.; Sharma, S.; Small, D. W.; Sodt. Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Mol. Phys.* **2015**, *113*, 184−215.

[181] Lu, G.; Liu, R. Y.; Yang, Y.; Fang, C.; Lambrecht, D. S.; Buchwald, S. L.; Liu, P. Ligand–Substrate Dispersion Facilitates the Copper-Catalyzed Hydroamination of Unactivated Olefins. *J. Am. Chem. Soc.* **2017**, *139*, 16548−16555.

[182] Thomas, A. A.; Speck, K.; Kevlishvili, I.; Lu, Z; Liu, P.; Buchwald, S. L. Mechanistically Guided Design of Ligands That Significantly Improve the Efficiency of CuH-Catalyzed Hydroamination Reactions. *J. Am. Chem. Soc.* **2017**, *140*, 13976 – 13984.

[183] Bickelhaupt, F. M.; Houk, K. N. Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. *Angew. Chem., Int. Ed.* **2017**, *56*, 10070−10086.

[184] Qi, X.; Diao, T. Nickel-catalyzed dicarbofunctionalization of alkenes. *ACS Catal.* **2020**, *10*, 8542 – 8556.

[185] Cao, H.; Liu, H.; Domling, A. Efficient Multicomponent Reaction Synthesis of the Schistosomiasis Drug Praziquantel. *Chem. Eur. J.* **2010**, *16*, 12296 – 12298.

[186] (a) Derosa, J.; Tran, V. T.; van der Puyl, V. A.; Engle, K. M. Carbon-Carbon pi Bonds as Conjunctive Reagents in Cross-Coupling. *Aldrichimica Acta*, **2018**, ***51*, 21 – 32**. (*b*) Giri, R.; KC, S. Strategies toward dicarbofunctionalization of unactivated olefins by combined heck carbometalation and cross-coupling. *J. Org. Chem.* **2018**, ***83***, 3013 – 3022. (c) Liao, L.; Jana, R.; Urkalan, K. B.; Sigman, M. S. A palladium-catalyzed three-component cross-coupling of conjugated dienes or terminal alkenes with vinyl triflates and boronic acids. *J. Am. Chem. Soc.*, **2011**, ***133***, 5784 - 5787.

(*d*) Qin, T.; Cornella, J.; Li, C.; Malins, L. R.; Edwards, J. T.; Kawamura, S.; Maxwell, B. D.; Eastgate, M. D.; Baran, P. S. A general alkyl-alkyl cross-coupling enabled by redox-active esters and alkylzinc reagents. *Science*, **2016**, *352*, 801 - 805. (*e*) García-Domínguez, A.; Li, Z.; Nevado, C. Nickel-catalyzed reductive dicarbofunctionalization of alkenes. *J. Am. Chem. Soc.*, **2017**, ***139***, 6835 – 6838.

[187] Tu, H.; Wang, F.; Huo, L.; Li, Y.; Zhu, S.; Zhao, X.; Li, H.; Qing, F.; Chu, L. Enantioselective three-component fluoroalkylarylation of unactivated olefins through nickel-catalyzed cross-electrophile coupling. *J. Am. Chem. Soc.* **2020**, *142*, 9604–9611.

[188] Yan, M.; Lo, J. C.; Edwards, J. T.; Baran, P. S. Radicals: Reactive Intermediates with Translational Potential. *J. Am. Chem. Soc.* **2016**, *138*, 12692–12714.

[189] Campbell, M. W.; Compton, J. S.; Kelly, C. B.; Molander, G. A. Three-component olefin dicarbofunctionalization enabled by nickel/photoredox dual catalysis. *J. Am. Chem. Soc.* **2019**, *141*, 20069 – 20078.

[190] Qin, T.; Cornella, J.; Li, C.; Malins, L. R.; Edwards, J. T.; Kawamura, S.; Maxwell, B. D.; Eastgate, M. D.; Baran, P. S. A general alkyl-alkyl cross-coupling enabled by redox-active esters and alkylzinc reagents. *Science* **2016**, *352*, 801 – 805.

[191] Basnetm P.; KC, S.; Dhungana, R. K.; Shrestha, B.; Boyle, T. J.; Giri, R. Synergistic Bimetallic Ni/Ag and Ni/Cu Catalysis for Regioselective γ,δ-Diarylation of Alkenyl Ketimines: Addressing β-H Elimination by in Situ Generation of Cationic Ni(II) Catalysts. *J. Am. Chem. Soc.* **2018**, *140*, 15586 – 15590.

[192] For representative examples of Pd and Ni catalyzed conjunctive cross-couplings, refer to the following. (a) Lovinger, G. J.; Morken, J. P. Ni-Catalyzed Enantioselective Conjunctive Coupling with C(sp^3) Electrophiles: A Radical-Ionic Mechanistic Dichotomy. *J. Am. Chem. Soc*. **2017**, *139*, 17293-17296. (b) Derosa, J.; Kleinmans, R.; Tran, V. T.; Karunananda, M. K.; Wisniewski, S. R.; Eastgate, M. D.; Engle, K. M. Nickel-catalyzed 1, 2-diarylation of simple alkenyl amides. *J. Am. Chem. Soc*. **2018**, *140*, 17878-17883. (c) Lovinger, G. J.; Aparece, M. D.; Morken, J. P. Pd-Catalyzed Conjunctive Cross-Coupling between Grignard-Derived Boron "Ate" Complexes and C(sp^2) Halides or Triflates: NaOTf as a Grignard Activator and Halide Scavenger. *J. Am. Chem. Soc*. **2017**, *139*, 3153-3160.

(d) Edelstein, E. K.; Namirembe, S.; Morken, J. P. Enantioselective conjunctive cross-coupling of bis (alkenyl) borates: a general synthesis of chiral allylboron reagents. *J. Am. Chem. Soc.* **2017**, *139*, 5027-5030. (g) Wu, L.; Wang, F.; Wan, X.; Wang, D.; Chen, P.; Liu, G. Asymmetric Cu-catalyzed intermolecular trifluoromethylarylation of styrenes: enantioselective arylation of benzylic radicals. *J. Am. Chem. Soc.* **2017**, *139*, 2904 – 2907. (h) Lin, J.; Li, T.; Liu, J.; Jiao, G.; Gu, Q.; Cheng, J.; Guo, Y.; Hong, X.; Liu, X. Cu/chiral phosphoric acid-catalyzed asymmetric three-component radical-initiated 1, 2-dicarbofunctionalization of alkenes. *J. Am. Chem. Soc.* **2019**, *141,* 1074 – 1083. (i) Kadam, A. A.; Metz, T. L.; Qian, Y.; Stanley, L. M. Ni-catalyzed three-component alkene carboacylation initiated by amide C–N bond activation. *ACS Catal.* **2019**, *9,* 5651 – 5656. (j) Qi, X.; Diao, T. Nickel-catalyzed dicarbofunctionalization of alkenes. *ACS Catal.* **2020**, *10,* 8542 – 8556. (l) Wang, X.; Lu, X.; He, S.; Fu, Y. Nickel-catalyzed three-component olefin reductive dicarbofunctionalization to access alkylborates. *Chem. Sci.* **2020**, *11,* 7950 – 7956. (o) Zhang, Y.; Chen, G.; Zhao, D. Three-component vicinal-diarylation of alkenes via direct transmetalation of arylboronic acids. *Chem. Sci.* **2019**, *10,* 7952 – 7957.

[193] Ni, D.; Brown, M. K. Three-Component Ni-Catalyzed Silylacylation of Alkenes. *ACS Catal.* **2021**, *11*, 1858 – 1862.

[194] Xu, S.; Chen, H.; Zhou, Z,; Kong, W. Three-Component Alkene Difunctionalization by Direct and Selective Activation of Aliphatic C− H Bonds. *Angew. Chem. Int. Ed.* **2021**, *60*, 7405 – 7411.

[195] Shu, W.; García-Domínguez, A.; Quiros, M. T.; Mondal, R.; Cardenas, D. J.; Nevado, C. Ni-catalyzed reductive dicarbofunctionalization of nonactivated alkenes: scope and mechanistic insights. *J. Am. Chem. Soc*. **2019**, *141*, 13812 – 13821.

[196] Stokes, B. J.; Liao, L.; Mendes de Andrade, A.; Wang, Q.; Sigman, M. S. A palladium-catalyzed three-component-coupling strategy for the differential vicinal diarylation of terminal 1, 3-dienes. *Org. Lett.* **2014**, *16,* 4666 – 4669.

[197] (a) Granger, B. A.; Wang, Z.; Kaneda, K.; Fang, Z.; Martin, S. F. Multicomponent Assembly Processes for the Synthesis of Diverse *Yohimbine*and *Corynanthe* Alkaloid Analogues. *ACS Comb. Sci.* **2013**, *15*, 379 – 386. (b) Li, T.; Liang, K.; Zhang, Y.; Hu, D.; Ma, Z.; Xia, C. Three-Component Minisci Reaction with 1, 3-Dicarbonyl Compounds Induced by Visible Light. *Org. Lett.* **2020**, *22*, 2386−2390.

(c) Wang, Q.; Qu, Y.; Tian, H.; Liu, Y.; Song, H.; Wang, Q. Trifluoromethylation and Monofluoroalkenylation of Alkenes through Radical–Radical Cross-Coupling. *Chem. Euro. J.* **2019**, *25*, 8686 – 8690.

[198] Guo, L.; Tu, H.; Zhu, S.; Chu, L. Selective, intermolecular alkylarylation of alkenes via photoredox/nickel dual catalysis. *Org. Lett.,* **2019**, *21*, 4771 – 4776.

[199] (a) García-Domínguez, A.; Mondal, R.; Nevado, C. Dual Photoredox/Nickel-Catalyzed Three-Component Carbofunctionalization of Alkenes. *Angew. Chem. Int. Ed.*, **2019**, *58*, 12286 –12290. (b) Shu, W.; García-Domínguez, A.; Quiros, M. T.; Mondal, R.; Cardenas, D. J.; Nevado, C. Ni-catalyzed reductive dicarbofunctionalization of nonactivated alkenes: scope and mechanistic insights. *J. Am. Chem. Soc*. **2019**, *141*, 13812 – 13821.

[200] Derosa, J.; Apolinar, O.; Kang. T.; Tran, V. T.; Engle, K. M. Recent developments in nickel-catalyzed intermolecular dicarbofunctionalization of alkenes. *Chem. Sci.,* **2020**, *11*, 4287 – 4296.

[201] Bauer, I.; Knölker, H. Iron catalysis in organic synthesis. *Chem. Rev.* **2015**, *115*, 3170-3387.

[202] (a) Liu, L.; Lee, W.; Yuan, M.; Acha, C.; Geherty, M. B.; Williams, B.; Gutierrez, O. Intra-and intermolecular Fe-catalyzed dicarbofunctionalization of vinyl cyclopropanes. *Chem. Sci.,* **2020**, *11*, 3146 – 3151. (b) Liu, L.; Lee, W.; Zhou, J.; Bandyopadhyay, S.; Gutierrez, O. Radical-clock α-halo-esters as mechanistic probes for bisphosphine iron-catalyzed cross-coupling reactions. *Tetrahedron*, **2019**, *75*, 129 – 136.

[203] Liu, L.; Lee, W.; Youshaw, C. R.; Yuan, M.; Geherty, M. B.; Zavalij, P. Y.; Gutierrez, O. Fe-catalyzed three-component dicarbofunctionalization of unactivated alkenes with alkyl halides and Grignard reagents. *Chem. Sci.* **2020**, *11*, 8301-8305.

[204] (a) Wang, J.; Sańchez-Roselló ,M.; Aceña, J. L.; del Pozo, C.; Sorochinsky, A. E.; Fustero, S.; Soloshonok, V. A.; Liu, H. Fluorine in pharmaceutical industry: fluorine-containing drugs introduced to the market in the last decade (2001–2011). *Chem. Rev.* **2014**, *114*, 2432−2506. (b) Hong, C. M.; Whittaker, A. M.; Schultz, D. M. Nucleophilic Fluorination of Heteroaryl Chlorides and Aryl Triflates Enabled by Cooperative Catalysis. *J. Org. Chem.* **2021**, 86, 3999 – 4006.

[205] Tu, H.; Wang, F.; Huo, L.; Li, Y.; Zhu, S.; Zhao, X.; Li, H.; Qing, F.; Chu, L. Enantioselective three-component fluoroalkylarylation of unactivated olefins through nickel-catalyzed cross-electrophile coupling. *J. Am. Chem. Soc.* **2020**, *142*, 9604–9611.

[206] Genoni, A.; Benaglia, M.; Puglisi, A.; Rossi, S. Chiral Bis-pyridinium Salts as Novel Stereoselective Catalysts for the Metal-Free Diels-Alder Cycloaddition of α,β-Unsaturated Aldehydes. *Synthesis* **2011,** *12,* 1926 – 1929.

[207] Font, D. ; Canta, M. ; Milan, M. ; Cussó, O. ; Ribas, X. ; Klein Gebbink, R. J. M. ; Costas, M. ; Readily Accessible Bulky Iron Catalysts exhibiting Site Selectivity in the Oxidation of Steroidal Substrates. *Dalton Trans.* **2016,** *55,* 5776 – 5779.

[208] Chen, M. S.; White, C. M. A Predictably Selective Aliphatic C–H Oxidation Reaction for Complex Molecule Synthesis. *Science* **2007**, *318*, 783 – 787.

[209] Millar, S. Liquid/liquid Diffusion or Layering Technique. In *Tips and Tricks for the Lab: Growing Crystals Part 3*. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, 2012.

[210] England, J.; Britovsek, G. J. P.; Rabadia, N.; White, A. J. P. Ligand Topology Variations and the Importance of Ligand Field Strength in Non-Heme Iron Catalyzed Oxidations of Alkanes. *Inorg. Chem.* **2007**, *46*, 3752.

[211] Becke, A. D. A new mixing of Hartree–Fock and local density-functional theories. *J. Chem. Phys.* **1993**, *98*, 1372.

[212] Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov,

T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[213] Improta, R.; Barone, V.; Scalmani, G.; Frisch, M. J. A state-specific polarizable continuum model time dependent density functional method for excited state calculations in solution. *J. Chem. Phys.* **2006,** *125*, 1.

[214] Zhao, Y.; Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.* **2006**, *125*, 194101.

[215] Grimme, S. Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J. Comp. Chem*. **2006**, *27*, 1787.

[216] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

[217] GaussView, Version5, Dennington, R., Keith, T. A., Millam, J. M., Semichem Inc., Shawnee Mission, KS, 2009

[218] Huang, H.; Okuno, T.; Tsuda, K.; Yoshimura, M.; Kitamura, M. Enantioselective Hydrogenation of Aromatic Ketones Catalyzed by Ru Complexes of Goodwin−Lions-type sp2N/sp3N Hybrid Ligands R-BINAN-R'-Py. *J. Am. Chem. Soc.,* **2006***, 128,* 8716 – 8717.

[219] (a) Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.*, **2008**, *120*, 215-241. (b) Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J. A complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-row atoms. *J. Chem. Phys*. **1988**, *89*, 2193-218. (c) Petersson, G. A.; Al-Laham, M. A. A complete basis set model chemistry. II. Open-shell systems and the total energies of the first-row atoms. *J. Chem. Phys.* **1991**, *94*, 6081-90.

(d) Hay, P. J.; Wadt, W. R. Ab initio effective core potentials for molecular calculations - potentials for the transition-metal atoms Sc to Hg. *J. Chem. Phys.* **1985**, *82*, 270-83. (e) Miertuš, S.; Scrocco, E.; Tomasi, J. Electrostatic Interaction of a Solute with a Continuum. A Direct Utilization of ab initio Molecular Potentials for the Prevision of Solvent Effects. *Chem. Phys.* **1981**, *55*, 117-29.

[220] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal solvation model based on solute electron density and a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B*. **2009**, *113*, 6378-96.

[221] McLean, A. D.; Chandler, G. S. Contracted Gaussian-basis sets for molecular calculations. 1. 2nd row atoms, Z=11-18. *J. Chem. Phys.* **1980**, *72*, 5639-48.

[222] (a) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648-52. (b) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, S. A consistent and accurate ab initio parametrization of density functional dispersion correction (dft-d) for the 94 elements H-Pu. *J. Chem. Phys.* **2010,** *132*, 154104. (c) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. V. R. Efficient diffuse function-augmented basis-sets for anion calculations. 3. The 3-21+G basis set for 1st-row elements, Li-F. *J. Comp. Chem.* **1983**, *4*, 294-301.

[223] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

[224] Anderson, T.L.; Kwan, E.E. *PyQuiver* **2016**, www.github.com/ekwan/PyQuiver.

[225] Singleton, D. A.; Wang, Z. H. Isotope Effects and the Nature of Enantioselectivity in the Shi Epoxidation. The Importance of Asynchronicity *J. Am. Chem. Soc.* **2005**, *127*, 6679 – 6685.

[226] (a) Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, *120*, 215-41. (b) Hay, P. J.; Wadt, W. R. Ab initio effective core potentials for molecular calculations - potentials for the transition-metal atoms Sc to Hg. *J. Chem. Phys.* **1985**, *82*, 270-83. (c) Tomasi, J.; Mennucci, B.; Cammi, R. Quantum mechanical continuum solvation models. *Chem. Rev.* **2005,** *105*, 2999-3093.

[227] (a) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648-52. (b) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, S. A consistent and accurate ab initio parametrization of density functional dispersion correction (dft-d) for the 94 elements H-Pu. *J. Chem. Phys.* **2010,** *132*, 154104. (c) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. V. R. Efficient diffuse function-augmented basis-sets for anion calculations. 3. The 3-21+G basis set for 1st-row elements, Li-F. *J. Comp. Chem.* **1983**, *4*, 294-301.

[228] (a) Neese, F. The ORCA program system, Wiley Interdiscip. Rev. *Comput. Mol. Sci.* **2012**, *2*, 73-78. (b) Riplinger, C.; Pinski, P.; Becker, U.; Valeev, E. F.; Neese, F., *J. Chem. Phys.* **2016**, *144*, 024109. (c) Hellweg, A.; Hattig, C.; Hofener, S.; Klopper, W. Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. *Theor. Chem. Acc.* **2007**, *117*, 587 – 597.

[229] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

[230] Wiechert, D.; Mootz, D.; Franz, R.; Siegemund, G. Amine-Poly(Hydrogen Fluoride) Solid Complexes: New Studies of Formation, Crystal Structures, and $H_{n-1}F_n^-$ Ion Diversity. *Chem. Eur. J.* **1998,** *4,* 1043 – 1047.

[231] (a) Becke, A. D. A new mixing of Hartree-Fock and local density-functional theories. *J. Chem. Phys.* **1993**, *98*,1372-1377. (b) Becke, A. D. Density-functional thermochemistry III. The role of exact exchange. *J. Chem. Phys.***1993**, *98*, 5648-5652. (c) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density. *Phys. Rev. B.* **1988**, *37*, 785-789. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. Ab initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields. *J. Phys. Chem.* **1994**, *98*, 11623-11627.

[232] Marenich, A. V.; Cramer, C. J.; Thrular, D. G. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *Phys. Chem. B,* **2009**,*113*, 6378- 6396.

[233] Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc*., **2008**, *120*, 215-241.

[234]Grimme, S. Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J. Comp. Chem.*, **2006,** *27***,**1787- 1799.

[235] Weigend, F.; Ahlrichs, R.; Balanced basis sets of split valence, triple zeta valence, and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys*. *Chem. Chem. Phys.* **2005**, *7*, 3297 – 3305.

[236] Hellweg, A.; Hattig, C.; Hofener, S.; Klopper, W. Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. *Theor. Chem. Acc.* **2007**, *117*, 587 – 597.

[237](a) Neese, F. The ORCA program system *Wiley Interdiscip. Rev.: Comput. Mol. Sci*. **2012**, *2*, 73 – 78. (b) Riplinger, C.; Sandhoefer, B.; Hansen, A.; Neese, F. Natural triple excitations in local coupled cluster calculations with pair natural orbitals. *J. Chem. Phys.* **2013**, *139*, 134101.

[238] (a)Liakos, D. G.; Sparta, M.; Kesharwani, M. K.; Martin, J. M. L.; Neese, F. Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. *J. Chem. Theory Comput.,* **2015**, *11*, 1525 – 1539; (b) Paulechka, E.;. Kazakov, A. Efficient DLPNO–CCSD(T)-Based Estimation of Formation Enthalpies for C-, H-, O-, and N-Containing Closed-Shell Compounds Validated Against Critically Evaluated Experimental Data. *J. Phys. Chem. A,* **2017**, *121*, 4379 – 4387.

[239] For selected examples, see: (a) Lu, Q.; Neese, F.; Bistoni, G. Formation of Agostic Structures Driven by London Dispersion. *Angew. Chem. Int. Ed.* **2018**, *57*, 4760-4764. (b) Riplinger, C.; Sampson, M. D.; Ritzmann, A. M.; Kubiak, C. P.; Carter, E. A. Mechanistic Contrasts between Manganese and Ruthenium Bipyridine Electrocatalysts for the Reduction of Carbon Dioxide. *J. Am. Chem. Soc.* **2014**, *136*, 16285-16298.

[240] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

[241] (a) Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.*, **2008**, *120*, 215-241. (b) Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J. A complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-row atoms. *J. Chem. Phys*. **1988**, *89*, 2193-218.

(c) Petersson, G. A.; Al-Laham, M. A. A complete basis set model chemistry. II. Open-shell systems and the total energies of the first-row atoms. *J. Chem. Phys.* **1991**, *94*, 6081-90. (d) Hay, P. J.; Wadt, W. R. Ab initio effective core potentials for molecular calculations - potentials for the transition-metal atoms Sc to Hg. *J. Chem. Phys.* **1985**, *82*, 270-83. (e) Miertuš, S.; Scrocco, E.; Tomasi, J. Electrostatic Interaction of a Solute with a Continuum. A Direct Utilization of ab initio Molecular Potentials for the Prevision of Solvent Effects. *Chem. Phys.* **1981**, *55*, 117-29.

[242] McLean, A. D.; Chandler, G. S. Contracted Gaussian-basis sets for molecular calculations. 1. 2nd row atoms, Z=11-18. *J. Chem. Phys.* **1980**, *72*, 5639-48.

[243] (a) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648-52. (b) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, S. A consistent and accurate ab initio parametrization of density functional dispersion correction (dft-d) for the 94 elements H-Pu. *J. Chem. Phys.* **2010,** *132*, 154104. (c) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. V. R. Efficient diffuse function-augmented basis-sets for anion calculations. 3. The 3-21+G basis set for 1st-row elements, Li-F. *J. Comp. Chem.* **1983**, *4*, 294-301.

[244] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

[245] a) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.*, **1993**, *98*, 5648-5652. b) Grimme, S. Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J. Comp. Chem.,* **2006**, *27,* 1787-1799. c) Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.,* **2005**, *7*, 3297-3305. d) Hay, P. J.; Wadt, W. R. Ab initio effective core potentials for molecular calculations - potentials for the transition-metal atoms Sc to Hg. *J. Chem. Phys.*, **1985**, *82,* 270-283.

[246] Tomasi, J.; Mennucci, B.; Cammi, R. Quantum mechanical continuum solvation models. *Chem. Rev.,* **2005**, *105*, 2999-3093.

[247] a) Weigend, F. Accurate Coulomb-fitting basis sets for H to Rn. *Phys. Chem. Chem. Phys.,* **2006**, *8*, 1057-1065. b) Fuentealba, P.; Preuss, H.; Stoll, H.; Szentpály, L. V. A Proper Account of Core-polarization with Pseudopotentials - Single Valence-Electron Alkali Compounds. *Chem. Phys. Lett.,* **1982**, *89*, 418-22.

[248] Mulliken, R. S., Electronic Population Analysis on LCAO–MO Molecular Wave Functions. I. *J. Chem. Phys.* **1955**, *23*, 1833-1840.

[249] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

[250] Lu, T.; Chen, F., Multiwfn: A multifunctional wavefunction analyzer. *J. Comp. Chem.* **2012,** *33*, 580-592.

[251] Humphrey, W.; Dalke, A.; Schulten, K., VMD – Visual Molecular Dynamics. *J. Mol. Graphics* **1996,** *14*, 33-38.

[252] (a) Horn, P. R.; Head-Gordon, M. Alternative definitions of the frozen energy in energy decomp**o**sition analysis of density functional theory calculations**.** *J. Chem. Phys.* **2016**, *144*, 084118. (b) Horn, P. R.; Mao, Y.; Head-Gordon, M. Defining the contributions of permanent electrostatics, Pauli repulsion, and dispersion in density functional theory calculations of intermolecular interaction energies. *J. Chem. Phys.* **2016**, *144*, 114107. (c) Horn, P. R.; Mao, Y.; Head-Gordon, M. Probing non-covalent interactions with a second-generation energy decomposition analysis using absolutely localized molecular orbitals. *Phys. Chem. Chem. Phys.* **2016**, *18*, 23067−23079.

[253] Shao, Y.; Gan, Z.; Epifanovsky, E.; Gilbert, A. T. B.; Wormit, M.; Kussmann, J.; Lange, A. W.; Behn, A.; Deng, J.; Feng, X.; Ghosh, D.; Goldey, M.; Horn, P. R.; Jacobson, L. D.; Kaliman, I.; Khaliullin, R. Z.; Kus, T.; Landau, A.; Liu, J.; Proynov, E. I.; Rhee, Y. M.; Richard, R. M.; Rohrdanz, M. A.; Steele, R. P.; Sundstrom, E. J.; Woodcock, H. L.; Zimmerman, P. M.; Zuev, D.; Albrecht, B.; Alguire, E.; Austin, B.; Beran, G. J. O.; Bernard, Y. A.; Berquist, E.; Brandhorst, K.; Bravaya, K. B.; Brown, S. T.; Casanova, D.; Chang, C.-M.; Chen, Y.; Chien, S. H.; Closser, K. D.; Crittenden, D. L.; Diedenhofen, M.; DiStasio, R. A.; Do, H.; Dutoi, A. D.; Edgar, R. G.; Fatehi, S.; Fusti-Molnar, L.; Ghysels, A.; Golubeva-Zadorozhnaya, A.; Gomes, J.; Hanson-Heine, M. W. D.; Harbach, P. H. P.; Hauser, A. W.; Hohenstein, E. G.; Holden, Z. C.; Jagau, T.-C.; Ji, H.; Kaduk, B.; Khistyaev, K.; Kim, J.; Kim, J.; King, R. A.; Klunzinger, P.; Kosenkov, D.; Kowalczyk, T.; Krauter, C. M.; Lao, K. U.; Laurent, A. D.; Lawler, K. V.; Levchenko, S. V.; Lin, C. Y.; Liu, F.; Livshits, E.; Lochan, R. C.; Luenser, A.; Manohar, P.; Manzer, S. F.; Mao, S.-P.; Mardirossian, N.; Marenich, A. V.; Maurer, S. A.; Mayhall, N. J.; Neuscamman, E.; Oana, C. M.; Olivares-Amaya, R.; O'Neill, D. P.; Parkhill, J. A.; Perrine, T. M.; Peverati, R.; Prociuk, A.; Rehn, D. R.; Rosta, E.; Russ, N. J.; Sharada, S. M.; Sharma, S.; Small, D. W.; Sodt. Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Mol. Phys.* **2015**, *113*, 184−215.

[254] Thomas, A. A.; Speck, K.; Kevlishvili, I.; Lu, Z; Liu, P.; Buchwald, S. L. Mechanistically Guided Design of Ligands That Significantly Improve the Efficiency of CuH-Catalyzed Hydroamination Reactions. *J. Am. Chem. Soc.* **2017**, *140*, 13976 – 13984.

[255] Bickelhaupt, F. M.; Houk, K. N. Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. *Angew. Chem., Int. Ed.* **2017**, *56*, 10070−10086.

[256] Manivasagam, S.; Laury, M. L.; Wilson, A. K. Pseudopotential-Based Correlation Consistent Composite Approach (rp-ccCA) for First- and Second-Row Transition Metal Thermochemistry. *J. Phys. Chem. A* **2015**, *119*, 6867−6874.

[257] For representative examples where pseudopotentials were used to describe Mo and W, refer to the following: (a) Ishiguro, Y.; Kudo, T.; Muraoka, T.; Ueno, K. Theoretical Study for the Reactions of (Silyl)(silylene)tungsten and molybdenum complexes with Ethylene Sulfide, *Organometallics* **2014**, *33*, 2704−2712. (b) Asako, S.; Ishikawa, S.; Takai, K. Synthesis of Linear Allylsilanes vis Molybdenum-Catalyzed Regioselective Hydrosilylation of Allenes. *ACS Catal.* **2016**, *6*, 3387−3395, (c) Itabashi, T.; Arashiba, K.; Tanaka, H.; Konomi, A.; Eizawa, A.; Nakajima, K.; Yoshizawa, K.; Nishibayashi, Y. Synthesis and Catalytic Reactivity of Bis(molybdenum-trihalide) Complexes Bridged by Ferrocene Skeleton toward Catalytic Nitrogen Fixation. *Organometallics* **2019**, *38*, 2863−2872. (d) Oztopcu, O.; Holzhacker, C.; Puchberger, M.; Weil, M.; Mereiter, K.; Veiros, L. F.; Kirchner, K. Synthesis and Characterization of Hydrido Carbonyl Molybdenum and Tungsten PNP Pincer Complexes. *Organometallics* **2013**, *32*, 3042−3052. (e) Bouhoute, Y.; Garron, A.; Grekov, D.; Merle, N.; Szeto, K. C.; Mallmann, A. D.; Rosal, I. D. Maron, L., Girard, G.; Gauvin, R. M.; Delevoye, L.; Taoufik, M. Well-Defined Supported Mononuclear Tungsten Oxo Species as Olefin Metathesis Pre-Catalysts. *ACS Catal.* **2014**, *4*, 4232−4241. (f) Chen, P.; Zhang, L.; Xue, Z.; Wu, Y.; Zhang, X. Density Functional Theory Study of the Reaction between d^0 Tungsten Alkylidyne Complexes and H_2O: Addition versus Hydrolysis. *Inorg. Chem.* **2017**, *56*, 7111−7119.