ABSTRACT

Title of Dissertation: Mechanistic Studies and Rational Catalyst Design of Nickel/Photoredox Dual-Catalyzed C–C Cross-Coupling Reactions

Mingbin Yuan, Doctor of Philosophy, 2022

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The merging of photoredox and nickel catalysis has revolutionized the field of C–C cross-coupling. However, in comparison to the development of synthetic methods, detailed mechanistic investigations of these catalytic systems are lagging. In this vein, computational tools have been applied to elucidate the mechanistic pictures, allowing for the rational design of new catalysts and the development of novel reactivity. Based on the reported studies, it appears that the mechanistic picture of catalytic systems is not generally applicable, but is rather dependent on the specific choice of substrate, ligands, photocatalysts, etc. Therefore, the challenges and opportunities of investigating the mechanisms of Ni/photoredox dual-catalyzed C–C cross-coupling reactions were first discussed (**Chapter 1**).

Using both quantum mechanics and molecular dynamics simulations, the mechanism of the tertiary radical cross-coupling between alkyl trifluoroborates and aryl bromides was then investigated, revealing the effect of ligands and the properties of alkyl radicals (**Chapter 2**). After exploring the mechanism of two-component Ni/photoredox dual-catalyzed C(sp^2)–C(sp^3) cross-couplings,

further mechanistic investigation was conducted for multicomponent cross-coupling reactions, revealing the factors controlling reactivity and selectivity in these complex catalytic transformations. In a multicomponent C–H activation/cross-coupling reaction, the origin of chemoselectivity between two-component versus three-component products was studied, showcasing the effect of intramolecular H-bonding (**Chapter 3**). Moreover, the mechanism of a novel enantioselective olefin difunctionalization was computationally investigated, identifying the radical addition step as the enantioselectivity-determining step (**Chapter 4**). Expanded to a wider scope of catalytic systems and reagents, the catalytic cycles of an enantioselective dicarbofunctionalization of vinylphosphonate were explored, demonstrating the origin of stereo- and enantioselectivity of this transformation (**Chapter 5**).

Given the complexity of the mechanistic pictures of these nickel metallaphotoredox systems, the need for more accurate computational methods, readily available and user-friendly dynamics simulation tools, and data-driven approaches is clear in order to understand at the molecular level of these transformations.

MECHANISTIC STUDIES AND RATIONAL CATALYST DESIGN OF NICKEL/PHOTOREDOX DUAL-CATALYZED C–C CROSS-COUPLING REACTIONS

by

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Chapter 1: Challenges and Opportunities of Ni/Photoredox Dual-Catalyzed C(sp^2)–C(sp^3) Cross-Couplings

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1.1 Abstract

The merging of photoredox and nickel catalysis has revolutionized the field of C–C cross-coupling. However, in comparison to the development of synthetic methods, detailed mechanistic investigations of these catalytic systems are lagging. In this vein, computational tools have been applied to elucidate the mechanistic pictures, allowing for the rational design of new catalysts and the development of novel reactivity.

Based on the reported computational studies, it appears that the mechanistic picture of catalytic systems is not generally applicable, but is rather dependent on the specific choice of substrate, ligands, photocatalysts, etc. Given the complexity of these systems, the need for more accurate computational methods, readily available and user-friendly dynamics simulation tools, and data-driven approaches is clear in order to understand at the molecular level the mechanisms of these transformations. In particular, we anticipate that such improvement of theoretical methods will become crucial to advance the understanding of excited-state properties and dynamics of key species, as well as to enable faster and unbiased exploration of reaction pathways. Further, with greater collaboration between computational, experimental, and spectroscopic communities, the mechanistic investigation of photoredox/Ni dual-catalytic reactions is expected to thrive quickly, facilitating the design of novel catalytic systems and promoting our understanding of the reaction selectivity.

1.2 Introduction

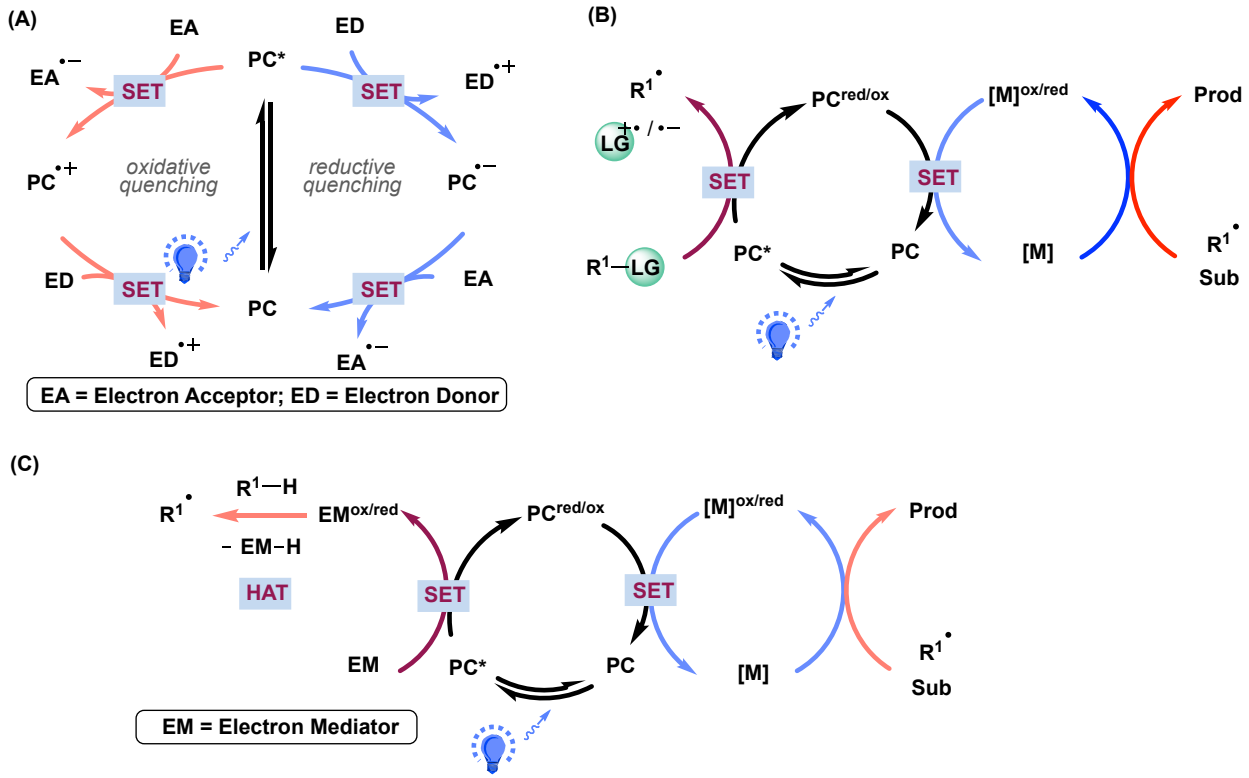

Figure 1.1 Commonly proposed mechanisms of photoredox/metal dual-catalyzed reactions. (A) Electron transfer events involved in light-irradiated conditions between the electron acceptor/donor and the excited photocatalyst (i.e., via oxidative or reductive quenching, respectively). (B) Proposed mechanism of metallaphotoredox-catalyzed carbon-carbon cross-coupling reactions, where radicals are generated via single-electron transfer between radical precursors and the excited photocatalyst. Sub = substrates; Prod = products. (C) Proposed mechanism of metallaphotoredox-catalyzed carbon-carbon cross-coupling reactions via H-atom abstraction in the presence of electron mediator.

Transition-metal-catalyzed C(sp^2)–C(sp^2) cross-coupling reactions have revolutionized the field of carbon-carbon bond formation in organic synthesis and are widely used in the pharmaceutical industry. However, the broader application of these synthetic strategies to the formation of C(sp^2)–C(sp^3) and C(sp^3)–C(sp^3) bonds remains a challenge due to, inter alia, unwanted side reactions from beta-hydride elimination and the requirement of harsh conditions (e.g., high temperature, strong bases, etc.).[1] To overcome these challenges, modifications to the

catalytic systems have focused on ligand design, manipulation of oxidation states, and electronic excitation.[2] In this vein, the merging of nickel and photoredox catalysis has become an attractive method to construct carbon-carbon bonds. Compared to traditional cross-coupling chemistry, they not only require milder conditions but also expand the chemical space by allowing the incorporation of sp^3-hybridized carbons into bioactive chemicals and drug candidates.[2-9] Moreover, photoredox-mediated radical generation has acted as an effective strategy to expand the toolbox of cross-coupling partners that are rarely utilized in transition metal-catalyzed protocols (**Figure 1.1A**). In this context, a broad variety of radical precursors have found applications in photoredox and nickel dual-catalyzed cross-coupling reactions, including alkyl halides,[10] carboxylic acids,[4] silicates,[11-12] 4-alkyl-1,4-dihydropyridines (DHPs),[13-15] trifluoroborates,[3, 16] and oxalates[17] (**Figure 1.1B**). In addition, sp^3-hybridized C–H bonds are also eligible as latent radical precursors in photoredox/Ni dual-catalyzed C–C cross-coupling reactions via the combination of photo-assisted hydrogen-atom-transfer (HAT) and nickel catalysts (**Figure 1.1C**).[18-19] The HAT process can be realized by the utilization of an external agent (e.g., quinuclidine), electrophile (heteroatom), or an excited photocatalyst (biphenylketone, decatungstate, etc.)

Overall, in stark contrast to the rapid growth of synthetic methods in this area, the knowledge about the molecular-level interactions in many of these catalytic reactions is rudimentary. On the contrary, the operating mechanisms in traditional transition-metal-catalyzed cross-couplings reactions (e.g. Pd-catalyzed cross-coupling reactions) have been successfully characterized by both experimental and computational methods and, in turn, one can argue that this information has led to more rational reaction design.[20-21] In all, palladium chemistry is found to mainly undergo electron transfer in pairs and change in oxidation states by two units, i.e., Pd^0/Pd^{II} and Pd^{II}/Pd^{IV} catalytic cycles. However, Ni is more accessible to multiple oxidation states

compared to Pd, involving Ni^0, Ni^I, Ni^{II}, Ni^{III}, and high-valent species Ni^{IV}, thus is more prone to undergo SET processes in the presence of suitable reagents.[1] In these dual catalytic systems, both polar and radical mechanisms might operate, and multiple species could undergo single electron transfers in the reaction system. Moreover, Ni complexes could also undergo electronic excitation in light-irradiated conditions, either via energy transfer (EnT) in the presence of an excited photocatalyst or via direct excitation by light, which is usually difficult to distinguish using traditional mechanistic tools.[22-29] As a consequence of the inherent complexity in these dual nickel/photoredox catalytic systems, information about the factors that control chemo-, regio- and stereoselectivity for many of these transformations remains virtually unknown.

To understand and design new photo-induced transition-metal-catalyzed reactions, novel aspects of mechanistic investigation need to be considered compared to traditional transition metal-catalyzed reactions. For example, multiple single-electron transfer events, different spin states of metal, excited-state properties of photosensitizers, and dynamical behaviors of high-energy photoexcited electronic states.[30] In this context, the computational study of these highly reactive species and complex reaction mechanisms can provide a blueprint for the rational design of catalyst and reaction. In this short overview, I first focus on commonly used methods (both experimental and computational) to investigate the mechanisms of these transformations. Next, I will briefly examine the encountered challenges in mechanistic exploration and the potential opportunities expected to enhance the understanding of photoredox/Ni dual-catalyzed reactions and facilitate the design of new catalysts. Then, I will highlight several computational studies on the area of $C(sp^2)$–$C(sp^3)$ bond-forming reactions (**Chapter 2–5**). Since I intend to provide an overview of my recent work on the computational study of the mechanisms of photoredox/Ni dual-catalyzed $C(sp^2)$–$C(sp^3)$ cross-coupling reactions, other reviews and representative computation

studies are recommended for extended interest, including the mechanism of C–heteroatom cross-coupling reactions (C–N,[31-35] C–O,[29, 36-41] and C–S bond-forming systems[42]) and the excited-state properties of Ni complexes[22, 24, 29, 32, 38, 40, 43-47]. Notably, compared to C(sp^2)–C(sp^3) cross-coupling reactions, C-heteroatom cross-coupling reactions likely proceed via significantly different catalytic mechanisms. For example, Maseras and coworkers showed that in a C–N cross-coupling reaction, the photocatalyst was involved in the change of oxidation state of Ni via single electron transfer prior to reductive elimination, and the iodide ion was not attached to the Ni center when aryl iodide was applied as electrophile.[33]

Nonetheless, similar to photoredox/Ni dual catalysis, nickel-catalyzed reductive coupling and nickel-catalyzed electrochemical reactions also show access to multiple oxidation states of Ni and the involvement of single-electron transfer events.[8] Therefore, mechanistic study of photoredox/Ni dual catalysis is expected to provide insight into the fundamental steps applicable to the other two fields.

1.3 Experimental Methods of Mechanistic Investigation

1.3.1 Study of ground-state and excited-state thermodynamics

Photoredox/Ni dual-catalyzed reactions often rely on the ability of a light-induced excited photoredox catalyst to undergo single-electron transfer with the quencher (substrate, metal catalyst, external reagent, etc.; **Figure 1.1A**). Therefore, mechanistic studies in this field have benefited from methods developed to study radical chemistry[48-50]and photochemistry[51-54].

Experimental methods to study the properties of ground-state species include UV-Visible (UV-vis) absorption spectroscopy[55] and cyclic voltammetry (CV)[56-57]. With these methods, the concentration of chromophores, and the redox potential of electron donors and electron acceptors

can be measured, respectively. Since many photocatalytic transformations are realized by the transfer of electrons (e.g., single-electron transfer),[58] the evaluation of the redox properties is critical to analyze the thermodynamic feasibility of such a process. Compared to the ground-state species, the excited-state entities are often significantly different (both structurally and electronically) from their ground-state counterparts.[59] Nonetheless, a range of spectroscopic methods[59-61] and photo-modulated voltammetry[62-63] can be used to study the properties of excited-state species and understand their reactivity.

Since the open-shell reactivity of transient species lies at the center of many photo-induced transformations, the mechanistic investigation of photocatalytic processes often relies on experimental methods that are typically used in the field of radical chemistry.[7, 49, 64] For example, radical trapping agents (e.g., phenyl *N*-*tert*-butylnitrone, PNB; 2,2,6,6-tetramethylpiperidine 1-oxyl, TEMPO)[65] and radical clock experiments[66-67] are used to probe the generation and lifetime of radical species. In particular, the latter method can provide kinetic information of a given radical pathway by incorporating the moieties that can undergo rapid unimolecular radical rearrangement pathways (e.g., ring-opening of cyclopropylmethyl radical and radical cyclization of 5-hexenyl radical).

However, due to the fleeting nature of short-lived species in photo-induced reactions, their isolation or trapping with organic species is often challenging. In these cases, spectroscopic methods are often applied to investigate the properties of these reactive open-shell species. In particular, electron paramagnetic resonance (EPR) spectroscopy is commonly used to detect and characterize paramagnetic organic and organometallic species.[68-70] In addition, NMR spectroscopy can be applied to detect the presence of radicals via Chemical Induced Dynamic Nuclear Polarization (CDNIP) spectroscopy that requires in situ illumination within the NMR

spectrometer.[71] Further, the application of more sensitive time-resolved spectroscopic methods like laser flash photolysis (LFP)[72-73] allows for the observation of species with lifespans in the order of pico/femtoseconds (i.e., singlet/triplet excited-state molecules and transient ionic radicals).[74]

1.3.2 Kinetic study of photochemical processes and radical reactivity

Although the thermodynamic preference of bimolecular radical processes can be assessed by determining the redox potentials, the feasibility of a redox event is also dependent on the kinetic parameters.[54] Common experimental methods used to investigate the excited-state kinetics in these transformations involve time-resolved spectroscopic methods like Stern-Volmer analysis[51, 75] and LFP analysis[72], where the kinetics of bimolecular events of emissive excited-state molecules can be obtained (e.g., rate constant of dynamic quenching processes). Apart from these methods, the kinetics of the overall photochemical processes can be studied by the method of initial-rate measurements.[76]

1.4 Computational Methods of Mechanistic Investigation

1.4.1 Density functional theory

The identification of the complex mechanistic scenarios using only with experimental methods is extremely challenging due to the short lifetime of relevant reactive intermediates, the competing side pathways of excited-state species, and the difficulty of assessing kinetic parameters of individual steps. As such, in addition to experimental methods, computational tools have become more common, practical, and powerful to study the molecular-level interactions of reactive species (i.e., excited-state species and radical intermediates) [21, 30, 77-80] involved in photoredox/Ni dual catalysis.[31-32, 81]

Advances in hardware, software, and algorithms in the past decades have led to wider application of quantum mechanical calculations to understand the operating mechanism and facilitate the design of novel catalysts and substrates in photoredox/Ni dual catalysis.[30, 82-83] In particular, density functional theory (DFT) is commonly used in locating intermediates and transition state structures due to its great balance between computational cost and chemical accuracy.[84-93] Moreover, recent efforts aiming to tackle some of the well-known drawbacks of DFT have led to increasing applications in catalysis. For example, DFT is well known for its poor performance in treating noncovalent interactions, which results from the failure of local and semilocal functions to correctly examine the dynamic electron correlation.[30] To overcome this issue, developments have been made in terms of optimized semilocal functions, effective one-electron potentials, density functionals with a nonlocal kernel, and the addition of (semi)empirical pairwise corrections for describing noncovalent interactions.[94-98] Notably, Grimme's D3 correction[97] with the Becke-Johnson damping function[99-100] has been widely used to treat noncovalent interactions in DFT calculations to mitigate the aforementioned issues.

Oftentimes, the choice of functional, basis set, and solvent for DFT calculations is based on prior literature, experience, and the intuition of computational chemists. However, methods appropriate for the study of organic molecules and closed-shell transition metals systems might not be suitable for investigating the electronic, structural properties, thermodynamics, and kinetics of open-shell 3d transition metal complexes.[30] As such, benchmarking and calibration with available experimental data are always recommended to study these systems.[101-102] To verify the accuracy of the computed structural properties and electronic configuration (e.g., spin states), the expectation value of the $\langle S^2 \rangle$ operator and frequency analysis of open-shell and closed-shell configurations is recommended.[30] The inspection of these parameters is important as multiple spin states are readily accessible for late 3d transition metal systems.[103-106] In sum, the development of a physically accurate, broadly applicable, and practical computational method remains one of the holy grails in computational chemistry.[107] Therefore, caution is advised when studying the mechanisms using purely computational tools, especially when related to nickel/photoredox catalysis, as the absolute energetics for each step in the catalytic cycles are likely to be dependent on the choice of DFT functional and basis set.[21, 30, 108-109]

1.4.2 Coupled-Cluster theory

Beyond DFT, coupled-cluster singles-and-doubles with perturbative triples (CCSD(T)) theory has been considered as the "golden standard" of quantum chemistry. However, this method remains virtually impractical for the analysis of (large) complex organic and organometallic systems (such as dual nickel/photoredox cross-coupling catalysis) due to its high computational cost.[110] To address this issue, Neese and coworkers have developed DLPNO-CCSD(T) method that involves domain-based local pair approximation.[111] Such a method can emulate CCSD(T) accuracy with the use of a suitable basis set with a low computational cost comparable to DFT methods and thus likely leads to wider application to studying nickel/photoredox dual catalysis.[112-116] In this vein, our group has applied this method to calculate the single-point energies of the full catalytic cycle of a challenging single-electron Tsuji-Trost reaction[117] and a three-component C–H activation/alkene dicarbofunctionalization reaction[118] in photoredox/Ni dual catalytic conditions (*vide infra*).

1.4.3 Multireference and multiconfigurational theories

Under photoredox/Ni dual catalytic conditions, nickel complexes can access different spin states and, as a consequence, single-reference methods like DFT could lead to erroneous conclusions. In these scenarios, the application of multireference or multiconfigurational methods including configuration interaction (CI) and multiconfigurational self-consistent-field (MCSCF) are essential to validate the computational method.[78] For example, the complete-active-space self-consistent-field (CASCCF) method builds its success on its proper description of the electronic structure and excited-state properties at the nonequilibrium geometries of mono- and polynuclear transition metal complexes.[119] In addition, multireference methods including CASPT2, NEVPT2,

and MRCI can also be used to intrinsically to analyze the conical intersections between various electronic states.[30, 78] An alternative method, DFT/MRCI method, uses Kohn-Sham orbitals to construct CSFs and to modify an MRCI-type Hamiltonian.[120-121] However, the applicability of these methods is limited by the dependence on the definition and size of active space. Thus, due to the generally greater computational cost of multireference methods, time-dependent DFT (TD-DFT) has been widely used in the study of electronic spectroscopy and photochemistry of transition metal complexes.[85, 122-123] However, the main error of TD-DFT arises from the erroneous long-range behavior of most density functionals, the lack of double and higher excitations, and the limited accuracy of higher spin states.[124] Regarding these issues, the computed results of TD-DFT are dependent on the choice of exchange-correlation functional, and the accuracy can be greatly promoted when it is combined with range-separated functionals or functionals with 100% HF exchange.[125]

1.5 Emerging Opportunities in the Computational Analysis of Mechanisms

1.5.1 More accurate and affordable computational methods for the description of excited-state and multiconfiguration properties

To facilitate the computational study of photoredox and Ni systems, multireference (MR) methods are needed to map the excited-state potential energy surface.[78] However, compared to single reference methods, application of MR methods usually require (or benefits from) more advanced knowledge (or assumptions) of the structural and electronic properties of the species under investigation.[78, 126-127] Therefore, the development of more accurate, faster multireference methods is needed to map the excited-state PES at the cost of similar computational efficiency to single-reference methods. In addition to the excited-state nature of electronic configurations under

photoexcited conditions, the multiconfigurational effect of Ni along with its ability to undergo spin crossover in reaction conditions necessitates the application of MR methods. Notably, under light irradiation, the properties of Ni intermediates in high spin states (i.e., triplet spin state) have been studied but the photophysics and dynamical properties of such intermediates are still not well-understood.[29, 38, 45] In all, increasingly accurate and efficient electronic structure calculation methods are needed for broader applicability to larger, more realistic (rather than highly truncated) catalytic systems.[30]

1.5.2 Study of ground-state and excited-state dynamical behavior

Quantum mechanical calculations are useful to examine the properties of static points on the potential energy surface (PES), including local minima (reactants, intermediates, and products) and saddle points (transition states). After obtaining the structures of stationary points, reactivity and selectivity of the reaction are often rationalized based on the calculated kinetics (i.e., barriers using transition state theory) and thermodynamics.[83, 108] However, sometimes transition state theory (TST) fails to rationalize or predict product selectivity.[128-131] In such scenarios, Born-Oppenheimer molecular dynamics (BOMD) calculations on the QM-calculated PES can be used to generate a statistically representative number of trajectories from the transition states, as well as to monitor the dynamics of reactive events of relevant metal species.[132] In addition, quasi-classical molecular dynamics has been applied with great success in both organic reactions with bifurcation points and homogeneous transition metal catalysis.[133-135] For smaller systems, *ab initio* molecular dynamics (AIMD) can also be utilized.[136-139] In addition, since excited-state PES is accessed under light irradiation, the commonly applied molecular dynamics simulation tools need to be modified to take into consideration the behavior of highly energetic species.[140] For example, the nonadiabatic molecular-dynamics (NAMD) simulation method was developed to describe the

nonadiabatic coupling effects between nuclear and electronic motions.[141] Recently, the Lopez group reported a study of the photoinduced denitrogenation of bicyclo azoalkanes with multireference calculations and non-adiabatic molecular dynamics (NAMD) simulations.[142] With simulations starting at the S_1 excited state of cyclic azoalkanes, its photophysics and reactivity were studied, revealing the stereoselectivity of such transformation. In all, with these dynamics simulation tools, opportunities to obtain more detailed information of the dynamical bond-forming and breaking processes of reactants and intermediates will likely lead to greater understanding of these transformations and rational design of dynamically-controlled systems.

1.5.3 Unbiased mapping of potential energy surface and exploration of potential reaction pathways

Apart from the challenges in describing the reactivity of excited-state species, determining speciation and conformation of solvated reactive transition metal species, the dynamical behavior of intermediates, and potential non-productive pathways remain difficult to study.[83] Further, to accelerate the study of *potential* reaction mechanisms, the initial inputs are often biased by chemical intuition and previous knowledge of related systems.[143] In this vein, automated reaction mapping methods are developed to realize the *unbiased* exploration of PES and exhaustively explore plausible reaction pathways.[143-147] However, the computation of excited-state PES becomes more complicated beyond the Franck-Condon region due to the strong mixing between different electronic configurations.[78] This situation becomes even more complicated with the consideration of possible interaction between excited-state species and transition metals.[30] Due to such challenges, improvements of automated mapping approaches of excited-state PES are of great potential with the addition of multireference calculations and the appropriate description of the entire excited-state surfaces. With the development of unbiased analysis of reaction networks, the

computational mechanistic study can be employed to describe the non-productive pathways accounting for the loss of reaction selectivity as well as the deactivation of catalysts.

1.5.4 Data-driven approaches for catalyst design and reaction optimization

Recently, data-driven approaches, benefiting from the large sets of chemical data from online and industrial databases and the improvement of applicable algorithms, have been developed and applied in the field of chemistry.[148-149] One of the advantages of data-driven approaches is that an in-depth mechanistic understanding of the catalytic system is not required, thus facilitates the study of complicated systems where multiple reaction pathways might exist. Common data-driven approaches applied in the field of chemistry include classical statistical analysis and supervised machine learning algorithms.[150] For example, multilinear regression analysis, employed by Sigman and coworkers in several studies, correlates a set of chemical descriptors (obtained through preliminary calculations) to reaction efficiency and, in turn, allows for the prediction of the performance of different substrates and catalysts.[151-153]

Apart from preliminary calculations, data applied for further analysis can also come from high-throughput experimentation (HTE) capable of rapidly generating enormous amounts of data.[154-156] As an example, Doyle and coworkers, in collaboration with Merck, applied a set of QM descriptors obtained from 4608 C–N cross-coupling reactions to random forest algorithm for supervised machine learning. As a result, mechanistic findings and prediction of reaction performance were achieved, which were also verified by experiments.[157] However, it raised a dispute on the algorithm's validity and the variety of dataset used to develop the algorithm by Keiser and Chuang.[158] In response, the authors argued that their model is valid to predict out-of-sample reactions.[159] Nonetheless, the application of data-analyzing approaches to chemistry need

to be done with care, which requires a broad collaboration between the communities of data scientists, synthetic chemists and computational chemists.[160]

1.5.5 Automated systems combined with data-driven approaches

The application of automated experimentation systems has revolutionized the reaction discovery process in synthetic chemistry.[161-162] To this end, the design of new experiments can be improved with adaption to new reaction outcomes in autonomous experimentation with the involvement of decision-making algorithms.[163-164] As an example of application to the field of visible-light photoredox catalysis, Noël and coworkers developed a Python-automated flow platform. Incorporating iniline UV/Vis spectroscopy and Stern-Volmer analysis, this platform not only identified the promising combinations of photocatalyst and quencher but also measured the quenching rate constants.[165]

Apart from automated experimentation, automated computation has also been developed based on data-driven approaches. As an example, Moitessier, Norrby, and coworkers developed the VIRTUAL CHEMIST program that helps bench chemists predict the outcomes of a series of asymmetric chemical reactions. Gratifyingly, it could achieve accuracies within ~1 kcal/mol and provided rapid analysis and a user-friendly working environment. Overall, this technology is expected to accelerate catalyst and reaction discovery.[166]

Moreover, the rapid development of data-driven approaches and related algorithms have facilitated computational chemists with the mechanistic investigation. Commonly, mechanistic exploration is performed based on quantum mechanical calculations to map out the potential energy surface and main reaction pathways based on the experimental findings. With the help of data-driven machine learning (ML) methods, qualitative reaction prediction models can be

generated based on the given data as training sets.[160] For cases where insight-dependent approaches and quantum mechanical calculations are challenging or time-consuming, data-driven approaches are powerful complements. Therefore, quantum mechanical calculations combined with machine learning methods can greatly expand the toolbox of computational methods for the mechanistic exploration of photoredox/Ni dual-catalytic systems.

1.6 Conclusion

Compared to traditional transition-metal-catalyzed cross-couplings, the merger of photoredox and Ni catalysis expands the chemical space, allowing the incorporation of C(sp^3) centers that are previously inaccessible due to side reaction pathways. Moreover, using light as energy input, dual photoredox/Ni catalysis has enabled mild reaction conditions and shows great tolerance of functional groups. Despite the rapid advancements in the field of photoredox/Ni dual catalysis and the growing number of mechanistic studies, the lack of in-depth mechanistic investigation limits the wider application and discovery of novel catalytic systems of this field. Based on the reported mechanistic studies of photoredox/Ni dual-catalyzed C(sp^2)–C(sp^3) cross-coupling reactions (**Chapter 2–5**), the mechanistic picture is dependent on the substrates and catalytic systems employed. Therefore, overgeneralization of mechanism should be avoided, and the analysis of selectivity of reaction needs to be performed based on the specific systems.

To promote the understanding of the complicated mechanistic pictures of developed systems, the use of computational methodologies is of great significance. In particular, properties and molecular-level interactions of the high-energy, short-lived intermediates can be learned with computational approaches. However, improvements need to be made to broaden the application of computational investigation and to facilitate the experimental chemists to take advantage of the

studied results. Regarding this issue, the accuracy and reliability of computational methods can be advanced to deepen the study of properties and dynamical behavior of the key species. Moreover, wider collaboration among computational, experimental, and spectroscopic groups is expected to accelerate reaction discovery, especially for asymmetric transformations. I expect that with the rapid development of many emerging computational tools and data-driven approaches, the mechanistic exploration of photoredox/Ni dual catalytic systems can advance and facilitate the design of novel catalytic systems.

Chapter 2: Mechanistic Study of the Nature of C(sp^3)–C(sp^2) Bond Formation in Nickel/Photoredox Dual-Catalyzed Tertiary Radical Cross-Couplings

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2.1 Abstract

The merger of photoredox and nickel catalysis has enabled the construction of quaternary centers. However, the mechanism, role of the ligand, and effect of the spin state for this transformation and related Ni-catalyzed cross-couplings involving tertiary alkyl radicals in combination with bipyridine and diketonate ligands remain unknown. Several mechanisms have been proposed, all invoking a key Ni(III) species prior to undergoing irreversible inner-sphere reductive elimination. In this work, I, and coworker Zhihui Song, have used open-shell dispersion-corrected DFT calculations, quasi-classical dynamics calculations, and collaborated with the Molander group to perform experiments to study in detail the mechanism of carbon−carbon bond formation in Ni bipyridine- and diketonate-based catalytic systems. Song was responsible for running calculations to explore the catalytic cycle of the diketonate-based (anionic ligand) system, while I ran the DFT calculations on the bipyridine (neutral ligand) system, performed quasi-classical dynamics calculations, and investigated the effect of different alkyl radicals on the reactivity of relevant transformations.

Overall, these calculations revealed that access to high spin states (e.g., triplet spin state tetrahedral Ni(II) species) is critical for effective radical cross-coupling of tertiary alkyl radicals. Further, a disparate mechanism was exhibited for the C−C bond formation between the neutral and

the anionic ligand systems. Specifically, contrary to the neutral Ni-bipyridyl system, diketonate ligands lead directly to the corresponding tertiary radical cross-coupling products via an outer-sphere reductive elimination step via triplet spin state from the Ni(III) intermediates. Implications to related Ni-catalyzed radical cross-couplings and the design of new transformations are discussed.

2.2 Introduction

Nickel-catalyzed cross-coupling reactions (CCRs) have been developed as powerful synthetic methods for the selective construction of carbon-carbon bonds in mild condition.[167] Although C(sp^2)−C(sp^2) couplings are highly reliable and well-established in common metal-catalyzed CCRs, significant limitations are often encountered in the utilization of sp^3-hybridized reagents, particularly in the incorporation of quaternary centers.[168-170] Notable examples (**Figure 2.1A**) are reported by the Glorius[171] and Biscoe[172] groups that used a Ni-based catalyst with N-heterocyclic carbene (NHC) ligands to perform C(sp^2)−C(sp^3) cross-couplings between aryl bromides and tertiary alkyl Grignard nucleophiles. Additionally, Fu employed a nickel/bipyridine system for the cross-coupling between unactivated alkyl bromides and organoboron compounds.[173] In Gong's system, a monodentate pyridine was used as ligand in combination with nickel catalyst for the reductive coupling between aryl halides and tertiary alkyl halides,[174-175] while Watson utilized a Ni/phosphine system for the cross-coupling between tertiary benzylic acetates and organoboron compounds.[176]

In the field of C(sp^3)–C(sp^2) bond formation, nickel/photoredox dual catalysis has developed rapidly since it can be performed in mild condition with great tolerance of functional groups. Since the pioneering reports from the Molander group and the MacMillan, Doyle groups, it's been utilized widely in incorporating C(sp^3) centers from primary and secondary alkyl precursors (**Figure 2.1B**).[3-4] More recently, this dual catalytic strategy has been expanded to the

cross-coupling of tertiary alkyl substrates — in 2017, the Molander group disclosed the first dual photoredox-Ni catalytic strategy for the construction of quaternary center from potassium tertiary alkyltrifluoroborates and aryl bromides (**Figure 2.1C**).[177] Notably, the bidentate bipyridyl-based ligand (4,4-di-*tert*-butyl-2,2-bipyridine; dtbbpy), which has proven effective in the dual photoredox-Ni catalyzed cross-coupling of secondary alkylboron reagents, was found ineffective with acyclic tertiary alkyltrifluoroborates in this case (inset). On the other hand, anionic diketonate-based bidentate ligands (e.g., 2,2,6,6-tetramethyl-3,5-heptanedionate TMHD and acetylacetonate acac) yielded the desired cross-coupling products between acyclic tertiary organoboron reagents and a wide range of electron-poor and electron-neutral aryl bromides. In this context, Baran also reported the use of anionic TMHD ligand in the nickel-catalyzed radical $C(sp^2)$–$C(sp^3)$ cross-coupling between tertiary alkyl redox-active esters and arylzinc reagents (**Figure 2.1A**) while Shenvi reported a dual Mn/Ni(acac)$_2$ system to form all-carbon arylated quaternary centers from tertiary radical precursors.[178-179]

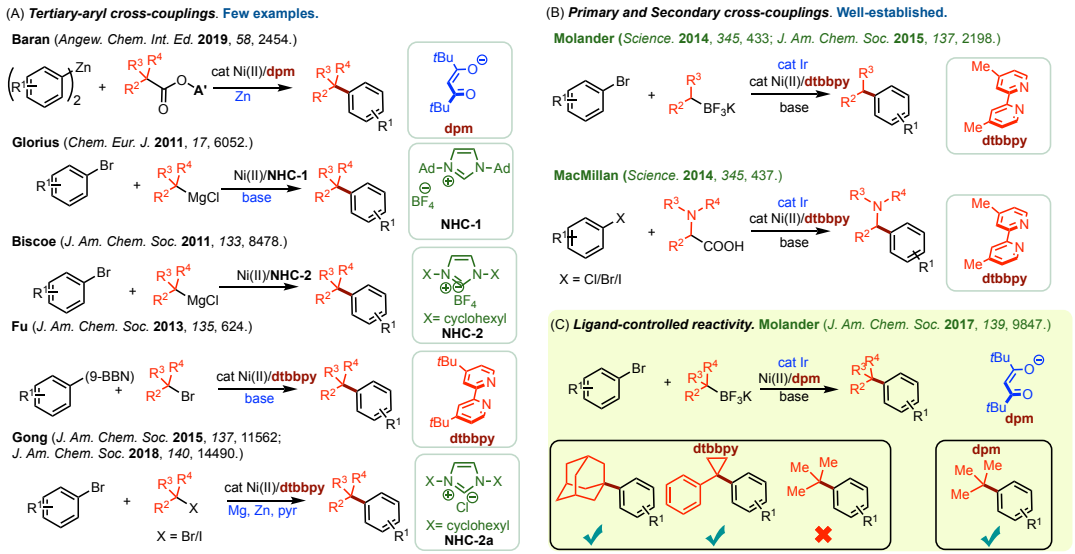


Figure 2.1 (A) Methods for the construction of all-carbon quaternary centers via Ni-catalyzed cross-couplings between tertiary alkyl precursors and aryl halides. (B) Pioneering examples of

Ni/photoredox dual-catalyzed primary and secondary cross-coupling reactions. (C) Ligand-controlled reactivity of tertiary cross-couplings in Ni/photoredox dual catalysis.

However, although the evidence for the presence of radical intermediates in these systems is strong,[3, 5, 180] the mechanism, effect of ligand (neutral versus anionic), and molecular-level understanding of the key C(sp^2)−C(sp^3) bond-forming step remain poorly understood. The use of quantum mechanical calculations to investigate the mechanisms, electronic properties, and dynamics of transition metal complexes has led to a deeper understanding of the molecular-level interactions controlling reactivity and selectivity in complex catalytic cycles.[21, 30, 181-185] Herein, a comprehensive computational study was reported on the mechanism of Ni-catalyzed CCRs between aryl halides and tertiary alkyl radicals using both neutral (dtbbpy) and anionic (TMHD) ligands. Specifically, I used quantum mechanical calculations to explore the operating mechanism of the bipyridine (neutral ligand) system, performed quasi-classical dynamics calculations to study the dynamics of key species, and investigated the effect of different alkyl radicals on their distinct reactivity of in the neutral ligand system. On the other hand, the other coworker Zhihui Song was responsible for running calculations to explore the catalytic cycle of the diketonate-based (anionic ligand) system.

Altogether, the computational results are expected to address such questions: (1) What is the effect of anionic diketonate-based ligands versus neutral bipyridine ligands in the commonly proposed Ni(0)/Ni(I)/Ni(III) and Ni(0)/Ni(II)/Ni(III) pathways?[81] (2) What are the factors responsible for the distinct reactivity of 2º vs. 3º alkyl radicals in the Ni-bipyridine system? (3) What is the role of spin state of the purported Ni complexes and the nature of C(sp^2)–C(sp^3) bond formation in the nickel radical cross-couplings? (4) What is the lifetime of Ni(III) intermediate prior to undergoing inner-sphere reductive elimination and dynamic effects on radical

dissociation/rebound? These knowledge can provide broad implications to the related Ni-catalyzed radical cross-couplings involving tertiary alkyl radicals as reported by Fu, Baran, and others.[173-175, 177, 186]

2.3 Results and Discussion

2.3.1 Computational Methods

All optimizations were performed without restrictions using open-shell, dispersion-corrected DFT (with guess=mix keyword) using THF with CPCM implicit solvation model [noted as UB3LYP-D3/def2-SVP-CPCM(THF)] as implemented in Gaussian 09 (see Appendix 1 for complete reference). Dispersion correction with Becke-Johnson damping (with EmpiricalDispersion=GD3BJ keyword) was also used to calculate the key pathway in the Ni-bipyridine system, and the results were consistent with those calculated with zero-damping (see **Figure A1.9** in Appendix 1 for comparison of calculated results). Stability tests were conducted (with stable keyword) on all singlet species to confirm that the wavefunctions are stable as implemented in Gaussian 09, and all singlet species were identified as closed-shell except **^{1}F'** and **^{1}G'** based on S^2 values (shown in Coordinates and Energetics section in the Supporting Information). Further, for comparison and to refine energetics, I also performed single point energy calculations using a larger basis set (def2-TZVPP), different solvents used experimentally (DMA and THF), other dispersion-corrected DFT functionals (e.g., UM06), and DLPNO-CCSD(T) method (in ORCA; see Supporting Information for complete reference). These methods have been used extensively to rationalize and predict reactivity and selectivity in transition metal-catalyzed transformations, including Ni-catalyzed cross-couplings.[117, 181, 183-184, 187] Overall, all methods lead to the same conclusions (see Supporting Information for details). For simplicity, only the energies

obtained from UB3LYP-D3/def2-TZVPP-CPCM (DMA or THF) will be discussed in the manuscript (See **Figure A1.1** in the Appendix 1 for energetics using other methods of Ni-TMHD system completed by Zhihui). For all purported intermediates, I considered both low and high spin states (i.e., singlet/doublet and triplet/quartet) and performed a manual conformational search to identify the lowest energy structure (See **Figure A1.2** in the Appendix 1). Initially, to reduce the computational cost, the 2,2,6,6-tetramethyl-3,5-heptanedionate TMHD ligand used experimentally (red; **Figure 2.1C**) was truncated as acetylacetonate (acac). Notably, the acac ligand has also enabled nickel-catalyzed cross-couplings with tertiary radicals albeit lower yields as demonstrated by the Molander group and Baran.[177-178] Nonetheless, to validate the proposed model, Song also compared the lowest energy pathways using the much bulkier TMHD ligand. The calculated energy values and the obtained structures with TMHD ligand are similar to those using the acac ligand (see **Figure A1.15** in the Appendix 1).

2.3.2 Ni-TMHD Catalytic System with tert-Butyl Radical

This part of computation is performed by Zhihui Song.

As shown in **Figure 2.2** (blue pathway), in the absence (or low concentration) of alkyl radical, (acac)Ni(I) intermediate ^{2}**A** could undergo facile oxidative addition (barrier of only 4.6 kcal/mol) to form Ni(III) ^{2}**B** intermediate (~11 kcal/mol downhill in energy). In turn, Ni(III) ^{2}**B** will then undergo an internal reorganization from distorted tetrahedral to distorted square planar conformation (see **Figure A1.10** in the Appendix 1) leading to Ni(III) ^{2}**C** (uphill in energy by ~6 kcal/mol from ^{2}**B**). The distorted square planar ^{2}**C** is now poised to undergo facile radical "outer-sphere" cross-coupling with the tertiary alkyl radical. Specifically, in this geometry, the tertiary alkyl radical is energetically favored to form a complex with ^{2}**C** rather than adding to the Ni center (^{3}**C**^{complex}). Finally, this radical will then undergo a spin-selective (barrier is only 3.1 kcal/mol from

^{3}**C**^{complex}) outer-sphere C(sp^2)−C(sp^3) bond formation to generate the desired product and the concomitant formation of bromo Ni(acac) species (^{3}**P**$_A$) downhill in energy by ~69 kcal/mol. The outer-sphere radical coupling via the singlet spin state was also explored by Song, but was found to be ~7 kcal/mol higher in energy than the calculated ^{3}**C-TS** and is thus not productive.[182]

Alternatively, when the pathways initiated from radical addition to the phenyl bromide Ni(acac) complex ^{2}**A**, it was found higher in energy. Specifically, as shown in **Figure 2.2** (red), in the presence of alkyl radical, radical addition to ^{2}**A** and concomitant displacement of phenyl bromide could lead to triplet ^{3}**D** which is exergonic by ~12 kcal/mol. ^{3}**D** can then undergo high-barrier (~22 kcal/mol) and rate-determining oxidative addition with phenyl bromide, leading to the formation of ^{3}**C'** that undergoes barrierless tertiary radical dissociation and generates distorted tetrahedral ^{2}**B**, thus merging both pathways. Ultimately, both of these pathways will lead to triplet spin, outer-sphere C(sp^2)–C(sp^3) bond formation from ^{3}**C**^{complex}. Based on the prior computational studies in the Gutierrez group,[81, 117, 183-184] the commonly proposed singlet spin state, inner-sphere reductive elimination directly accessed from singlet spin state of Ni(IV) intermediate was also explored, but was ruled out due to the higher barrier.

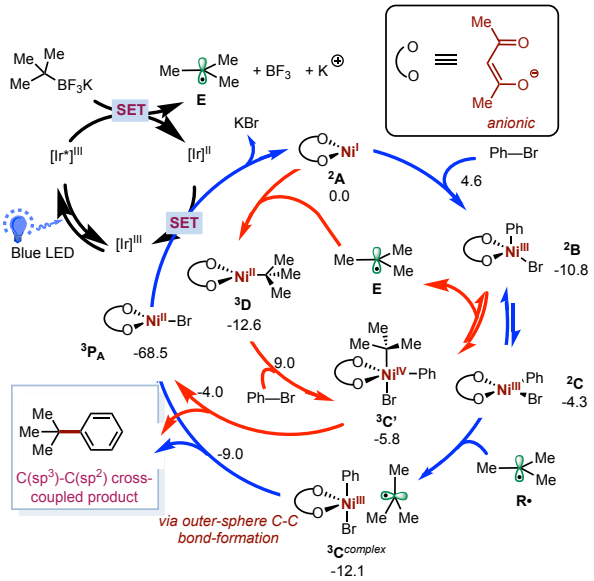


Figure 2.2 Proposed catalytic cycle with computed energetics of the Ni-catalyzed cross-coupling between *tert*-butyl radical and bromobenzene using truncated anionic acac ligand. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF). Calculations of this part was performed by Zhihui Song.

Song also considered the likelihood of explicit DMA solvent coordinating to the key nickel species ^{2}**A** or ^{2}**C** and promoting ligand dissociation, while the calculations showed that the DMA solvent is unlikely to cause ligand dissociation during the transition metal catalytic cycle (see **Figure A1.14** in the Appendix 1). Moreover, experiments using excess TMHD anionic ligand was carried out by the collaborator (Molander group), where excess TMHD ligand (50 and 100 mol %), presumably saturating the nickel intermediates coordinatively, had a minor effect on the efficiency of the system (*vide infra*). Finally, the electronic properties of the aryl bromide do not change the overall mechanistic conclusions (see **Figure A1.3** in the Appendix 1).

In sum, for anionic diketonate-Ni systems involving tertiary alkyl radicals (i.e., as reported by Molander[177], Baran[178], Shenvi[179]), these computational results strongly support a novel, low barrier, spin-selective "outer-sphere" radical cross-coupling pathway via triplet spin state. In contrary to commonly proposed pathways, the formation of sterically hindered halo-aryl-alkyl-Ni

intermediates using anionic ligands are disfavored (see **Figure A1.21–A1.22** in the Appendix 1 for calculations with other substrates). These results could be applied to a wide range of experimental observations in which privileged anionic ligands, in combination with nickel complexes, allow radical cross-coupling with tertiary radical precursors.[177-179]

2.3.3 Ni-Bipyridine Catalytic System with tert-Butyl Radical

This part of computation is performed by me.

Previously, neutral bipyridine ligands in combination with nickel as catalyst failed to undergo C(sp^2)–C(sp^3) cross-couplings with *acyclic* tertiary radical under dual photoredox/nickel catalysis (**Figure 2.1C**). Nonetheless, this bipyridyl-nickel system has found success for a wide range of Ni-catalyzed radical C(sp^2)–C(sp^3) cross-couplings with *secondary* and *cyclic* tertiary alkyl radical precursors, and many groups[81, 117, 188] have taken advantage of this reactivity to promote selective dicarbofunctionalization of olefins.[185, 188-190] However, despite the widespread utility of bipyridyl-nickel system in organic synthesis with tertiary alkyl radicals, the mechanism and, in particular, the nature of the critical C–C bond formation is not known. To gain insights from this divergent reactivity with tertiary alkyl radicals, I examined the competing reaction pathways in the bipyridyl-nickel system (**Figure 2.3**, see **Figure A1.4** in the Apppendix 1 for energetics using other methods).

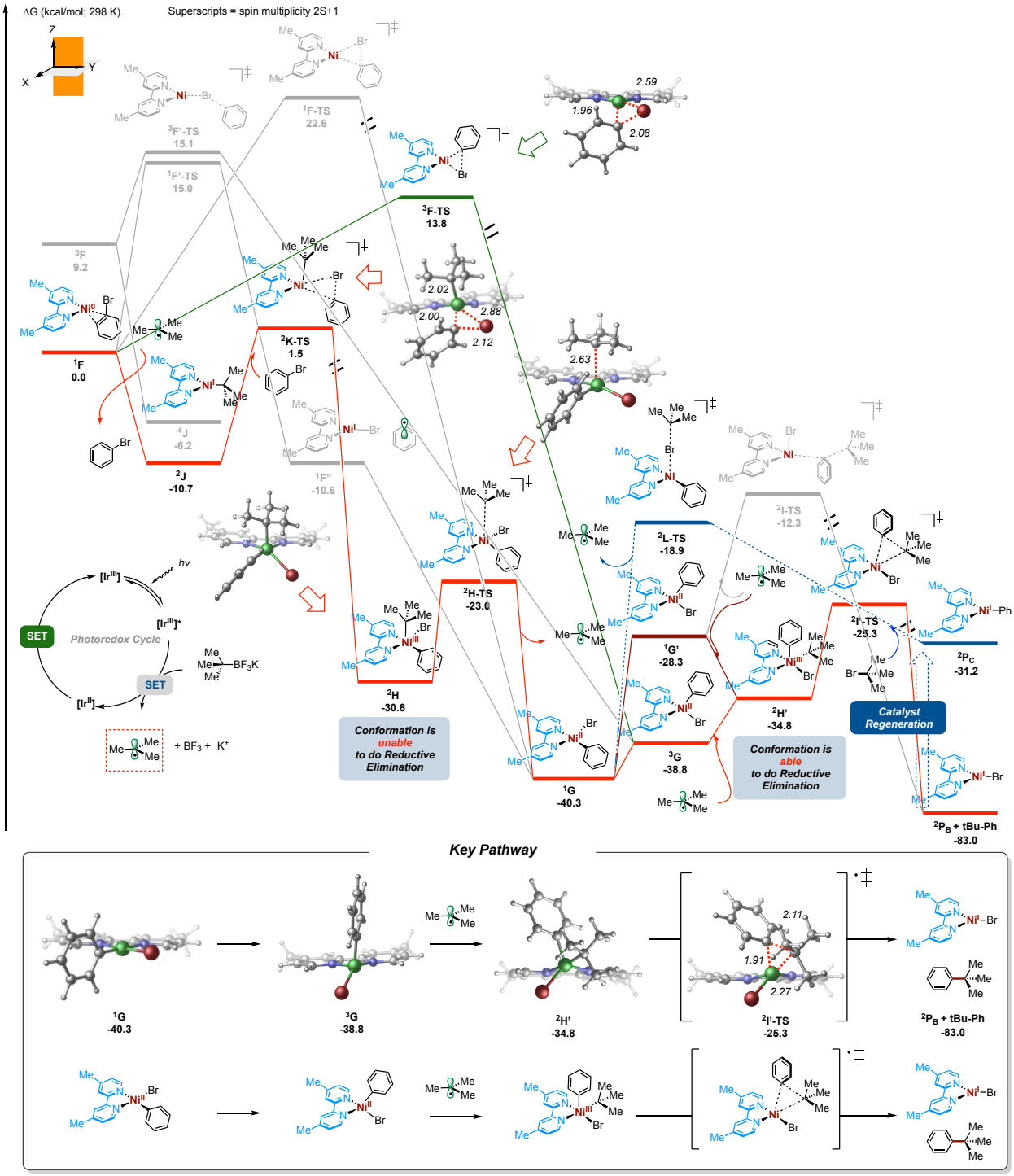


Figure 2.3 Calculated energetics of the Ni-catalyzed cross-coupling between *tert*-butyl radical and bromobenzene using neutral bipyridine as ligand. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) level of theory. All calculations of the bipyridyl-nickel system were performed by me.

Similar to the results in the anionic system, in the presence of alkyl radical, overall the lowest energy pathway (red) proceeds via barrierless *tert*-butyl radical addition to Ni(0), leading to Ni(I) intermediate ^{2}**J**. In turn, Ni(I) ^{2}**J** undergoes oxidative addition to aryl halide via ^{2}**K-TS** — the overall barrier is ~12 kcal/mol from ^{2}**J**, leading to Ni(III) intermediate ^{2}**H**. However, despite numerous attempts, I was unable to locate the direct, inner-sphere reductive elimination from this isomer. Instead, a very low barrier tertiary alkyl radical dissociation (via ^{2}**H-TS**) was found that leads to the formation of square planar Ni(II) intermediate ^{1}**G**. This square planar aryl halo Ni(II) intermediate is favored to undergo an intersystem crossing/conformational change to form the *tetrahedral, triplet spin state* Ni(II) intermediate ^{3}**G**. In turn, ^{3}**G** is now poised to undergo radical addition to form Ni(III) intermediate ^{2}**H'** followed by *inner-sphere* reductive elimination (via ^{2}**I'-TS**), leading to the desired products ^{2}**P$_{B}$** and ***t*-Bu-Ph**, which is exergonic by 83 kcal/mol. After the C(sp^{2})–C(sp^{3}) bond-forming step, SET can occur between the bromo Ni species and the reduced Ir photocatalyst to regenerate the Ni(0) catalytic species ^{1}**F** with concomitant formation of KBr complex and restart the transition-metal catalytic cycle (see **Figure A1.17** in Appendix 1 for details).

Given the prevalence of proposed Ni(I)/Ni(III)/Ni(I) pathways by the community and the lack of understanding of the dynamic effects in nickel-catalyzed radical cross-coupling reactions, I conducted preliminary quasi-classical dynamics simulations on the transition state of oxidative addition ^{2}**K-TS** and that of reductive elimination ^{2}**I'-TS**, respectively (see **Figure A1.13** in the Appendix 1). Simulated results suggest that starting from ^{2}**K-TS** in the forward direction, 60% of the trajectories resulted in the formation of a Ni(III) intermediate, while 40% formed the *square planar* Ni(II) intermediate and *concomitant dissociation of tert-butyl radical*. No cross-coupling product (***t*-Bu-Ph**) was observed in any simulated trajectory (see **Figure A1.13a** in Appendix 1 for

details). These observations support my static DFT calculations that the Ni(III) intermediate obtained from direct oxidative addition on the alkyl Ni(I) intermediate *cannot undergo reductive elimination*, but rather undergoes radical dissociation to generate the *square planar* Ni(II) intermediate **^{1}G**. On the other hand, within dynamics calculations propagated from **^{2}I'-TS** in the reverse direction, all trajectories ended up in forming Ni(III) intermediate without radical dissociation from the Ni center or structural rearrangement (see **Figure A1.13b** in Appendix 1 for details). This is also consistent with my assumption concerning the overall process because the radical addition to Ni involves a change of spin state of the Ni(II) species, while quasi-classical dynamics simulations only operate in a single spin state. From a broader perspective, these results suggest a novel Ni(0)/Ni(I)/Ni(III)/Ni(II)/Ni(III)/Ni(I) pathway in bipyridine-nickel radical cross-couplings with tertiary alkyl radicals.

Within the dynamics simulations, I also investigated the possibility of ligand dissociation from Ni(III) intermediate, which might invoke structural rearrangement of Ni(III) intermediates. However, based on our calculations the complete ligand dissociation is unlikely to occur on neither **^{2}H** nor **^{2}H'** since these processes are both uphill in energy (see **Figure A1.19** for energetic details in the Appendix 1). In addition, although transient decoordination of one of the pyridine ligands was observed in quasi-classical dynamics simulations on **^{2}K-TS** in forward direction (see **Figure A1.20** for an example trajectory), *the Ni(III) intermediates didn't undergo any structural rearrangement*, but rather stayed the same conformation until the end of simulation (60% of trajectories) or underwent radical dissociation of *t*Bu radical from axial position of Ni center (40% of trajectories).

Ni(0)/Ni(II)/Ni(III) Pathway: In the absence (or low concentration) of *tert*-butyl radical, Ni(0) could undergo oxidative addition via *triplet* spin state (**^{3}F-TS**; green) leading directly to the

productive *tetrahedral*, *triplet* spin state Ni(II) ^{3}**G** intermediate, thus merging both Ni(0)/Ni(I)/Ni(III)/Ni(II) (red) and Ni(0)/Ni(II) (green) pathways. I also considered the possible *outer-sphere* C-C bond formation pathway between *tert*-butyl radical and Ni(II) intermediate, but the transition states of both of the doublet (^{2}**I-TS**) and quartet spin state pathways (^{4}**I-TS**) are higher in energy compared to ^{2}**I'-TS** (see **Figure A1.4** in the Appendix 1 for details). Therefore, *inner-sphere* reductive elimination via Ni(III) intermediate ^{2}**H'** is preferred to that of the *outer-sphere* pathway from Ni(II) intermediate in Ni-bipyridine catalytic systems.

Ni(I)/Ni(II)/Ni(III) Pathway: Previously, alkyl halide activation by Ni(I) species (akin to ^{2}**Pc**) have been proposed in a range of Ni-catalyzed cross-couplings.[8, 191-194] As shown in **Figure 2.3** (blue), in these cases, aryl bipyridine-Ni(I) could undergo halogen abstraction (via ^{2}**L-TS**; barrier ~12 kcal/mol from ^{2}**Pc**) leading to the Ni(II) ^{1}**G**, thus also merging the cross-coupling cycles. Finally, Ni(II) ^{1}**G** will need to undergo an isomerization/spin-crossing to form the productive tetrahedral Ni(II) ^{3}**G** which, after barrierless radical addition, will form the productive Ni(III) ^{2}**H'**. Finally, inner-sphere reductive elimination (via ^{2}**I'-TS**) will lead to the desired product and bromo Ni(I). *From a broader perspective, although the pathway for catalyst regeneration from the bromo Ni(I) varies among nickel-catalyzed cross-coupling methods (e.g., it could undergo SET by photocatalyst or external reductant to form a Ni(0)* ^{1}***F*** *or, alternatively, could undergo transmetalation to form the Ni(I)* ^{2}***Pc***[173]*), calculations show that these systems involving tertiary alkyl radicals share the same critical C(sp^{2})–C(sp^{3}) formation step!*

As an example, the phenyl bpy-Ni(I) species was proposed to be obtained via transmetalation in Fu's experiments.[173] The overall key findings of these calculations are summarized as follows (**Figure 2.3**; inset): after *singlet spin square planar* Ni(II) species ^{1}**G** forms, this species needs to undergo intersystem crossing/conformational change to generate the *triplet*

spin tetrahedral ^{3}**G** complex followed by tertiary alkyl radical addition to form Ni(III) intermediate ^{2}**H'** (see **Figure A1.6** in the Appendix 1 for more detailed analysis). The requirement for the tetrahedral Ni(II) conformation to undergo Ni(II)/Ni(III) radical addition was also reported in a recent paper with neutral bis(oxazoline) ligand, in which phenyl bromo Ni(II)-bis(oxazoline) is in a *square planar* geometry, while the radical adds to a *tetrahedral* phenyl bromo Ni(II) species.[195] Moreover, the results of my preliminary quasi-classical dynamics calculation are consistent with this suggested pathway (see **Figure A1.7** and **Figure A1.8** in the Appendix 1). Finally, ^{2}**H'** will undergo *doublet spin, inner-sphere* reductive elimination pathway via ^{2}**I'-TS** to generate the desired C(sp^2)−C(sp^3) cross-coupling product and bromo Ni(bipyridine) (^{2}**P$_B$** + ***t*-Bu-Ph**).

2.3.4 Origin of the Difference in the C(sp^2)–C(sp^3) Bond-Forming Step in Ni-TMHD and Ni-Bipyridine Catalytic Systems

As shown above, independent of the operative catalytic active species, all pathways converge at the Ni(II) and tertiary radical. Thus, assuming facile intersystem crossing/conformational change, the barrier for *inner-sphere* tertiary radical C(sp^2)–C(sp^3) cross-coupling using neutral bipyridine nickel-system (~15 kcal/mol from ^{1}**G**) is much higher in energy than using anionic diketonate nickel-system (~4 kcal/mol). These relative barriers are consistent with the experiments that prevented the formation of the desired C(sp^2)–C(sp^3) bond using acyclic tertiary radicals under the Ni-bipyridyl/PC system.[177] Moreover, the higher barrier could lead to unwanted side reactions with tertiary radicals like the H-atom abstraction with the solvent, as observed by us.[177] Further calculations suggest that these side reactions are feasible in the reaction system, which could explain the observation of THF-Ar adduct and Ar-H in the stoichiometric studies of aryl bromo Ni(II) with *t*Bu-BF$_3$K in experiment[177] (see **Figure A1.11** and **A1.12** in the Appendix 1 for the calculation of possible side reaction pathways). Moreover, in accord with

experiments by Fu,[173] switching to solvent systems with high bond dissociation energies (BDE) (e.g., benzene) likely increases the barrier for H-abstraction and, in turn, allows for favorable kinetics to promote C(sp^2)−C(sp^3) bond formation with tertiary alkyl radicals. The competence of alkyl radical undergoing H-abstraction (e.g., with solvent or other reagents) or C(sp^2)−C(sp^3) bond formation is not only seen in Ni-bipyridine system in Fu's report,[173] but also observed in Ni-TMHD(acac) system.[178-179] Altogether, this suggested that the H-abstraction reactions with alkyl radical are competing with C–C bond formation in related cross-coupling reactions and the efficiency of C–C bond formation (e.g., H-abstraction versus C–C cross-coupling) is likely system-dependent.

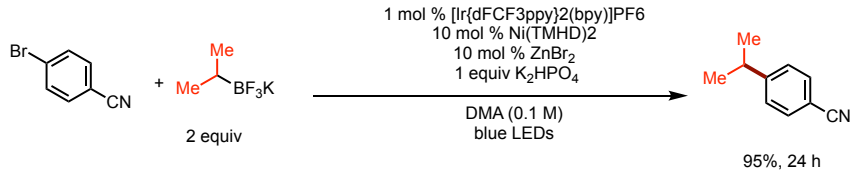


Figure 2.4 Cross-coupling of secondary alkyltrifluoroborates with Ni-TMHD performed by the collaborator (Molander group). NMR yield was calculated using 1,3,5-trimethoxybenzene as the internal standard.

On the other hand, the cross-coupling barrier for the diketonate-nickel system is only ~3 kcal/mol from the respective nickel complex and tertiary alkyl radical (computed by Song). Thus, the efficiency of Ni-diketonate systems with tertiary alkyl radicals under photocatalytic conditions [177-179] was attributed to the nature of the *outer-sphere* C–C bond formation that avoids the formation of a high energy, sterically congested aryl-alkyl-halo-Ni intermediate. Experiments using less sterically hindered secondary alkyltrifluoroborates also led to the desired product in 95% yield (**Figure 2.4**; conducted by collaborator). However, in contrast to tertiary alkyl radicals, from DFT calculations it was found that the favored pathway for less sterically secondary alkyl radicals

is via inner-sphere C–C bond formation with overall barriers for C–C bond formation ~9 kcal/mol (see **Figure A1.21** in the Appendix 1; computed by Song). Presumably, the less sterically hindered secondary alkyl radical (in contrast to the tertiary alkyl radical) does not pay a penalty to form the aryl-alkyl-halo-Ni species and can quickly undergo inner-sphere C–C bond formation. In contrast to bipyridyl-Ni system, these results suggest that for acac/TMHD-Ni systems, the nature of the C–C bond formation and whether inner- or outer-sphere $C(sp^2)$–$C(sp^3)$ is operative is dependent on the sterics properties of the alkyl radical.

Surprisingly, for cyclic tertiary systems, we found that this system did not undergo aryl substrate activation in the experiment, leading, after 24 hours, to the recovered starting material (done by collaborator). Although the reasons for lack of reactivity are not completely understood, computations showed that, if the cyclic radical were to engage with the nickel in the cross-coupling cycle, the formation of 1-bromoadamantane via inner-sphere C–Br bond formation is favored over C–C bond formation (see **Figure A1.22** in the Appendix 1; computed by Song). However, since substoichiometric additives (e.g., LiBr, $ZnBr_2$, $ZnCl_2$, etc.) were found to influence the reactivity of substrates in the Ni-TMHD system where bicyclic substrate (adamantyl-like) also failed,[178-179] the exact reason for the failure of adamantyl substrate remains unknown and is under exploration.

To better understand the origins of the distinct reactivity (i.e., ligand effect on C–C bond formation), the activation strain-distortion/interaction analysis was conducted, where I targeted the neutral bipyridyl-nickel system and Song computed the anionic-nickel system.[196-199] As shown in **Table 2.1**, comparing inner-sphere and outer-sphere C–C bond formation transition states in the Ni-bipyridine catalytic system (green background), the relative activation electronic energy of inner-sphere transfer is negative (-3.9 kcal/mol) while that of outer-sphere transfer is positive, meaning that the C–C bond formation is favorable via inner-sphere pathway (see **Table A1.1** in

the Appendix 1 for energetics using other methods). Despite the larger distortion energy of the inner-sphere compared to the outer-sphere pathway, its interaction energy compensates for the larger distortion energy and makes the overall process favorable.

On the other hand, for the Ni-TMHD system (blue background; computed by Song) both inner-sphere and outer-sphere transition states possess negative activation electronic energies, and both of their distortion energy and interaction energy are close to each other. Although the inner-sphere and outer-sphere pathways of the Ni-TMHD system do not show as large a difference as those of the Ni-bipyridine system, the *triplet spin state outer-sphere* pathway is still found most favorable (-13.3 kcal/mol) because of its lower distortion energy (18.4 kcal/mol) and larger interaction energy (-31.7 kcal/mol).

Table 2.1 Activation Strain-Distortion/Interaction analysis of C(sp^2)–C(sp^3) bond formation step.[a] Ni-bipyridine system was computed by me and Song targeted the Ni-TMHD system.

		$\Delta E_{activation}$ (kcal/mol)	$\Delta E_{distortion}$ (kcal/mol)	$\Delta E_{interaction}$ (kcal/mol)
Outer-Sphere	^{2}I-TS	19.1	28.6	-9.6
	^{4}I-TS	12.2	17.1	-4.9
Inner-Sphere	^{2}I'-TS	-3.9	41.0	-44.9
Outer-Sphere	^{1}C-TS	2.7	16.0	-14.0
	^{3}C-TS	-13.3	18.4	-31.7
Inner-Sphere	^{1}C'-TS	-13.2	20.8	-34.0

[a]Relative electronic energy values were computed with respect to the separate corresponding phenyl-bromo-Ni-ligand species and *tert*-butyl radical at the UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(THF) level of theory.

2.3.5 Origin of the Distinct Alkyl Reactivity in the Ni-Bipyridine Catalytic System

This part is performed by me.

Because of the observed experimental differences of structurally different alkyl radicals in Ni-bipyridine systems,[177] I became interested in exploring the potential reactivity of different alkyl radicals in the above key pathways (**Table 2.2**). Specifically, in the dual photoredox-Ni catalytic system, C(sp^2)–C(sp^3) cross-coupling succeeded with aryl bromides as the electrophile and potassium 1-adamantyltrifluoroborate and potassium 1-phenylcyclopropyltrifluoroborate as the nucleophile (**Figure 2.1C**).[177] Therefore, I compare here the reactivity of *tert*-butyl radical, isopropyl radical, 1-phenylcyclopropyl radical, and 1-adamantyl radical in the key *inner-sphere* reductive elimination step (see **Figure A1.6** in the Appendix 1 for the comparison of different radicals in other steps). As shown in **Table 2.2** (gray), using distinct Ni(II) species **^{1}G** and the purported alkyl radicals as a reference, I observed that the relative energy values of Ni(III) **^{2}H'** intermediates, which are reactive towards inner-sphere reductive elimination, vary for different alkyl radicals. First, the Ni(III) intermediate with *tert*-butyl radical (black) is found to be endergonic by 5.6 kcal/mol, while all other Ni(III) intermediates with tertiary and secondary alkyl radicals (red, blue, and green) are exergonic (by 2-3 kcal/mol). *These results suggest that tert-butyl radical is more favorable to dissociate from Ni(III) center to form Ni(II) and tert-butyl radical, while for the other tertiary and secondary alkyl radicals the energetics favor the formation of Ni(III) complex*. This trend is also observable in the barriers for reductive elimination. Specifically, the barriers for *inner-sphere* reductive elimination of cyclic and secondary alkyl radicals are significantly lower (by 7-12 kcal/mol) than with *tert*-butyl radical. This observation is consistent with the results in experiments by Fu, where 1-iodoadamantane, with the assumption of 1-adamantyl radical being generated *in situ*, can also be cross-coupled in non-photocatalytic

condition despite their slightly higher barrier of reductive elimination (7.3 kcal/mol) compared to secondary *iso*-propyl radical.[173]

Table 2.2 Analysis of distinct alkyl radical reactivity in Ni-bipyridine system.[a]

	ΔG (kcal/mol; 298K)			BDE of Ni-C(sp^3) (ΔH; kcal/mol)	$\Delta E_{activation}$ (kcal/mol)	$\Delta E_{distortion}$ (kcal/mol)	$\Delta E_{interaction}$ (kcal/mol)
	^{1}G	^{2}H'	^{2}I'-TS				
	0.0	5.6	15.0	11.0	-3.9	41.0	-44.9
		-2.3	4.2	18.3	-13.9	37.4	-51.2
		-3.4	2.7	17.9	-14.2	33.1	-47.3
		-3.3	7.3	18.3	-8.0	32.4	-40.4

[a]White: calculated energetics on inner-sphere reductive elimination step with different alkyl radicals; Blue: related analysis on bond dissociation energy of Ni(III) intermediate; Yellow: activation strain-distortion/interaction analysis on reductive elimination transition state [relative electronic energy values were calculated with respect to the separate corresponding Ni(II) species and tert-butyl radical]. Relative free energy values were computed concerning the Ni(II) species at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) level of theory, bond dissociation energy and relative electronic energy values were calculated at the UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(THF) level of theory.

Further, to gain insight into the observed trends, I computed the bond dissociation energy (BDE) of Ni–C(sp^3) bond with different alkyl radicals. As shown in **Table 2.2** (blue), I found that Ni-C(*tert*-butyl) bond has the lowest BDE (11.0 kcal/mol), which indicates that the dissociation of *tert*-butyl radical from the Ni(III) center is easier than the dissociation of secondary and cyclic tertiary alkyl radicals (~18 kcal/mol). Also, from an activation strain-distortion/interaction analysis on the reductive elimination step (yellow), the transition state with *tert*-butyl radical shows a less negative activation energy and larger distortion energy compared to the rest of the systems. This suggests that reductive elimination with *tert*-butyl radical is less favorable because it needs to pay a higher energy penalty for distortion to reach the geometry in the C(sp^2)–C(sp^3) bond-forming step. Although the exact mechanism of bipyridyl-nickel-involved radical cross-coupling reactions

could be significantly different depending on the experimental condition and applied substrates/additives, my findings on the nature of C(sp^2)−C(sp^3) bond formation can be used to explain some of the observed selectivity in the selective dicarbofunctionalization of olefins with a broad variety of *secondary* and *tertiary* alkyl radical precursors.[81, 185, 188-190]

2.4 Conclusion

In summary, quantum mechanical calculations and quasi-classical direct dynamics simulations have been used to investigate the mechanism of dual photoredox-Ni-catalyzed C(sp^2)–C(sp^3) cross-coupling reactions between tertiary alkyltrifluoroborates and aryl halides with Ni bipyridine- and diketonate-based catalytic systems. Calculations showed the prominent effect of the charge on the ligand on key catalytic intermediates and the C(sp^2)–C(sp^3) bond-forming step in such transformations. Specifically, as outlined in **Figure 2.5**, in the Ni-TMHD (anionic ligand) system, the tertiary alkyl radical can directly interact with the aryl-bromo-Ni species to obtain the desired product via *high-spin, outer-sphere* reductive elimination pathway without engaging the Ni center first. In the Ni-bipyridine (neutral ligand) system, as shown by transition state calculations and supported by quasi-classical dynamics, the Ni(III) intermediate directly obtained from oxidative addition on alkyl Ni(I) species needs to undergo radical dissociation to form the *singlet-spin square planar* Ni(II) intermediate. Then, it needs to undergo a conformational change/intersystem crossing followed by radical addition to gain access to the productive Ni(III) intermediate, followed by subsequent *low-spin, inner-sphere* reductive elimination to generate the desired product and halo Ni(I). *From a broader perspective, although the pathway for catalyst regeneration from the halo Ni(I) varies among different nickel-catalyzed cross-coupling methods (e.g., it could undergo SET by photocatalyst or external reductant to form a Ni(0) or, alternatively,*

could undergo transmetalation to form an aryl Ni(I)), calculations show that these systems share the same critical C(sp^2)−C(sp^3) formation step!

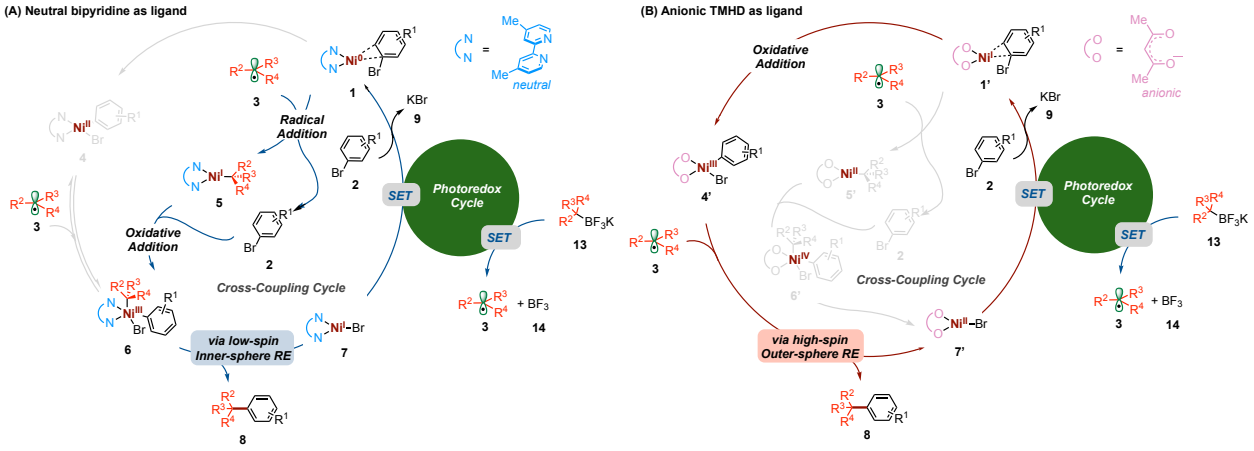


Figure 2.5 Catalytic cycle for photoredox/Ni dual catalytic system using (A) neutral (blue) and (B) anionic (pink) ligands.

The reactivity of different alkyl radicals was also compared in the Ni-bipyridine system. This information suggests that relatively subtle changes in the alkyl radical precursors and ligands have a dramatic effect on the mechanism of the reactions. Nonetheless, this investigation sheds light on mechanistic possibilities that were never considered previously and inspires the design of catalytic systems and modification of substrates for Ni-catalyzed C(sp^2)–C(sp^3) cross-coupling reactions. Further exploration will be focused on the comparison of more neutral and anionic ligand systems and the behavior of different alkyl radicals based on the mechanistic models proposed here.

Chapter 3: Mechanistic Study of Nickel-Catalyzed Olefin Dicarbofunctionalization Enabled by Photochemical C–H Activation

Excerpts from this chapter were published in: Campbell, M. W.; **Yuan, M.**; Polites, V. C.; Gutierrez, O.*; Molander, G. A.* *J. Am. Chem. Soc.* **2021**, *143*, 3901-3910.

3.1 Abstract

Alkenes, ethers, and alcohols account for a significant percentage of bulk reagents available to the chemistry community. The petrochemical, pharmaceutical, and agrochemical industries each consume gigagrams of these materials as fuels and solvents each year. However, the utilization of such materials as building blocks for the construction of complex small molecules is limited by the necessity of prefunctionalization to achieve chemoselective reactivity. In this chapter, in collaboration with the Molander group, we reported the implementation of efficient, sustainable, diaryl ketone hydrogen-atom transfer (HAT) catalysis to activate native C–H bonds for multicomponent dicarbofunctionalization of alkenes. The ability to forge new carbon–carbon bonds between reagents typically viewed as commodity solvents provides a new, more atom-economic outlook for organic synthesis. Through detailed experimental and computational investigation, the critical effect of hydrogen bonding on the reactivity of this transformation was uncovered. Using dispersion-corrected DFT and DLPNO-CCSD(T) calculations, I studied the mechanism and revealed the origin of the chemoselectivity of this transformation.

3.2 Introduction

Among the most prevalent materials available to the chemistry community are hydrocarbons (alkanes and alkenes) and their oxygenated derivatives (alcohols and ethers). Despite their ubiquity in nature and chemical industries, the preparation of complex small molecules from these commodity materials remains a pertinent synthetic challenge.

Prefunctionalization, typically requiring multistep sequences, is often necessary for promoting selective reactivity of simple building blocks. In an effort to overcome the inefficiency of non-native functional group installation, several research programs have been initiated that focus on the selective functionalization of C–H bonds.[200]

Despite significant advancements in this arena, multicomponent C–H functionalizations are still exceedingly rare.[201] This stands in stark contrast to the advances in the field of multicomponent, transition metal-mediated cross-couplings that utilize prefunctionalized substrates.[202-203] Dicarbofunctionalizations (DCF) are a subset of multicomponent cross-coupling reactions that employ an alkene or alkyne as a "linchpin", facilitating the regioselective construction of two C–C bonds. Early work in the field of nickel-catalyzed DCF employed aryl- and alkylmetallic coupling partners (e.g., organozinc and organoboron reagents).[189, 204-207] Significant advancement in functional group compatibility has been achieved in nickel-catalyzed DCF reactions by leveraging radical-based mechanisms.[208] More recently, photoredox/Ni dual catalysis has dramatically expanded the suite of installable fragments by exploiting a well-developed library of divergent radical precursors.[17, 188, 209-214]

Although synthetically enabling, even the most modern DCF reactions do not address the longstanding challenge of utilizing commodity reagents in multicomponent reactions, instead relying on prefunctionalized radical precursors, typically exhibiting poor atom-economy. To address these limitations, in collaboration with the Molander group, I sought to develop a radical-based DCF strategy enabled by the selective homolysis of C–H bonds. At the outset, various intermolecular hydrogen-atom transfer (HAT) catalysts (e.g., tertiary amines or tungsten-based salts) were considered to achieve the desired transformation, but these either require activation via organometallic photocatalysts or lack sufficient chemoselectivity.[215-220] Notably, diaryl ketones

have been identified as effective HAT catalysts that are photoactive, sustainable, and chemoselective, thus overcoming the inherent challenges of the aforementioned HAT agents. In this vein, diaryl ketone HAT catalysis has been used in the hydroalkylation of activated alkenes as well as the arylation of C–H bonds via Ni-catalyzed cross coupling.[221-224] It's envisioned that the merger of these two fundamental transformations, achieved by synergistic diaryl ketone/Ni dual catalysis, could overcome the inherent limitations of prefunctionalized radical precursors in multicomponent cross-coupling reactions. In addition to developing this transformation, I performed state-of-the-art quantum mechanical calculations to provide insight into the mechanism and the origin of selectivity of this protocol. Hydrogen-bonding interaction was found to be the key in controlling the chemoselectivity of this transformation.

3.3 Results and Discussion

Based on the optimization studies of the HAT catalysts by the Molander group, diaryl ketones bearing on electron-rich and one electron-poor arene were found the most effective.[118] Notably, quantum mechanical calculations revealed a general trend between the DCF product yield (determined by crude ^{1}H NMR, done by collaborator) and the calculated triplet state energy of a range of benzophenone derivatives (see **Table A2.1** in Appendix 2).

After figuring out the optimal HAT catalyst, the desired hydrogen atom transfer-mediated DCF was envisioned to operate via the mechanism outlined in **Figure 3.1**. Photoexcitation of a diaryl ketone (**I**) would access the triplet-state diradical **II**. This persistent radical would perform selective homolysis of an activated C–H bond (BDE = 90.4 kcal/mol; see **Figure A2.1** in Appendix 2 for further details about the regioselectivity of the C–H activation), generating the desired carbon-centered radical (**IV**) with concomitant formation of ketyl radical **III**. In turn, this alkyl

radical would undergo regioselective Giese addition to an activated alkene **V**, leading to the corresponding radical adduct **VI**. The newly formed radical adduct (**VI**) could be captured by a Ni^0 species (**VII**), and undergo subsequent oxidative addition with an aryl halide, affording Ni^{III} complex **IX** (blue pathway). Alternatively, the aryl halide could first undergo oxidative addition with the Ni^0 species prior to radical capture (**VII**; green pathway). After reversible square planar-tetrahedral isomerism, **VI** could then add to the productive tetrahedral Ni^{II} intermediate **X**,[225] forming complex **IX**. Reductive elimination from **IX** would produce the desired DCF product **XII** and Ni^{I} complex **XI**.[81] Finally, single-electron transfer (SET) from ketyl radical **III** to **XI** would regenerate **VII** and **I**, completing both catalytic cycles.

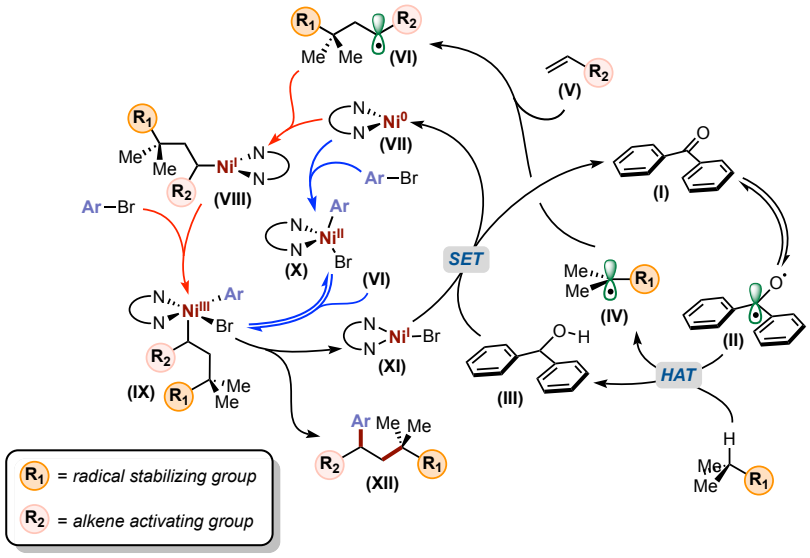
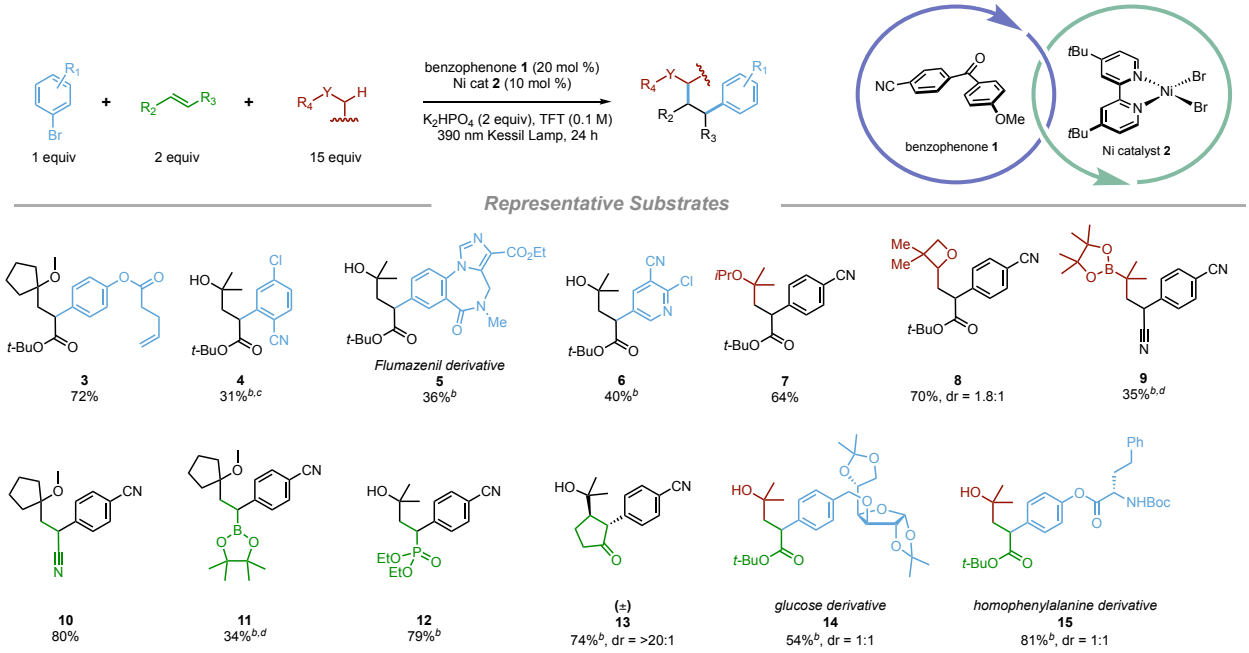


Figure 3.1 Proposed mechanism for three-component HAT-mediated photoredox/nickel dual-catalyzed DCF of alkenes.

After optimizing a suitable set of reaction conditions for this DCF reaction, the scope of reaction components were evaluated by our collaborator,[118] with the representative substrates shown in **Table 3.1**. Apart from mono- and disubstituted arenes (**3–5**), heteroaryl bromides were also found employable (**6**). In terms of the scope of C–H precursors, alcohols (**4–6**) and ethers (**7**,

8) were both utilized with good success, including the challenging α-pinacol boronate (**9**) that can be used as a synthetic building block for a wide array of transformations of alkyl boronates. Moreover, diverse vinyl functional groups can be incorporated from the starting alkene materials (**10**–**12**), even including the internal alkenes that showed superb diastereoselectivity (**13**). As a validation of the synthetic value of this DCF strategy, more complex substrates based on natural product scaffolds (**14**, **15**) were prepared by our collaborator, showcasing the rapid assembly of substrates containing such highly functionalized motifs.

Table 3.1 Representative substrates of the three-component HAT-mediated photoredox/nickel dual-catalyzed DCF strategy done by Molander[a]



[a]Values indicate yield of the isolated product. Unless otherwise noted: aryl halide (1 equiv, 0.5 mmol), alkene (2 equiv, 1.0 mmol), C−H precursor (15 equiv, 7.5 mmol), Ni **2** (10 mol %, 0.05 mmol), benzophenone **1** (20 mol %, 0.10 mmol), K_2HPO_4 (2 equiv, 1.0 mmol), TFT (0.1 M), 24 h, irradiating with 390 nm Kessil lamp. Variation in reaction components was illustrated by the change in color (aryl bromides: blue; alkenes: green; C−H precursor: red). [b]Using a 1:1 v/v ratio of C−H precursor/TFT. [c]Reaction time extended to 48 h. [d]Using 4 equiv of alkene.

After exploring the synthetic value of this strategy, we investigate its mechanistic picture by first investigating the mechanisms of C–C bond formation in this DCF reaction. Because of the potential for alkyl radicals to undergo either direct two-component cross-coupling (CC) or three-component DCF, DLPNO-CCSD(T) and dispersion-corrected DFT calculations were used to provide further insight into the mechanism and selectivity (**Figure 3.2**; see Appendix 2 for full computational details). Such calculations have recently been used by our group to study the mechanism of a nickel-catalyzed photoredox single-electron Tsuji-Trost reaction[117] and provide accuracy at the level of coupled cluster theory at the cost of DFT calculations.[226] Consistent with previous results,[225] calculations showed that both the $Ni^0/Ni^{II}/Ni^{III}$ and $Ni^0/Ni^{I}/Ni^{III}$ mechanisms are energetically feasible for two- and three-component pathways, (see **Figure A2.3** and **Figure A2.4** in Appendix 2) as observed in related systems,[225] and converge on the singlet, square planar Ni^{II} oxidative addition complex, ^{1}**C** (**Figure 3.2**, inset). Two plausible mechanisms for two-component cross-coupling (CC) of radical fragment **A** are outlined in **Figure 3.2** (left; blue/green pathways). After formation of the singlet, square planar complex ^{1}**C**, this species is expected to equilibrate rapidly under photocatalytic conditions to the triplet, tetrahedral complex ^{3}**C**.[29, 38, 225] Based on prior work,[225] **A** is expected to add to either the "axial" position of ^{1}**C** (blue pathway, via **A-TS-B**, barrier of 12.8 kcal/mol) or the "equatorial" position of ^{3}**C** (green pathway, via **A-TS-B'**, barrier of 11.5 kcal/mol), the latter being more energetically favorable. On the basis of these calculations, at low concentration of alkene, alkyl radical **A** is expected to produce the direct cross-coupling product (**P^{cc}**) via the green pathway. However, at higher concentration of alkene, alkyl radical **A** is expected to undergo *irreversible* Giese addition to methyl acrylate via **A-TS-D**, which is isoenergetic to the barrier for metallation of **A** (**A-TS-B'**). We also considered radical addition of A to Ni^0-bound alkene but found this pathway less likely because of the inherent higher

concentration of alkene in the system with respect to nickel, as well as the low barrier for the oxidative addition of aryl bromide to the Ni^0 center (see **Figure A2.5** in Appendix 2 for more detailed discussion). Finally, subsequent metalation of ^{3}**C** with **D** affords the key Ni^{III} intermediate **E**, which will quickly undergo reductive elimination (via **E-TS-F**) to form the desired, three-component product ($\mathbf{P^{DCF}}$) and bromo-Ni^I species **F**. Notably, both metalation (via **A-TS-B'**) and Giese addition (via **A-TS-D**) of radical **A** were found to be irreversible, and their transition states were higher in energy than the subsequent reductive eliminations (via **B'-TS-F** and **E-TS-F**, respectively). Thus, *these calculations demonstrate that the kinetic product selectivity for the competing pathways (DCF vs CC) is determined by the relative energy difference between the metalation (**A-TS-B'**) versus Giese addition (**A-TS-D**) transition states and, given the small energetic difference between these, is highly dependent on the relative concentration of nickel to alkene.* Analysis of a secondary α-ether system (THF, see **Figure A2.6** in Appendix 2) is also in agreement with these findings.

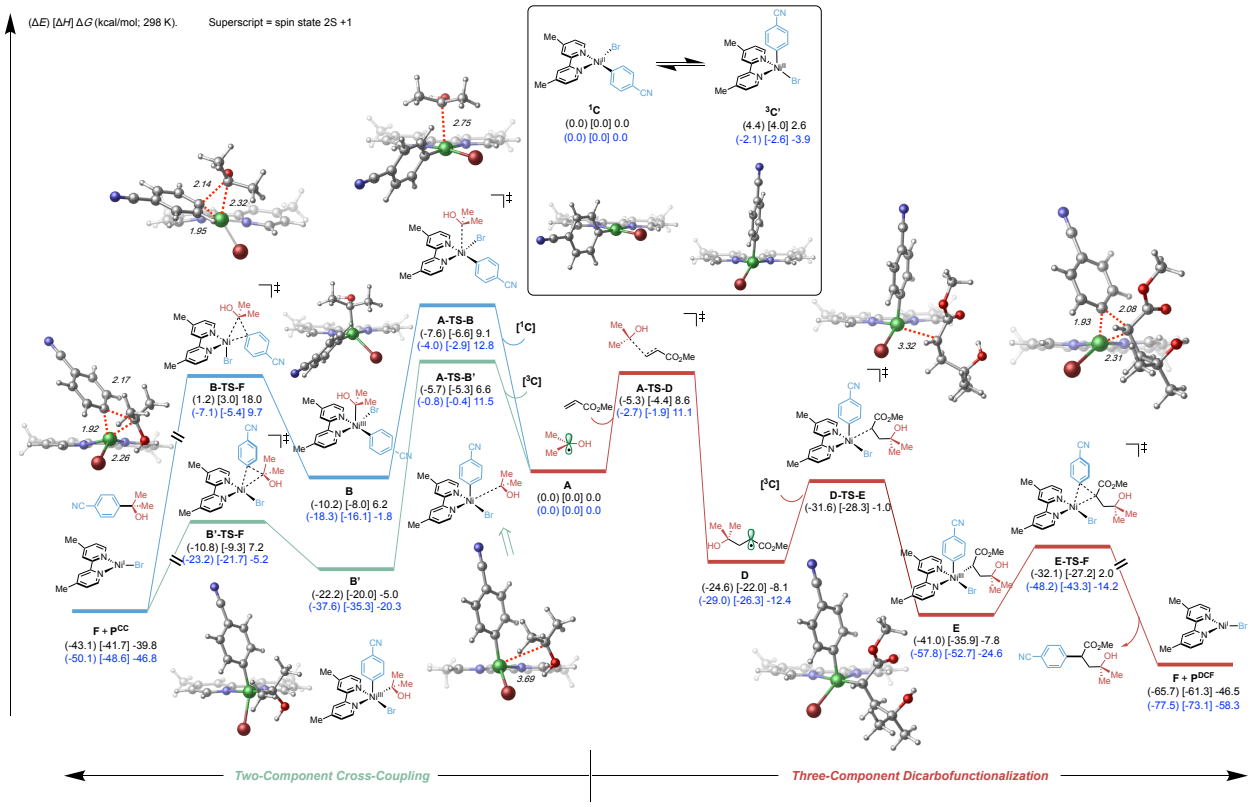
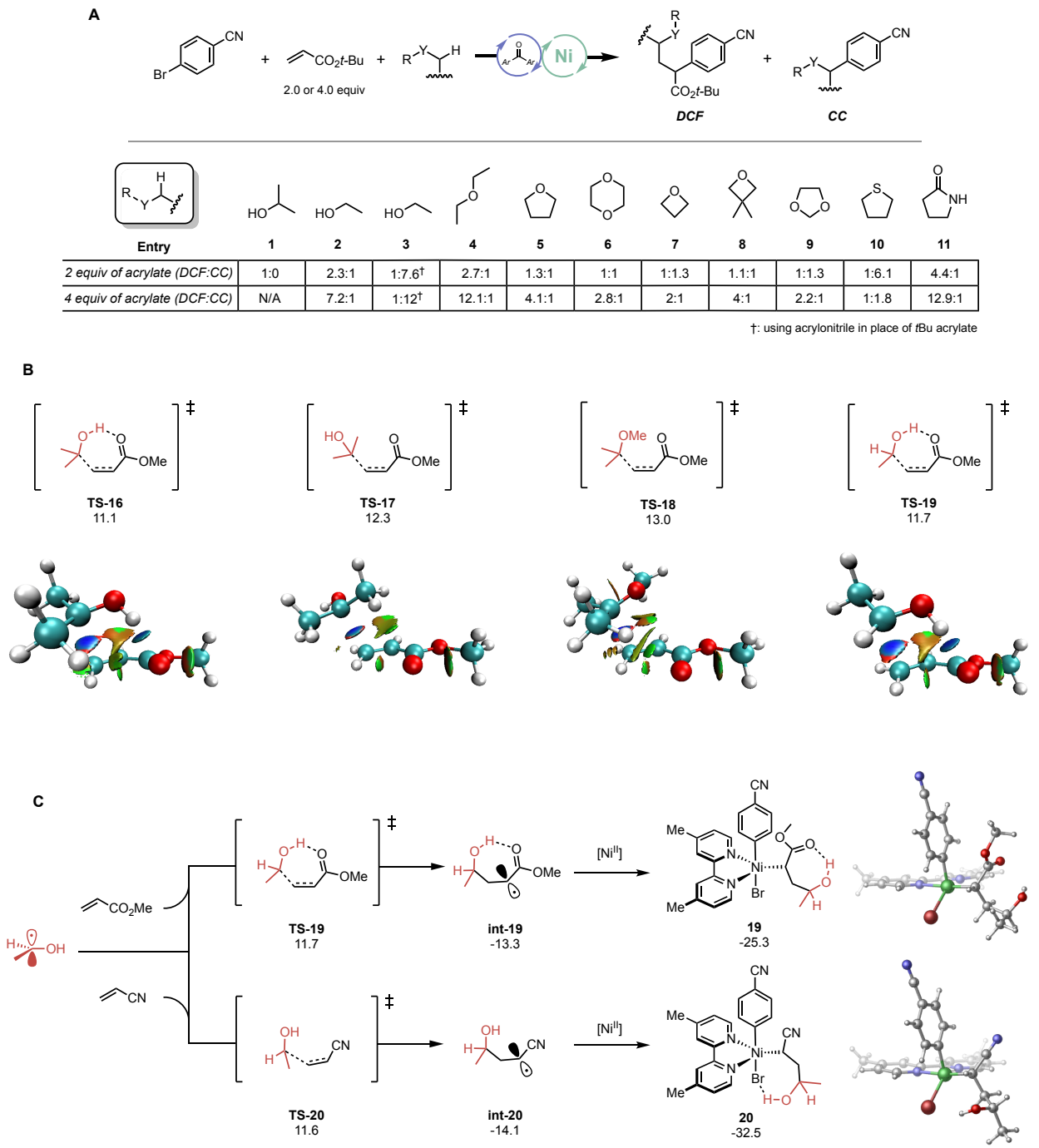


Figure 3.2 Computational analysis of the divergent reactivity of alkyl radical in the isopropyl alcohol system. Electronic (in parenthesis), enthalpy (in bracket) and free energies (kcal/mol; 298 K) given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-D3/def2-SVP-CPCM(benzene) (black) and DLPNO-CCSD(T)/def2-TZVPP//(U)B3LYP-D3/def2-SVP-CPCM(benzene) (blue) levels of method.

We then examined the DCF:CC selectivity for a range of sterically and electronically unique alkyl radicals. As established previously by our group and others, tertiary radicals are reluctant to directly metalate nickel,[177, 225] and undergo exclusive Giese addition in the presence of an activated alkene (**Figure 3.2**, red pathway). Under similar conditions in our previous report,[188] we observed that direct two-component CC was favored over three-component DCF (~3:1 NMR ratio) for unstabilized, secondary alkyl radicals generated from organotrifluoroborates. In contrast, secondary α-alkoxy radicals gave approximately equimolar ratios of DCF to CC products (**Figure 3.3A**, entries 4–9). These results suggest that the presence of an α-oxygen increases the nucleophilic character of the radical, accelerating the Giese addition. Notably, the secondary

radical generated from EtOH gave a significantly higher DCF:CC ratio than cyclic α-alkoxy radicals. The DCF selectivity was also severely eroded in the case of the α-thiyl radical derived from tetrahydrothiophene (entry 10). Satisfyingly, α-amido radicals exhibited the highest DCF:CC selectivity among all the examined secondary radicals (entry 11). Further, we found that the trends of experimentally observed DCF:CC selectivities is also consistent with the computed barriers (see **Table A2.2** in Appendix 2). That is, in general, the DCF:CC selectivity arises from competitive alkyl radical Giese addition versus metalation to the tetrahedral Ni^{II} species, which could be operative in related transformations involving secondary α-hetero-substituted alkyl radicals.



Entry	1	2	3	4	5	6	7	8	9	10	11
2 equiv of acrylate (DCF:CC)	1:0	2.3:1	1:7.6†	2.7:1	1.3:1	1:1	1:1.3	1.1:1	1:1.3	1:6.1	4.4:1
4 equiv of acrylate (DCF:CC)	N/A	7.2:1	1:12†	12.1:1	4.1:1	2.8:1	2:1	4:1	2.2:1	1:1.8	12.9:1

†: using acrylonitrile in place of *t*Bu acrylate

Figure 3.3 Selectivities of various secondary radicals for competing DCF and CC pathways. **A:** Values indicate ratio of DCF to CC product determined by crude ^{1}H NMR (performed by Molander and coworkers). Reaction conditions: 4-bromobenzonitrile (1 equiv, 0.1 mmol), *tert*-butyl acrylate or acrylonitrile (2 equiv or 4 equiv, 0.2 or 0.4 mmol), C–H precursor (15 equiv, 1.5 mmol), Ni **2** (10 mol %, 0.01 mmol), benzophenone **1** (20 mol %, 0.02 mmol), K_2HPO_4 (2 equiv, 0.2 mmol), TFT (0.1 M), 24 h, irradiating with 390 nm Kessil® lamp. **B:** NCI plots and the computed energetics (free energy, in kcal/mol) for corresponding Giese addition transition states of various alkyl radicals to acrylate. **C:** Proposed hydrogen bonding facilitates Giese-type addition *vs* direct

metalation in the reaction of secondary ethoxy radical. Free energies (kcal/mol; 298 K) given were calculated at the DLPNO-CCSD(T)/def2-TZVPP//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of method.

Given the unique reactivity exhibited by secondary α-hydroxy radicals (e.g., derived from EtOH), we speculated that hydrogen bonding could influence the selectivity for the two competing pathways. Prior studies revealed that the presence of hydrogen bonding significantly accelerates radical addition of alcohols into alkenes,[216, 227-228] presumably by weakening the α-hydroxy C–H bond in the presence of exogenous hydrogen bond acceptors. However, there are very few computational studies that examine the role of hydrogen bonding between the radical component and Giese acceptor.[229] We hypothesized that this type of hydrogen bonding interaction could play a paramount role in controlling selectivity for this DCF protocol. Based on our calculations, we attribute the increased DCF selectivity in entry 2 compared with entries 5–9 to an accelerated Giese addition via hydrogen bonding as demonstrated by the NCI plots (**Figure 3.3B**, demonstrated as blue cloud between the hydroxyl and carbonyl groups).[230] In the case of the α-alkoxy systems, the higher barrier for Giese addition (owing to the lack of hydrogen bonding) and the lower barrier for direct radical addition to the Ni center results in the increased formation of the CC product (see **Table A2.2** in Appendix 2 for the computed barriers of each system). Further support for the influence of hydrogen bonding was found when replacing *tert*-butyl acrylate with acrylonitrile as the Giese acceptor (entry 2 vs 3). The dramatic erosion of DCF to CC selectivity could be attributed to the inability of acrylonitrile to engage in hydrogen bonding with the hydroxyl group. However, considering the similar barrier of Giese addition for acrylonitrile and an acrylate (**Figure 3.3C**, **TS-19** *vs* **TS-20**), we propose that the carbonyl of the acrylate "locks" the hydroxyl via an intramolecular hydrogen bond, facilitating efficient arylation of α-carboxy radical **int-19**. Upon closer inspection of the Ni^{III} intermediates that result from metalation of radical adducts **int-19** and

int-20, we found that the hydroxyl group remains oriented toward the carbonyl in **19**, while pointing to Br atom in **20**. We presume that the alternate orientation of the hydroxyl in complex **20** negatively impacts the arylation step, leading to hydroalkylation of acrylonitrile. The exact mechanistic details concerning the formation of this hydroalkylation product have not yet been fully elucidated. Interestingly, the α-thiyl radical (**Figure 3.3A**, entry 10) shows a low barrier for metalation but a much higher barrier for Giese addition, which makes the generation of cross-coupling product more favorable (see **Table A2.2** in Appendix 2). Overall, these results convincingly demonstrate an unappreciated, yet critical, effect of hydrogen bonding in controlling product formation in metallaphotoredox radical cross-couplings.

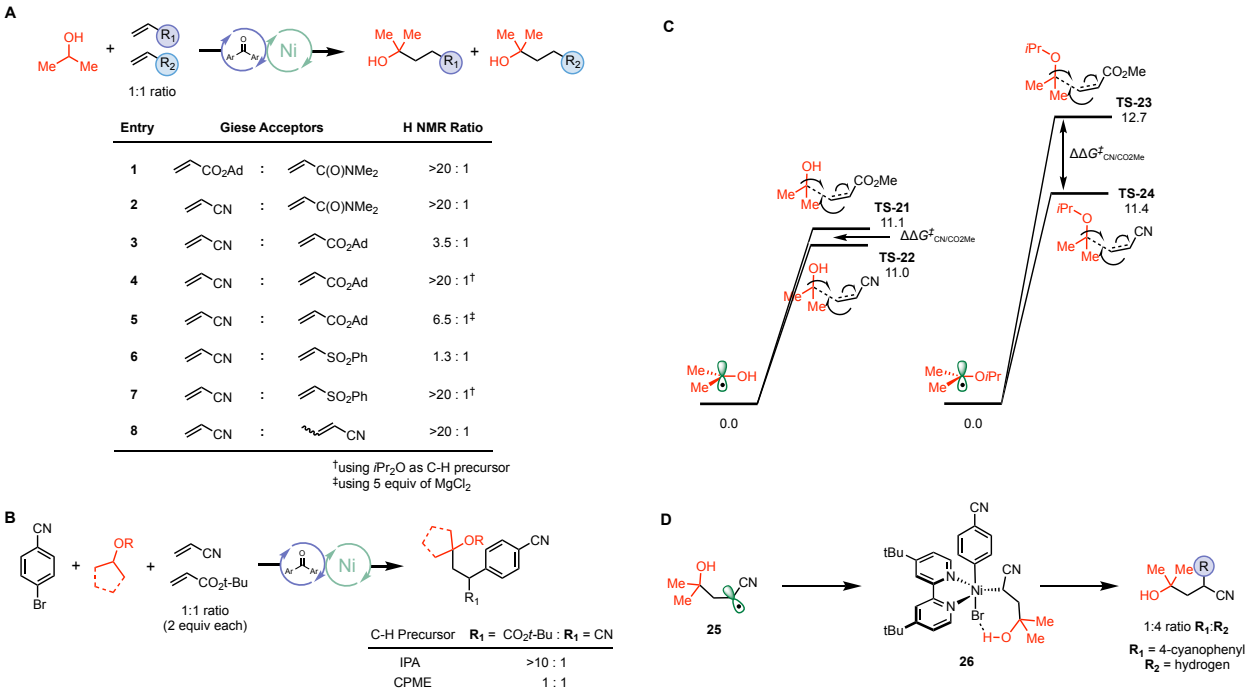


Figure 3.4 Competition reactions and related computational details. **A:** Hydroalkylation competition reactions (performed by Molander and coworkers), alkenes (1 equiv each, 0.1 mmol), C-H precursor (15 equiv, 1.5 mmol), Ni **2** (10 mol %, 0.01 mmol), benzophenone **1** (20 mol %, 0.02 mmol), TFT (0.1 M), irradiating with 390 nm Kessil® lamp for 30-90 min, reactions carried out to ~25% conversion. **B:** DCF competition reactions, standard reaction conditions as in **Table 3.1** (performed by Molander and coworkers). **C:** Computed energetics for the Giese addition processes. Free energies (kcal/mol; 298 K) given were calculated at the DLPNO-CCSD(T)/def2-TZVPP//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of method. **D:** Experimental results of reaction of *i*-PrOH/acrylonitrile/*p*-BrC_6H_4CN (performed by Molander and coworkers).

In an effort to more fully understand the hydrogen bonding interactions between various radical and alkene components in the Giese addition step, hydroalkylation competition reactions were performed (**Figure 3.4**). Isopropanol preferentially engaged acrylates and acrylonitrile in hydroalkylation compared to the less electrophilic acrylamide (**Figure 3.4A**; entries 1 and 2). However, *i*-PrOH underwent hydroalkylation with only a slight preference for acrylonitrile over adamantyl acrylate. Complete selectivity for addition to acrylonitrile over adamantyl acrylate was observed using diisopropyl ether as a C–H precursor (**Figure 3.4A**, entry 4). The calculations in **Figure 3.4C** rationalized the dissimilar selectivities of alcohols and ethers observed in the hydroalkylation competition reactions. In particular, we attribute the significant decrease in $\Delta\Delta G^{\ddagger}_{CN/CO2R}$ for *i*-PrOH compared to diisopropyl ether to the presence of hydrogen bonding between the hydroxyl and the acrylate. Addition of a chaotropic reagent ($MgCl_2$) in entry 5 resulted in high selectivity for hydroalkylation of acrylonitrile with *i*-PrOH. We attribute the dissimilar selectivities in entries 3 and 5 to the disruption of hydrogen bonding between *i*-PrOH and adamantyl acrylate when $MgCl_2$ is present. A control reaction demonstrated that hydroalkylation of adamantyl acrylate with *i*-PrOH is not inhibited by the presence of excess $MgCl_2$. Furthermore, a similar trend in chemoselectivity for *i*-PrOH and diisopropyl ether was observed in competition reactions between acrylonitrile and phenyl vinyl sulfone, which is again attributed to the presence/absence of hydrogen bonding in the Giese addition transition states (entries 6 and 7).

As evident in entry 8, the presence of β-substitution on the alkene significantly retards the rate of Giese addition. Next, equimolar ratios of acrylonitrile and *tert*-butyl acrylate were subjected to the standard DCF conditions using either *i*-PrOH or CPME as the C-H precursor (**Figure 3.4B**). When *i*-PrOH was used as the C–H precursor, the ratio of DCF products greatly favored the

acrylate. However, CPME exhibited an equivalent ratio of DCF products. Because of these unexpected results, we conducted a DCF reaction of *i*-PrOH with acrylonitrile under standard conditions, which produced an atypically high ratio of hydroalkylation/DCF products (**Figure 3.4D**). Based on these experiments and the calculated transition state energies in **Figure 3.4C**, it is apparent that the ratio of DCF products is not solely governed by the rates of each Giese addition. As such, we conclude that the arylation step is significantly impacted by the steric and electronic nature of Giese adducts (**21–24**) as well as the presence or absence of hydrogen bonding in Ni^{III} complexes (**18**, **20**, **26**). We are currently pursuing further detailed calculations (including quasi-classical molecular dynamics simulations) to probe this hypothesis and these results will be reported in due course.

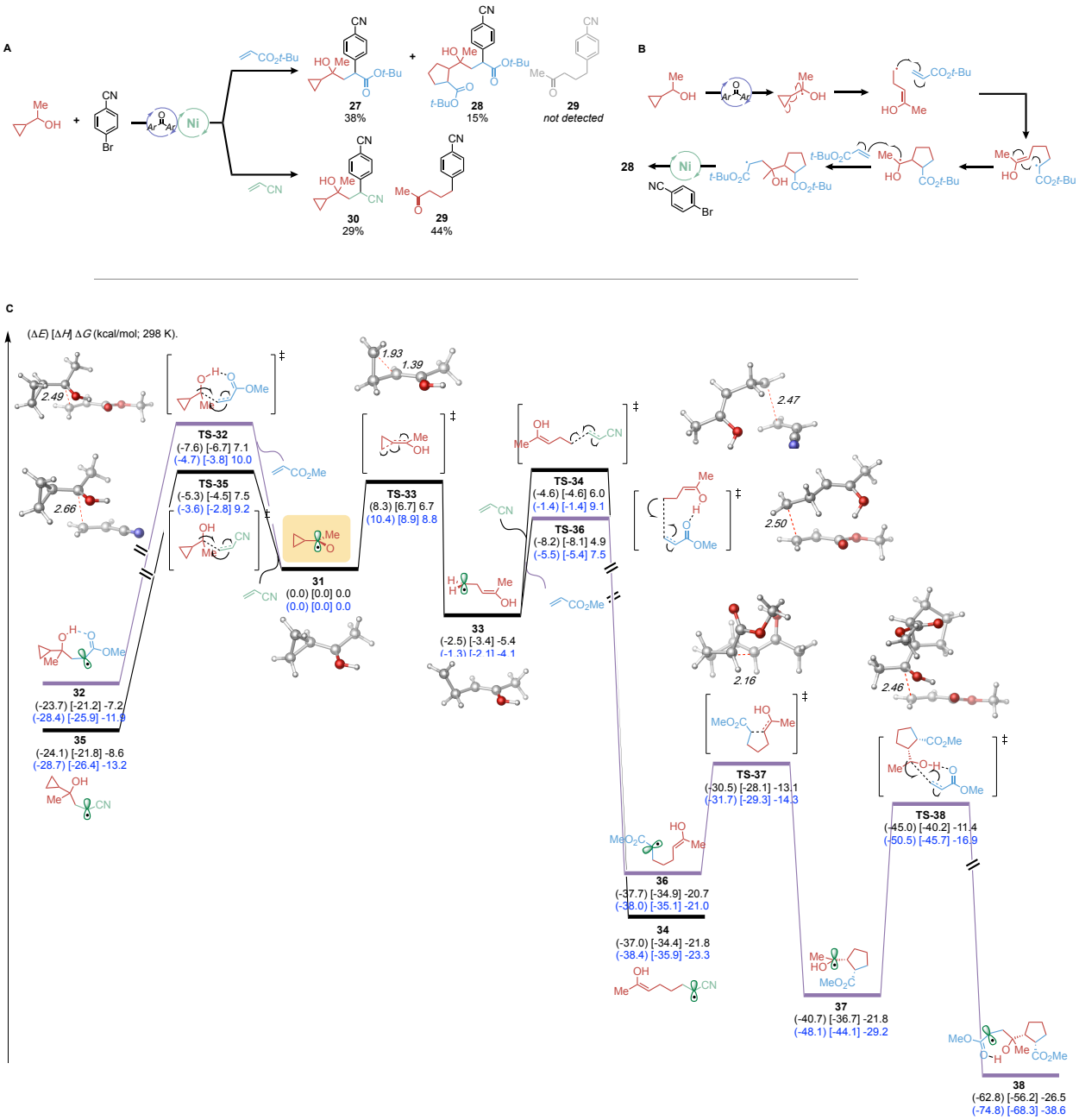


Figure 3.5 Experimental and computational results with 1-cyclopropylethanol as C–H precursor. **A:** DCF reactions with 1-cyclopropylethanol; standard reaction conditions as in **Table 3.1** (performed by Molander and coworkers). **B:** Proposed pathway of the formation of cyclopentane-containing DCF product. **C:** Computational analysis of the competing ring-opening and Giese addition of tertiary radical in acrylate and acrylonitrile systems. Electronic (in parenthesis), enthalpy (in bracket), and free energies (kcal/mol; 298 K) given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-D3/def2-SVP-CPCM(benzene) (black) and DLPNO-CCSD(T)/def2-TZVPP//(U)B3LYP-D3/def2-SVP-CPCM(benzene) (blue) levels of method.

Finally, we employed 1-cyclopropyl ethanol as a C-H precursor, anticipating that the resultant alkyl radical could trigger ring-opening of the α-cyclopropane ring prior to undergoing Giese addition and/or metalation (**Figure 3.5A**). To our astonishment, the *major* product from the reaction of with *tert*-butyl acrylate under standard conditions was the *three-component* cyclopropane-containing adduct **27**. An additional product, a [3+2] cycloaddition adduct (**28**), was isolated as well. This product was presumably generated from cyclopropane ring opening followed by Giese addition and *cis*-selective 5-exo-*trig* cyclization to achieve a cyclopentane-containing α-hydroxy radical (*vide infra*), which could undergo subsequent DCF reactivity (**Figure 3.5B**).[231] Similar reactivity was observed in our previous DCF report when employing an organotrifluoroborate derived from (*S*)-verbenone, which produced a [4+2] cycloaddition adduct.[188] Under identical conditions, reaction with acrylonitrile produced some cyclopropane-containing DCF product (**30**). However, the *major* product obtained in this system was a *two-component* cross coupled product (**29**), which stemmed from α-cyclopropyl radical ring opening. Computed energetics for these systems (**Figure 3.5C**) shows that ring opening of the α-cyclopropyl radical (**TS-33**) is competitive with Giese addition to either acrylate or acrylonitrile and thus account for the mixture of both cyclopropyl DCF products (**27** and **30**) and various ring opened products (**28** and **29**). We propose that **28** and **29** stem from primary radical **33** (generated from reversible cyclopropane ring opening), which could undergo either Giese addition to the corresponding alkene or metalation to the Ni center (not calculated). The formation of **29** as the major product in the reaction with acrylonitrile suggests that **TS-34** is higher than the barrier for metalation of **33**. Conversely, the absence of **29** and the formation of **28** in the reaction with *tert*-butyl acrylate is rationalized by the significantly lower barrier of Giese addition of **33** to the acrylate. As demonstrated by the transition state structure (**TS-36**), hydrogen bonding between **33**

and acrylate is responsible for the accelerated Giese addition leading to **36**. We therefore conclude that hydrogen bonding is again a prevailing factor in determining product selectivity in this DCF protocol.

3.4 Conclusion

In summary, a novel multicomponent DCF strategy has been developed that relies on a sustainable and chemoselective mode of HAT catalysis. New insights into the nature and effect of hydrogen bonding in radical/alkene reactivity as well as metallaphotoredox cross-coupling has been discovered. We anticipate that these findings will not only provide a new and efficient strategy for small molecule synthesis but also that the mechanistic insights will prompt further discovery in the area of radical reactivity mediated by hydrogen bonding.

Chapter 4: Mechanistic Study of Enantioselective Three-Component Carboarylation of Alkenes Enabled by Visible-Light Dual Ni/Photoredox Catalysis

Excerpts from this chapter were published in: Guo, L.[#]; **Yuan, M.**[#]; Zhang, Y.; Wang, F.; Zhu, S.; Gutierrez, O.*; Chu, L.* *J. Am. Chem. Soc.* **2020**, *142*, 20390-20399.

4.1 Abstract

A visible-light-promoted photoredox/nickel protocol for the enantioselective three-component carboarylation of alkenes with tertiary and secondary alkyltrifluoroborates and aryl bromides is described. This redox-neutral protocol allows for facile and divergent access to a wide array of enantioenriched β-alkyl-α-arylated carbonyls, phosphonates, and sulfones in high yields and excellent enantioselectivities from readily available starting materials. We also report a modular and enantioselective synthesis of flurbiprofen analogs and piragliatin lead compound to demonstrate synthetic utility. Experimental and computational mechanistic studies were performed to gain insights into the mechanism and origin of chemo- and enantioselectivity.

4.2 Introduction

Chiral α-aryl carbonyls are prevalent structural motifs found in bioactive molecules, pharmaceuticals, and versatile intermediates in organic synthesis (**Figure 4.1A**).[232-234] Thus, the development of catalytic asymmetric approaches for direct construction of enantioenriched α-aryl carbonyls has attracted remarkable attention but remains a significant challenge due to the facile racemization of such stereocenters under basic conditions.[235-239] Recently, Ni-catalyzed asymmetric cross-couplings with aryl organometallic reagents have emerged as effective protocols to forge these chiral tertiary carbon centers.[1, 195, 240-247] A complementary asymmetric cross-electrophile coupling strategy, that bypasses the employment of moisture-sensitive metallic

reagents, has also been reported.[248-253] However, these examples generally focus on catalytic enantioconvergent cross-couplings between two components. In this context, the development of catalytic asymmetric multi-component cross-coupling reactions, that utilize robust and readily available starting materials, could allow for rapid access to diverse functionalized chiral α-aryl carbonyls and related structural motifs.

During the last several years, nickel-catalyzed intermolecular carboarylation of alkenes has emerged as an efficient and attractive approach for the rapid construction of diverse carbon frameworks.[185, 189-190, 203, 254-271] Notably, Baran reported a Ni-catalyzed three-component alkylarylation of acrylates using phenylzinc and tertiary alkyl carboxylic esters, forging functionalized α-aryl carbonyls from simple alkenes.[189] Later, several groups, including ours, utilized the synergistic visible-light dual-photoredox/nickel catalytic approach[7, 272-276] to engage diverse alkyl radical precursors with three-component reactions with alkenes (**Figure 4.1B**).[188, 210, 277-279] However, enantioselective control of the newly formed pro-chiral α-carbonyl carbon centers using these methods remains challenging. On the other hand, transition metal-catalyzed asymmetric intermolecular difunctionalization of alkenes has begun to emerge as a powerful strategy for the construction of complex molecular skeletons with enantioselective control,[280-283] but the use of chiral nickel catalysis in the asymmetric multicomponent transformations of alkenes has only recently been described (**Figure 4.1C**).[284-288]

Herein we report an asymmetric dual photoredox/Ni-catalyzed[81, 253, 289-296] three-component alkylarylation of a wide range of diverse alkenes with aryl bromides and alkyltrifluoroborates under redox-neutral conditions (**Figure 4.1D**). This visible-light-induced synergistic strategy represents a highly enantioselective approach to forge the valuable enantiopure α-aryl carbonyls from readily available starting materials.

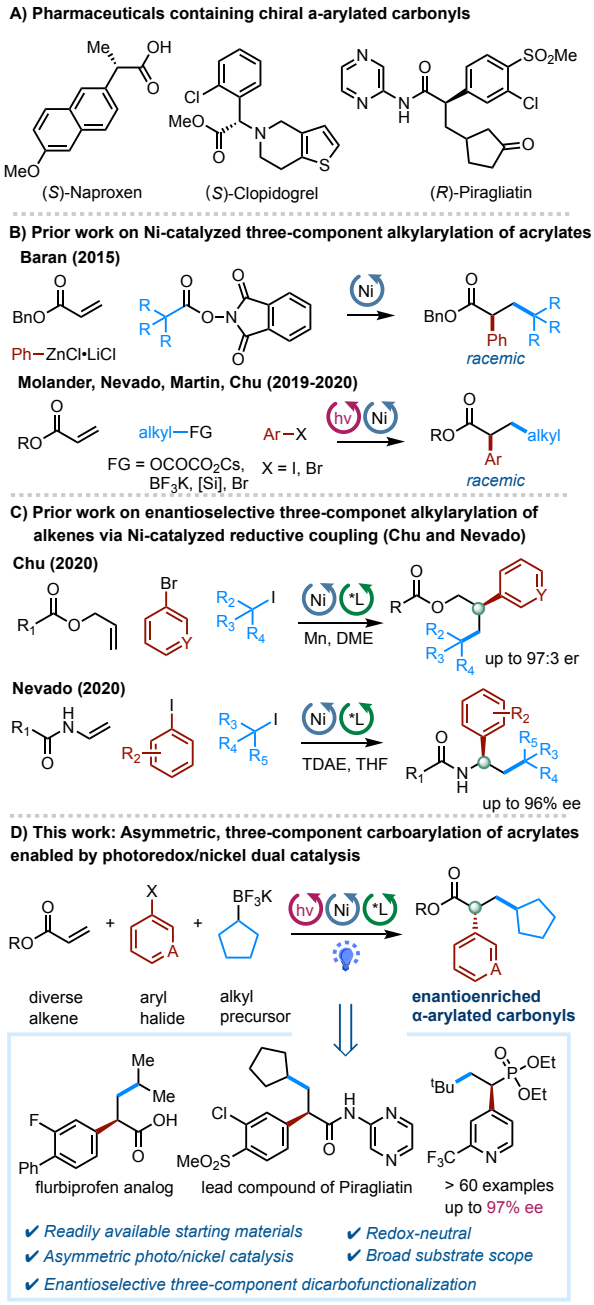


Figure 4.1 Enantioselective, three-component 1,2-alkylarylation of alkenes enabled by dual photoredox/nickel catalysis.

4.3 Results and Discussion

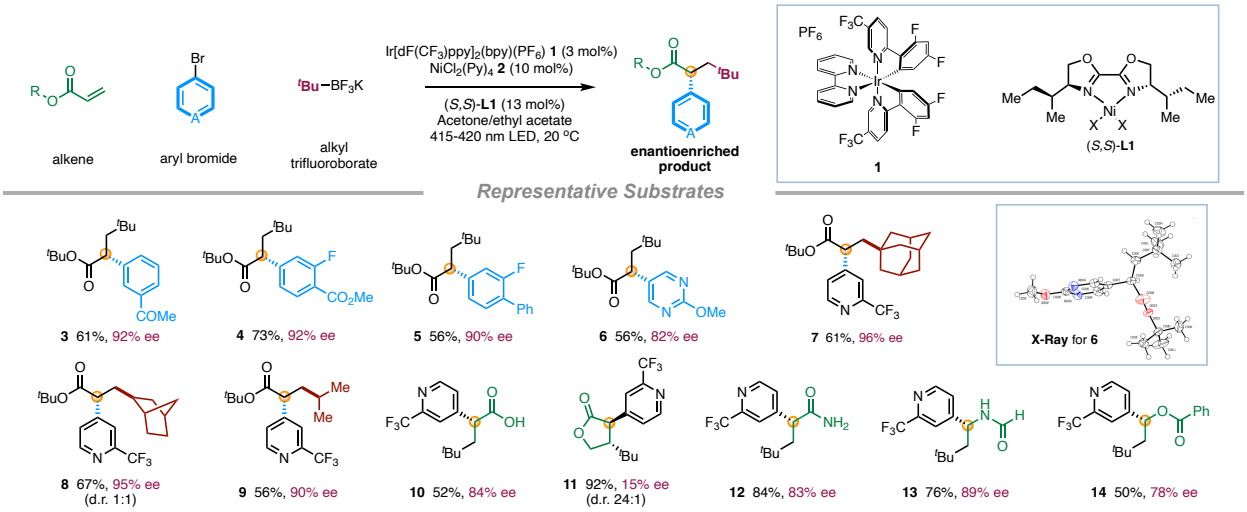


Figure 4.2 Representative substrates of the enantioselective three-component carboarylation of alkenes performed by Chu.[297] Reactions conditions: aryl bromide (0.2 mmol), alkene (2 equiv.), alkyl-BF_3K (2.5 equiv.), Ir[dF(CF_3)ppy]$_2$(bpy)(PF_6) **1** (3 mol%), $NiCl_2(Py)_4$ **2** (10 mol%), (*S,S*)-**L1** (13 mol%), acetone/ethyl acetate [0.05 M], 10 W 415-420 nm LED, 20 °C, 24 h. Isolated yields. The ee values were determined by HPLC on a chiral stationary phase.

After optimizing a suitable set of reaction conditions for this asymmetric dicarbofunctionalization reaction, the scope of reaction components were evaluated by our collaborator,[297] with the representative substrates shown in **Figure 4.2**. Apart from mono- and disubstituted arenes (**3–5**), heteroaryl bromides were also found employable (**6**). In terms of the scope of alkyl precursors, both tertiary linear (**3**–**6**) and cyclic (**7**) alkyl trifluoroborates were both coupled with high yields and excellent enantioselectivity (up to 96% ee). Notably, secondary alkyl trifluoroborates (**8**, **9**) could be also applicable to this asymmetric photoredox/nickel protocol (up to 95% ee). Moreover, a wide range of alkenes was found to be viable substrates, including the unprotected acrylic acid (**10**), internal alkene (**11**), acrylamide (**12**) and the more challenging electron-rich alkenes vinylamine (**13**) and vinyl ether (**14**). The outstanding tolerance of functional groups and the capability to functionalize alkenes with varied electronic and structural properties

embodies the importance of this asymmetric photoredox/nickel three-component dicarbofunctionalization protocol in synthesizing highly valuable structural motifs.

To gain insight into the mechanism and elucidate the factors controlling selectivity, we turned to quantum mechanical calculations. Specifically, we used dispersion-corrected DFT to identify: (1) the preference of the three-component carboarylation over the direct arylation of the generated alkyl radical; (2) the factors controlling the enantioselectivity.

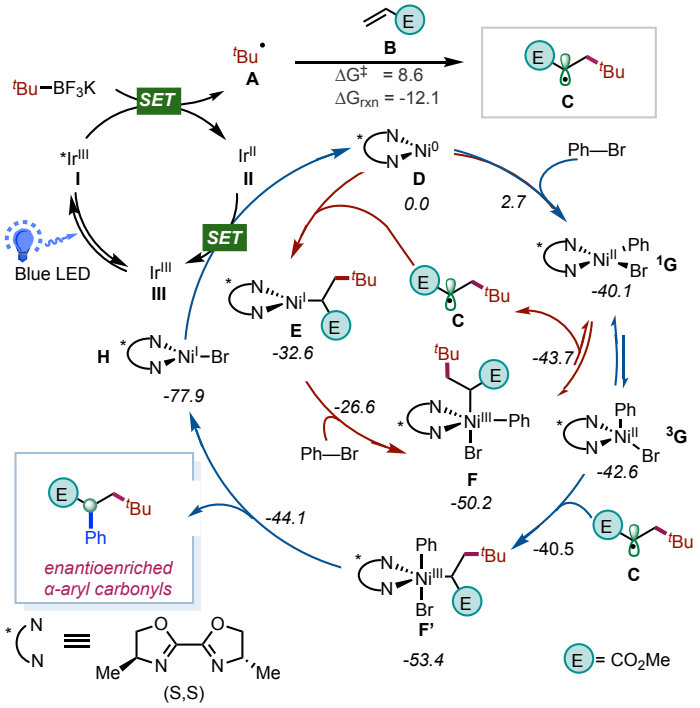


Figure 4.3 Mechanistic proposal based on computations [UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)]. All free energies are in kcal/mol (298K).

Initially, to reduce the computational cost, the (*S*,*S*)-Me-BiOx, phenyl bromide, and methyl acrylate were used as model substrates in our calculations. All optimizations were performed with open-shell, dispersion-corrected DFT (with Becke-Johnson damping) in THF using the CPCM implicit solvent model [noted as UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)]. To compare energetics, we also performed calculations at the UB3LYP-D3(BJ)/def2-TZVPP-

CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) level of theory but, for simplicity, only UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) will be discussed in the text (see **Figure A3.1** in Appendix 3). Calculations show that alkyl radical **A,** presumably generated from favorable single-electron oxidation of alkyl trifluoroborate reagent with Ir* **I**, can undergo *fast and irreversible* radical addition to methyl acrylate **B** (via **A-TS-C**, barrier of 8.6 kcal/mol) to form α-ester radical **C**, which is 12.1 kcal/mol downhill in energy (**Figure 4.3**). Based on prior work in dual nickel/photoredox cross-coupling reactions, we explored both Ni(0)/Ni(I)/Ni(III), Ni(0)/Ni(II), and alternative mechanisms to understand the fate of alkyl radical **C** (see **Figure A3.1** in Appendix 3 for full energy diagrams). As found with the bipyridyl-Ni systems (blue),[225] a chiral Ni(0) **D** species could undergo rapid oxidative addition (barrier of only 2.7 kcal/mol) with phenyl bromide to give a *square planar singlet* Ni(II) species ^{1}**G**. In turn, this species can then equilibrate with a *triplet tetrahedral* Ni(II) ^{3}**G** prior to interacting with the alkyl radical **C** to undergo *productive* C–C bond formation (*vide infra*). Alternatively, as shown in red, alkyl radical **C** can be intercepted by the Ni(0) **D** to generate a Ni(I)-alkyl species **E** that is downhill in energy by 32.6 kcal/mol. As observed with related transformations, Ni(I) **E** can then undergo oxidative addition with phenyl bromide to afford Ni(III) species **F**, which, as previously found before for related transformations,[225] will undergo *reversible* radical dissociation (barrier of 6.5 kcal/mol) to form a *square planar singlet* Ni(II) species ^{1}**G**. We also located a reductive elimination transition state from **F** with a barrier of 8.7 kcal/mol (see **Figure A3.7** in the Appendix 3). Considering the lower barrier for **F** to undergo radical dissociation (6.5 kcal/mol), the latter process is more favorable.

Altogether, independent of the species responsible for intercepting the alkyl radical **C**, these pathways will converge at a *singlet square planar Ni(II)* prior to undergoing *irreversible* C–C bond formation (*vide infra*). Specifically, we found that the Ni(II) ^{1}**G** can undergo isomerization

and intersystem crossing to form the more stable *tetrahedral* triplet spin state Ni(II) ^{3}**G** species. Precedent reports for this singlet-triplet conversion of Ni^{II} species in photoredox/Ni system has been made by many groups in related nickel transformations.[29, 38, 225] In turn, ^{3}**G** can then rapidly and *irreversibly* intercept the α-ester radical **C** to form the productive Ni(III) **F'** species. Finally, subsequent reductive elimination will lead to the observed three-component alkylarylation product and Ni(I) **H** which, after SET will restart the dual catalytic cycle.

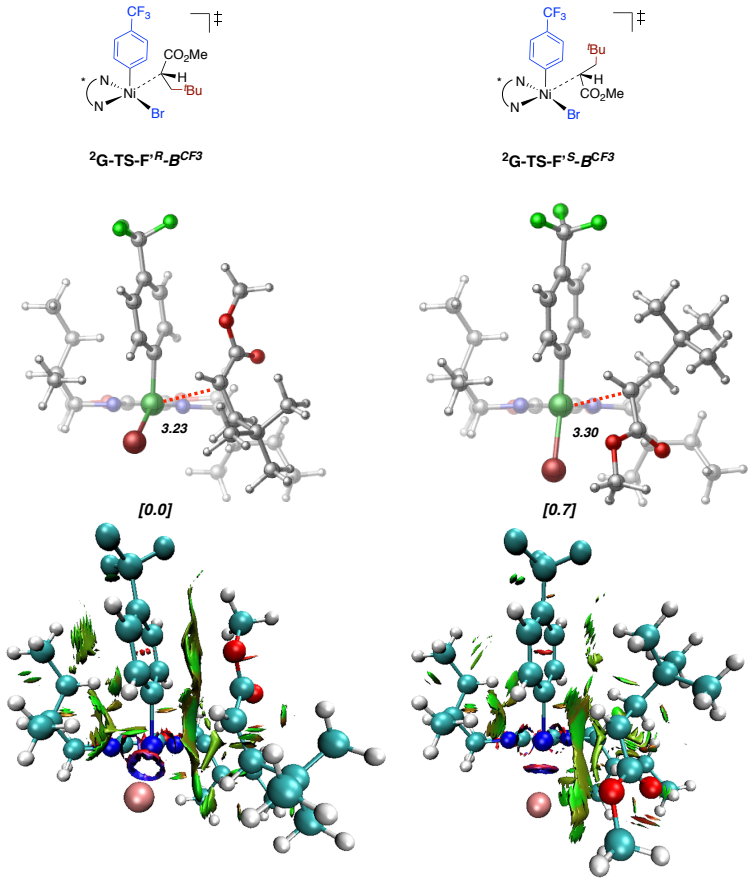


Figure 4.4 Origin of enantioselectivity in the radical addition step. The electronic energy values shown were calculated at the UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) level of method.

Closer inspection of the catalytic cycle reveals that the energy for the radical addition step (^{3}**G** to **F'**) is higher than the energy for the reductive elimination transition state (**F'** to **H**). These results suggest that the *radical addition to tetrahedral Ni(II) center, not the reductive elimination,*

is the stereodetermining step. Similarly, Fu reported that the radical addition to Ni^{II} center is the stereodetermining step and that the alkyl radical adds to the tetrahedral Ni^{II} center instead of the square planar Ni^{II} center in the chiral Ph-Box system.[195, 288] We have also found similar stereodetermining step in Fe-catalyzed cross-couplings involving α-ester radicals computationally.[298]

After identifying the radical addition as the stereodetermining step, we went further to investigate the origin of the enantioselectivity as well as the effect of chiral ligand in this step (see **Figure A3.2** in Appendix 3). Specifically, using the full chiral ligand (*S,S*)-*sec*-Bu-BiOx **L1** and *p*-CF_3-ArBr as model substrate, we investigated in detail the stereodetermining radical addition step. Overall, we considered numerous rotamers of the alkyl chains on the chiral ligand and performed a Boltzmann calculation using nine of the lowest energy radical addition transition states (see **Figure A3.3** in Appendix 3),[230] which, in agreement with the experiment, these results predicted the correct enantiomer albeit underestimated the observed enantiomeric ratio (~ 80:20 vs. ~95:5). To study the controlling factor in the radical addition step, we also conducted NCI analysis on only the lowest-energy competing diastereomeric transition states to investigate the possible effects of noncovalent interactions as implemented in Multiwfn (**Figure 4.4**).[230] This analysis revealed a stronger van der Waals interaction [green cloud, created as color-filled Reduce Density Gradient (RDG) isosurface] between the aryl ring and the alkyl chain as well as the ester group, which can be attributed to the C-H•••π interaction and the π-π interactions, respectively. Overall, these noncovalent interactions play an important role in this enantioselective olefin dicarbofunctionalization protocol (see Appendix 3 for detailed discussion). Notably, Doyle and Sigman also pointed out the important contribution of C-H•••π interaction between the alkyl chain

of chiral BiOx ligand and the aryl ring to the reductive asymmetric Ni catalysis through multivariate analysis.[299]

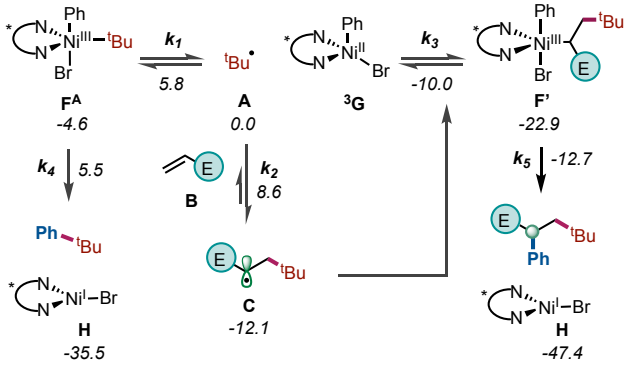


Figure 4.5 Origin of chemoselectivity of the model system. All free energies (kcal/mol; 298 K) were calculated at the UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) level of method.

Next, to gain insights into the divergent reactivity of *tert*-butyl radical **A** in this system (i.e., two-component versus three-component cross-coupling), we performed calculations to study the separate pathways of forming the three-component alkylarylation product and the two-component arylation product **Ph-^{t}Bu** (**Figure 4.5**). Based on the calculated results, we found that the radical addition of *tert*-butyl radical **A** to *tetrahedral* Ni^{II} ^{3}**G** is *reversible* (barrier of 5.8 kcal/mol), while the subsequent reductive elimination to form **Ph-^{t}Bu** has a barrier of 10.1 kcal/mol with respect to **F^A**. In contrast, although the barrier of the *irreversible* Giese addition of *tert*-butyl radical **A** to methyl acrylate is slightly higher (8.6 kcal/mol), it's still feasible and will lead to the generation of α-carbonyl radical **C** that is 12.1 kcal/mol downhill in energy. Given that the *relative* concentration of π-component **B** during catalytic turnover is significantly higher than that of Ni^{II} ^{3}**G** species, we expect a higher rate for the trapping of *tert*-butyl radical by the acrylate than the catalytic tetrahedral Ni(II) under catalytic turnover conditions. Finally, this Giese addition adduct can then undergo fast addition to Ni^{II} ^{3}**G** (barrier of only 2.1 kcal/mol) followed by subsequent reductive elimination (barrier of 10.2 kcal/mol) to form the three-component product. Taken

together, the preference of the three-component pathway is not only driven by the relative concentration of olefins in the system during catalytic turnover, but also by the low barrier of radical addition to the tetrahedral Ni^{II} ^{3}**G**.

Finally, we also performed preliminary calculations on the barriers and the thermodynamic drive of the Giese addition step between *tert*-butyl radical **A** and a series of different olefins that were tested in experiment as shown in **Figure 4.2**. These results showed that the barrier for Giese addition to π-components varies from 6.9 kcal/mol to 12.7 kcal/mol and the process is irreversible (see **Figure A3.5** in Appendix 3). In general, olefins with calculated higher barriers for Giese addition generally gave lower yields (e.g., methyl (*E*)-but-2-enoate, vinyl amines and vinyl ether) but more in-depth calculations on the competing cross-coupling pathways are needed since the chemoselectivity likely depends not only on the barrier for Giese addition but also on the concentration of olefins and the competing side-reactions (i.e., cross-coupling, H-atom abstraction, etc). To probe the mechanism experimentally, we also performed a series of preliminary experiments to study the relative lifetime of alkyl radical since it might also affect the chemoselectivity in this system (**Figure 4.6**). Consistent with the involvement of discrete alkyl radical intermediates and facile Giese addition prior to nickel cross-coupling addition, we observed that the addition of TEMPO completely shut down the desired alkylarylation reaction, whereas affording 32% yield of compound **19**, which might be generated via alkyl radical addition to acylate followed by TEMPO trapping (**Figure 4.6A**).

Moreover, based on our previous experience in studying the divergent reactivity of intermolecular cross-coupling and intramolecular radical cascade in Fe-catalysis, we performed the reaction with ester-substituted cyclopropyl alkene **20** under the optimal conditions (**Figure 4.6B**).[300] As expected from analysis of the enantiodetermining steps (**Figure 4.4**), the ester is

expected to play a critical role in controlling the enantioselectivity. Gratifyingly, we found that this reaction proceeded with a sequential radical addition/ring opening and *enantioselective aryl coupling* process to furnish product **21** in moderate yield and ee. Further, consistent with the experimental results, the barrier for radical addition was found to be 12.9 kcal/mol with DFT calculations leading to the formation of **22** that is 8.1 kcal/mol downhill in energy. From **22**, fast *intramolecular* ring-opening (barrier of only 3.2 kcal/mol) is expected to outcompete the *intermolecular* radical addition to Ni^{II} (not calculated), resulting in the generation of α-carbonyl C-radical **23**. In turn, **23** can add, in enantioselective fashion, to the chiral Ni catalyst to form the desired product **21**.

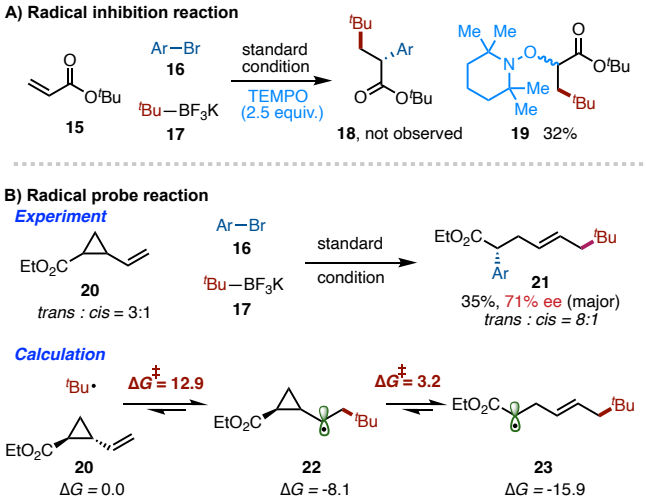


Figure 4.6 Mechanistic experiments. (A) Radical inhibition reaction. (B) Experimental results of radical probe reaction and the computed energetics of relevant pathways.

4.4 Conclusion

In conclusion, we developed an enantioselective three-component alkylarylation reaction of alkenes with secondary and tertiary alkyl trifluoroborates and aryl bromides via asymmetric photoredox/nickel dual catalysis. This visible light-enabled synergistic platform allows for direct and versatile synthesis of enantioenriched α-arylated carbonyls with high efficiency and excellent

enantioselectivity from readily accessible starting materials under redox-neutral conditions. The synthetic application of this asymmetric protocol has also been demonstrated via divergent and enantioselective synthesis of flurbiprofen analogs and lead compound of piragliatin. Computational and experimental studies were carried out that were consistent with a Ni(0)/Ni(II)/Ni(III) catalytic cycle with the radical addition to tetrahedral Ni(II) species as the stereodetermining step.

Chapter 5: Mechanistic Study of Enantioselective Three-Component Alkenylation of Organophosphonates via Nickel Metallaphotoredox Catalysis

This chapter contains unpublished data.

5.1 Abstract

The development of new and efficient catalytic multicomponent reactions (MCRs), a powerful technology for the rapid construction of molecular complexity from readily available starting materials, is highly sought-after in chemical synthesis. However, catalytic asymmetric MCRs, particularly involving radical species, remain largely underdeveloped due to the exceptionally high reactivity of open-shell radical species. Herein the Gutierrez group and the Lingling Chu group together report a metallaphotoredox-catalysed asymmetric three-component method to access a diverse array of enantioenriched α-alkenyl phosphonates from readily available vinyl phosphonates, alkenyl halides, and alkyl trifluoroborates under mild conditions. This operationally simple and redox-neutral protocol exhibits broad substrate scope and high to excellent chemo-, regio-, stereo-, and enantioselectivity. Further, by simple modification of the triplet energy of photocatalyst employed, both enantioenriched *trans* and *cis* α-alkenyl phosphonates can be divergently accessed from the same starting material. Moreover, aryl- and heteroaryl bromides can be utilized as effective coupling partners in this MRC for the expedient construction of the corresponding α-aryl phosphonates in good yields and excellent enantioselectivity. To provide insight into the operating mechanism, I performed detailed computational studies to elucidate the mechanism and origin of the observed regio-, stereo-, and enantioselectivity of this dual asymmetric nickel/photoredox-catalyzed MCR. Based on the computational data, this transformation operates via a radical cascade sequence with α-

phosphonate radical capture by a chiral tetrahedral alkenyl nickel(II) species as the enantioselectivity-determining step.

5.2 Introduction

Catalytic multicomponent reactions (MCRs) represent a powerful and efficient technology for the rapid construction of molecular complexity in one single operation, thus expanding the synthetic toolbox by providing novel retrosynthetic strategies to access natural products, drugs, and functionalized polymers.[301-304] Therefore, the development of new catalytic MCRs is highly sought-after in chemical synthesis.[305] Recently, significant attention has been devoted to the catalytic MCRs involving highly reactive open-shell (e.g., alkyl radicals and first-row transition metal) species, which complement the reactivity and selectivity patterns of classical two-electron MCRs.[306-309] In particular, the merger of visible-light photoredox catalysis and transition metal catalysis[272-274] has dramatically expanded the diversity of radical precursors as abundant feedstocks in catalytic MCRs.[257-258] However, the exceptionally high reactivity of open-shell radical species poses significant challenges in controlling reactivity and selectivity.[310-312] In particular, controlling enantioselectivity of the resulting chiral stereogenic centers remains a longstanding challenge in MCRs[310] and, not surprisingly, catalytic asymmetric radical MCRs still remain largely underexploited.

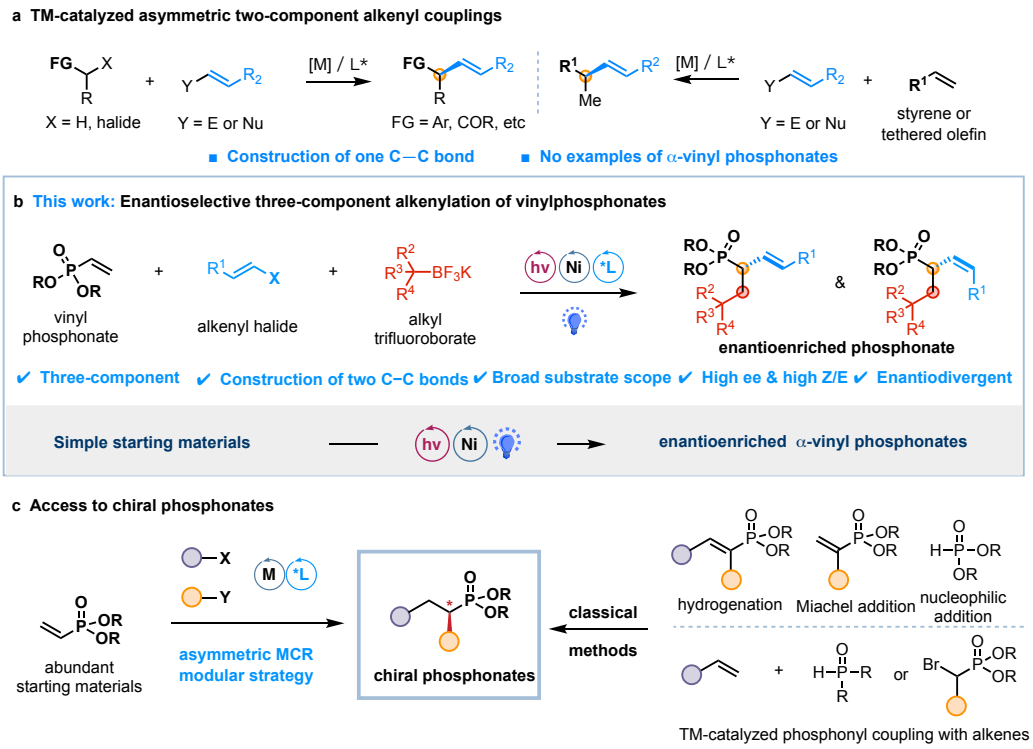


Figure 5.1 Enantioselective three-component carbo-vinylation of vinylphosphonates via dual photoredox/nickel catalysis. **a**, transition metal-catalyzed asymmetric two-component alkyl-alkenyl couplings; **b**, design of dual photoredox/nickel catalyzed enantioselective three-component carbo-vinylation of vinylphosphonates; **c,** previous methods to access chiral phosphonates.

Significant progress has been made in asymmetric radical difunctionalizations of alkenes enabled by chiral metal complexes and activated radical precursors under thermal conditions.[260, 281-282, 309] To date, however, scarce examples of enantioselective three-component dicarbofunctionalization of alkenes driven by dual visible light photoredox and transition metal catalysis have been disclosed.[297, 313-314] Notably, these methods are largely restricted to the construction of enantioenriched benzylic centers with the use of (hetero)aryl nucleophiles or electrophiles as coupling partners.[297, 313] Thus, the utilization of alkenyl coupling partners in multicomponent asymmetric cross-couplings is still significantly underexploited,[315] despite impressive progress in metal-catalyzed asymmetric two-component alkyl–alkenyl couplings to

forge chiral α-alkenyl/vinyl moieties (**Figure 5.1a**).[244, 316-326] Herein, the Gutierrez group and the Chu group together demonstrate that a combination of photoredox catalyst and chiral nickel catalyst can achieve enantioselective and divergent three-component carbo-vinylation of alkenyl phosphonates with alkyl nucleophiles and vinyl halides to deliver enantioenriched α-vinyl phosphonates under redox-neutral and mild conditions (**Figure 5.1b**). In terms of the mechanism of this novel transformation, I used dispersion-corrected DFT calculations to shed light on the mechanism and determine the origin of enantioselectivity. We anticipate that these combined experimental and computational results will accelerate the development of asymmetric multicomponent radical cross-coupling reactions using sustainable transition metals.

Organophosphonates and derivatives are important structural motifs in medicinal and pharmaceutical chemistry[327-329] and serve as privileged ligand scaffolds in (asymmetric) catalysis, [330] thus, the demand for stereo-chemically well-defined organophosphonates is of particular interest in chemical synthesis.[331-332] Generally, chiral organophosphonates can be accessed via asymmetric catalytic hydrophosphonylation with phosphites,[333] Michael addition of alkenyl phosphonates,[334-335] and hydrogenation of ethenylphosphonic acids.[336-337] Recently, transition metal-catalyzed cross-coupling reaction with alkenes has emerged as an attractive platform to assess these important motifs (**Figure 5.1c**).[338-339] However, these methods are limited to the use of two-component systems to form a net one C–C or C–heteroatom bond. The three-component protocol disclosed herein provides a new and complementary approach to these methods with diverse reactivity and selectivity leading to formation of two new C–C bonds, three stereogenic centers, and one asymmetric carbon.

5.3 Results and Discussion

5.3.1 Experimental results

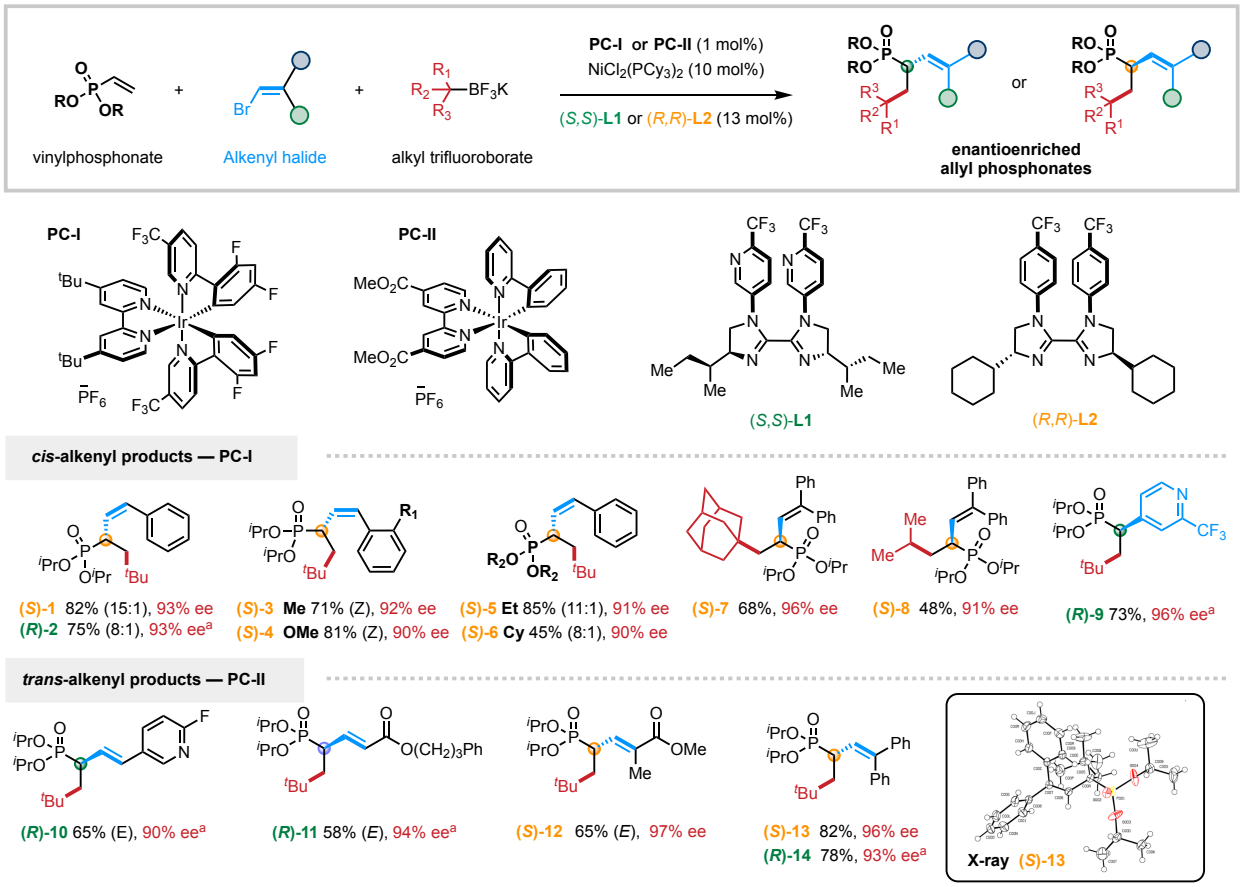


Figure 5.2 Representative substrate scope performed by collaborator. Reaction conditions: vinyl halide (0.1 mmol), vinylphosphonate (2.0 equiv.), alkyl-BF_3K (2.5 equiv.), $Ir[dF(CF_3)ppy]_2(dtbbpy)(PF_6)$ (**PC-I**) or $Ir(ppy)_2(di\text{-}CO_2Me\text{-}bpy)(PF_6)$ **PC-II** (1 mol%), $NiCl_2(PCy_3)_2$ (10 mol%), bis(2-CF_3-pyridyl)-biimidazoline (BiIm) ligand (*S,S*)-**L1** or (*R,R*)-**L2** (13 mol%), acethyl acetate/DMA or DME [0.05 M], 90 W LED, -15 °C or 20 °C, 12 h. Isolated yields. The ee values were determined by HPLC on a chiral stationary phase. [a]Using (*S,S*)-**L1** as chiral ligand.

After optimizing a suitable set of reaction conditions for this asymmetric dicarbofunctionalization reaction (by the collaborator), it was found that the photocatalyst can control the *Z*/*E* selectivity of the formed allyl product while the chiral ligand is responsible for the enantioselectivity of this three-component dicarbofunctionalization reaction. Specifically, mainly chiral *Z*-allyl phosphonates (e.g., **(*S*)-1**) were obtained when **PC-I** was employed, while *E*-allyl

phosphonates (e.g., **(*R*)-10**) became the major product when **PC-II** was the photocatalyst. In the same photocatalytic system, different enantiomers could be obtained when different chiral ligands were utilized (e.g., **(*S*)-1** versus **(*R*)-2**).

With the optimized reaction conditions in hand, the scope of reaction components was evaluated by our collaborator. As shown in **Figure 5.2**, when **PC-I** was employed, unsubstituted (**(*S*)-1** and **(*R*)-2**) and substituted styrenyl substrates can be coupled to generate *E*-selective products (**(*S*)-3**, **(*S*)-4**). In terms of the scope of alkoxy groups on the vinylphosphonates, both ethyl (**(*S*)-5**) and cyclohexyl (**(*S*)-6**) groups were both applicable with high yields and similar stereoselectivity and enantioselectivity (up to 91% ee). Notably, cyclic tertiary (**(*S*)-7**) and secondary alkyl trifluoroborates (**(*S*)-8**) could be also applicable to this asymmetric photoredox/nickel MCR protocol (up to 98% ee). Similar to the previous report,[297] (hetero)aryl bromides can also be coupled with high yields and excellent enantioselectivity (**(*R*)-9**). When switching to **PC-II** as the photocatalyst, *Z*-allyl phosphonates can be obtained. Apart from the products with different stereoselectivity as the other system (**(*R*)-10**), substituents other than aryl groups can also be incorporated, generating enantioselective α,β-unsaturated products open to late-stage modification (**(*R*)-11**). Moreover, multisubstituted alkenes can be generated with success (**(*S*)-12**, **(*S*)-13**, **(*R*)-14**).

To gain insight into the mechanism and origin of selectivity, the collaborator has done a series of experimental mechanistic experiments and I have performed dispersion-corrected DFT calculations. Specifically, to shed light on the photocatalytic cycle, our collaborator performed a series of Stern-Volmer fluorescent quenching studies. They found that photoexcited ***PC-I** (as well as ***PC-II**) was strongly quenched by vinyl bromide on the order of $5.38*10^8$ $M^{-1}S^{-1}$, which is significantly faster than *tert*-butyl trifluoroborate (Kq = $7.6*10^5$ $M^{-1}S^{-1}$). Further, cyclic

voltammogram (CV) analysis disclosed the redox potential of vinyl bromide ($E_{p/2}$ = -2.0 V vs Ag/AgCl) is much lower than photoexcited **PC-I** ($E_{p/2}$ = -1.05 V vs Ag/AgCl), suggesting that it's less likely to proceed via oxidative fluorescent quenching process. Therefore, it was surmised that an energy transfer event between photoexcited **PC** and vinyl bromide could be involved. Next, in the control reactions performed by the collaborator, both pure *trans*- or *cis*-vinyl bromides were efficient coupling partners to react with vinyl phosphonate and alkyl trifluoroborate under standard conditions. These results further indicated that ground-state two-electron oxidative addition of vinyl bromide with nickel species is likely slower than photoexcited oxidative interaction. This hypothesis is further corroborated by my computations (*vide infra*) in which oxidative addition of excited spin state vinyl bromide is lower in energy (~10 kcal/mol) while ground state oxidative addition proceeds via a much higher barrier (~17-24 kcal/mol).

5.3.2 Computational results

Based on the prior computational and experimental results related to the dual nickel/photoredox-catalyzed three-component systems,[81, 118, 225, 297] I hypothesized that this transformation could proceed via the mechanism shown in **Figure 5.3**. First, alkyl radical **A**, generated from the single-electron oxidation of the corresponding alkyl trifluoroborate by excited photocatalyst $*Ir^{III}$, can undergo fast and *irreversible* Giese addition (barrier of 13.2 kcal/mol) to vinyl phosphonate to afford α-phosphonate alkyl radical **B** (exergonic by 4.7 kcal/mol; inset in **Figure 5.3**). In parallel, Ni(0) can engage with vinyl bromide **C** to undergo direct oxidative addition to generate singlet-spin, square planar Ni(II) **E** (blue pathway), which can then isomerize to the tetrahedral, triplet spin state Ni(II) before trapping Giese adduct **B** to form the key Ni(III) species **G.** Ni(III) species **G** is prone to undergo productive reductive elimination to give the

desired product **I** and bromo Ni(I) **H**. Alternatively, as shown by the Stern-Volmer quenching studies (*vide supra*), in addition to participating in single electron transfer events (SET), photocatalysts can also engage in energy transfer (EnT) events with in-cycle and off-cycle species (e.g., in this case alkene *E*/*Z* isomerization). Calculations show that photoexcited $^{*}Ir^{III}$ could, in principle, undergo energy transfer with vinyl bromide **C** to generate triplet excited state ^{3}**C** (triplet energy = 50.4 kcal/mol), which could then revert back to *E* or *Z* alkene (i.e., to promote substrate isomerization) or, alternatively, add to the Ni(0) catalytic species **D**. Specifically, prior (or in competition) to undergoing intersystem crossing to singlet spin state, ^{3}**C** can complex to Ni(0) and then undergo facile oxidative addition to form the key triplet-spin, tetrahedral Ni(II) ^{3}**F** (black pathway; *vide infra*).

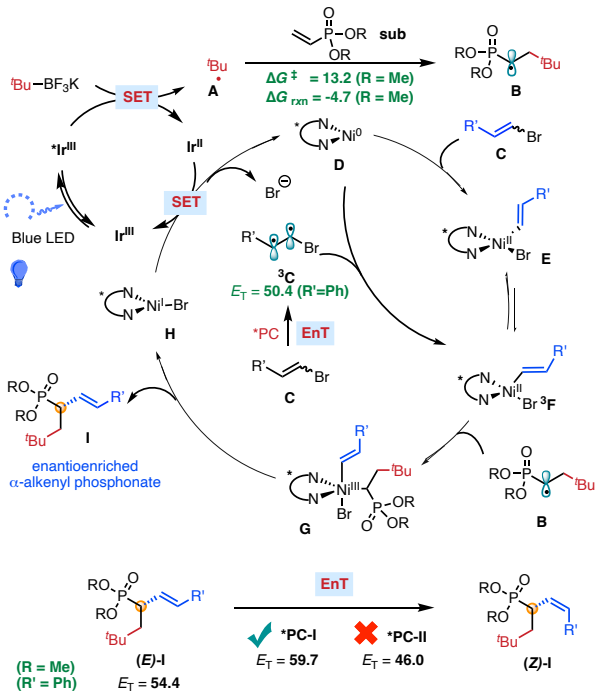


Figure 5.3 Proposed catalytic cycle of enantioselective three-component carbo-vinylation of vinylphosphonates based on computational studies. All free energies (kcal/mol; 298K) are computed at the (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP level of theory.

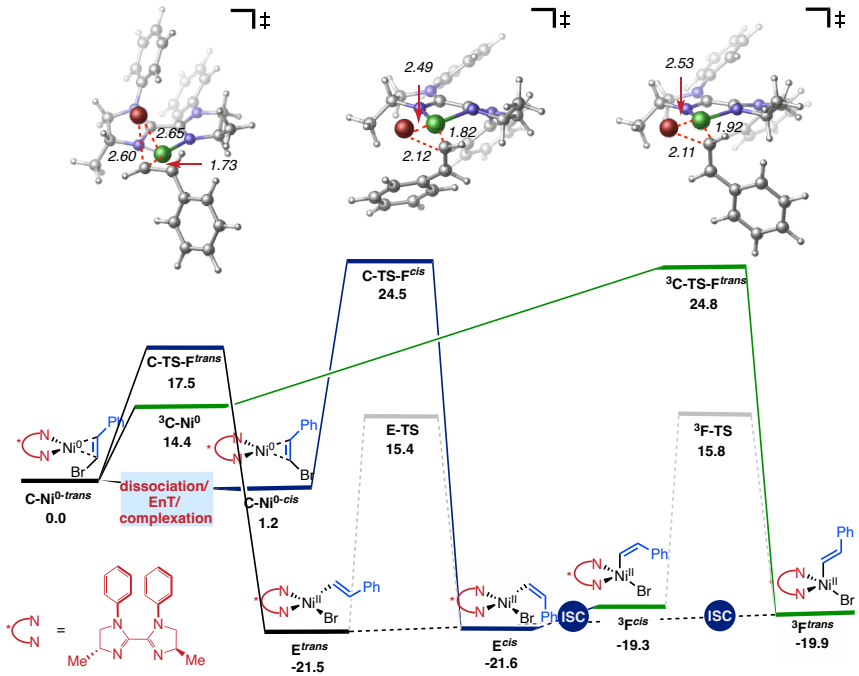


Figure 5.4 Mechanism of quenching of photocatalysts by vinyl bromide and the generation of Ni(II) species. All free energies (kcal/mol; 298K) are computed at the (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP level of theory.

To probe the feasibility of this catalytic cycle, the nature of quenching of vinyl bromide with photocatalysts, and the origin of regio-, stereo-, and enantio-selectivity of this transformation, I turned to dispersion-corrected DFT calculations. All optimizations were performed with open-shell, dispersion-corrected DFT (with Becke-Johnson damping) [noted as (U)B3LYP-D3(BJ)/def2-SVP].[97, 100, 340-343] To account for solvation effects, single-point energy calculations were conducted in ethyl acetate/DMA solvent as employed in experiment using the SMD implicit solvation model (see **Figure A4.1**–**A4.2** in Appendix 4 for the comparison of computational results to experimental values of redox potentials and triplet state energies). To reduce the computational cost, I initially used a truncated chiral BiIm ligand (see **Figure A4.3** in Appendix 4 for further computational details). As shown in **Figure 5.4**, I first focus on the putative oxidative addition steps via singlet and triplet spin states. Starting from complex **C-Ni$^{0\text{-}trans}$**, direct ground-state oxidative addition via **C-TS-F^{trans}** proceeds with a barrier of 17.5 kcal/mol to generate singlet-spin,

square planar *trans*-vinyl bromo Ni(II) **E**^{trans} (downhill by 21.5 kcal/mol) while oxidative addition of the *cis*-isomer complex (also present in the reaction and/or from photocatalyzed *E*/*Z* isomerization of **C**)[344-345] is higher in barrier (via **C-TS-F**^{cis}, barrier of 24.5 kcal/mol). Alternatively, under photoexcitation, triplet state ^{3}**C** can form, complex to Ni(0), and undergo facile oxidative addition (via ^{3}**C-TS-F**^{trans}, barrier is only 10.4 kcal/mol from ^{3}**C-Ni**^{0}) to afford triplet-spin, tetrahedral *trans*-vinyl bromo Ni(II) ^{3}**F**^{trans} directly (**Figure 5.4**; green pathway). I note that while *both ground-state and excited state oxidative addition pathways are feasible* (black and green pathways, via **C-TS-F**^{trans} and ^{3}**C-TS-F**^{trans}, respectively) and provide a direct route to the formation of isomeric Ni(II) species, the *trans-cis* isomerization of the singlet and triplet vinyl Ni(II) species is energetically unfeasible (barriers ~35 kcal/mol via **E-TS** and ^{3}**F-TS**). However, due to the close energetics of singlet and triplet vinyl Ni(II) species, these isomeric Ni(II) species could, in principle, rapidly interconvert via intersystem crossing (ISC).[29, 38, 225, 297] If so, the overall product selectivity will be ultimately determined by the subsequent radical addition/reductive elimination steps between the alkyl radical **B** and isomeric Ni(II) species.

Exhaustive DFT calculations on competing pathways (as shown in **Figure A4.4** in Appendix 4) demonstrate that the most energetically favorable pathway is alkyl radical **B** engaging with *trans*-vinyl triplet Ni(II) ^{3}**F**^{trans} species to form *trans*-vinyl α-phosphonate Ni(III) **G** which can then undergo facile reductive elimination to form the desired product and Ni(I) **H**. Finally, consistent with the previous mechanistic proposal,[118, 225, 297, 346] radical addition to triplet, tetrahedral Ni(II) species is found as the enantiodetermining step (see **Figure A4.4**).

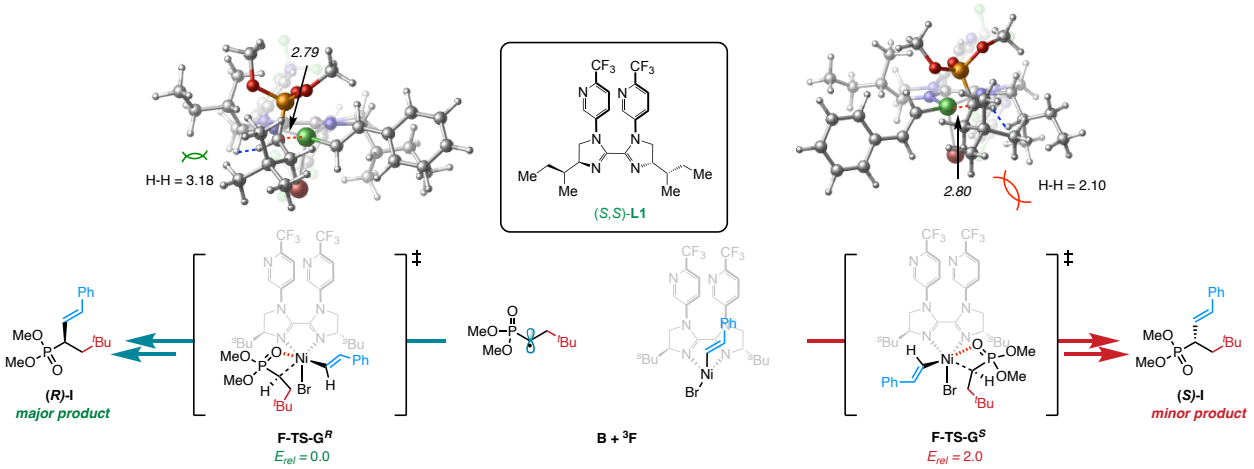


Figure 5.5 Models for the divergent enantioselectivity of different catalytic systems. Relative electronic energies (kcal/mol; 298K) are computed at the (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP level of theory.

To gain insights into the origin of enantioselectivity, we next model the enantiodetermining radical addition transition using the full chiral BiIm ligands (*S*,*S*)-**L1** and (*R*,*R*)-**L2**. For simplicity, only the lowest energy diastereomeric transition states for (*S*,*S*)-**L1** system are shown [see **Figure A4.5** in Appendix 4 for the corresponding diastereomeric transitions states for the (*R*,*R*)-**L2** system]. Overall, the computational results are in excellent agreement with experiments leading to *trans* **(*R*)-I** as the major product (93% exp. vs. 93% ee calc.) Moreover, a closer look at the lowest energy diastereomeric transition states (**F-TS-G^R** and **F-TS-G^S**) reveals that the steric hindrance between the ^{t}Bu group and the alkyl chain on the ligand as the major factor in controlling the enantioselectivity. Notably, computations show that the coordinating ability of the P=O moiety with nickel center controls the *trajectory of radical addition* to the Ni center leading to exclusive addition. Specifically, unlike previous study on the asymmetric three-component carboarylation,[297] the directing group P=O occupies the axial position of Ni center (**Figure 5.5**) and, as a consequence, directs the trajectory of radical addition exclusively to the *equatorial position*. I anticipate that this unappreciated role of directing group to guide trajectory of radical

addition additions will open new opportunities towards design and control of asymmetric radical cascades/cross-couplings. Finally, in agreement with experiments, calculations also show that the *E*/*Z* stereoselectivity of *trans*- versus *cis*- products is controlled by the feasibility of the *trans* product to undergo *trans-cis* alkene isomerization via energy transfer with the photocatalysts (as determined by their triplet state energy)[344, 347] *without racemization on the chiral center* (**Figure 5.3**).

5.4 Conclusion

In conclusion, a dual photoredox and nickel catalyzed asymmetric three-component coupling method have been developed for the straightforward construction of enantioenriched α-alkenyl phosphonates from simple vinyl phosphonates, alkenyl halides, and alkyl trifluoroborates. By taking advantage of photoinduced energy transfer process can further enable stereodivergent access to both *cis*- and *trans*-α-alkenyl phosphonates. The operationally simple and mild, redox-neutral protocol shows a broad substrate scope with good compatibility of diverse functional groups. Based on computational mechanistic studies, this transformation is likely to operate via a radical cascade sequence, where directing group shows an influence in guiding the trajectory of radical metalation in the enantioselectivity-determining step.

Chapter 6: Conclusion and Future Directions

The merging of photoredox and Ni catalysis has greatly expanded the chemical space of C–C cross-coupling reactions compared to traditional transition-metal-catalyzed cross-couplings. Specifically, it allows for the incorporation of C(sp^3) centers that are previously inaccessible due to the unwanted side reaction pathways. Since light is used as energy input, dual photoredox/Ni catalysis has enabled mild reaction conditions and shows great tolerance of functional groups in the system. However, in comparison to the rapid advancements of synthetic methodologies, the in-depth mechanistic investigation is lagging and limits the wider application and discovery of novel catalytic systems. In this vein, computational tools can be utilized to elucidate the mechanistic pictures, allowing for the rational design of new catalysts and the development of novel reactivity.

According to my mechanistic studies of photoredox/Ni dual-catalyzed C(sp^2)–C(sp^3) cross-coupling reactions (**Chapter 2–5**), the mechanistic picture is not generally applicable, but rather depends on the specific choice of substrate, ligands, photocatalysts, etc. Therefore, overgeneralization of mechanism should be avoided, and the analysis of selectivity of reaction needs to be performed based on the specific systems (i.e., multicomponent cross-coupling systems).

To improve the understanding of the complicated mechanistic pictures of targeted systems, the use of computational methodologies is of great significance. In particular, the high-energy, short-lived intermediates can be learned in detail with computational approaches on their properties and molecular-level interactions. Moreover, enhancements are needed to increase the application of computational investigation as well as to help the experimental chemists to interpret and utilize the computational results.

Regarding this issue, the accuracy and reliability of computational methods can be developed to strengthen the study of varied properties and dynamical behavior of the key species. On the other hand, wider collaboration among computational, experimental, and spectroscopic groups is expected to accelerate reaction discovery, especially for (multicomponent) asymmetric transformations. I expect that with the rapid development of currently emerging computational tools and data-driven approaches, the mechanistic exploration of photoredox/Ni dual catalytic systems can facilitate the design of novel reagents and catalytic systems.

Appendix 1: Computational Methods, Results, Coordinates and Energies from Chapter 2 (Mechanistic Study of the Nature of C(sp^3)–C(sp^2) Bond Formation in Nickel/Photoredox Dual-Catalyzed Tertiary Radical Cross-Couplings)

A1.1 Methods

Details of computational methods and quasi-classical direct-dynamics simulations

All geometry optimizations of intermediates and transition states were achieved using spin-unrestricted UB3LYP[340-341]-D3[100]/def2-SVP[342-343] method, in THF solvent using the CPCM solvent model[348] with "opt=noeigen" and "guess=mix" keywords as implemented in Gaussian09[5]. Frequency calculations were also conducted at the same level of theory to obtain vibrational frequencies to determine the identity of stationary points as intermediates (no imaginary frequencies) or transition states (only one imaginary frequency), as well as obtaining the thermal corrections to enthalpy ($H_{correction}$) and free energy ($G_{correction}$) at the temperature of 298 K. Energies were refined by computing single point energies in implicit solvent with UB3LYP-D3/def2-TZVPP[342-343] method using larger basis set compared to optimization method. To explore the effect of DMA solvent in Ni-TMHD catalytic system, single point energy was also calculated in implicit DMA solvent as labeled as UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF). For comparison, single point energies were also computed using UM06[349]/def2-TZVPP method using Gaussian 09. Moreover, domain-based local pair-natural orbital coupled-cluster calculations using single and double excitations with perturbative triple excitations (DLPNO-CCSD(T))[111, 116] were performed with def2-TZVPP as basis set and def2-TZVPP/C as auxiliary basis set using ORCA software.[350] This method was used to obtain energy with high accuracy at affordable computational cost compared to DFT calculations. Free energies obtained with each method was calculated generally as $G^{method\text{-}solvent} = E^{method\text{-}solvent} + G_{correction}$. In part **E**,

single point energies obtained directly with each method ($E^{method\text{-}solvent}$ computed with UB3LYP-D3 and UM06 methods, and $E^{DLPNO\text{-}CCSD(T)\text{-}gas}$ computed with DLPNO-CCSD(T) method) would be shown. All structural figures were generated with CYLview.[351] Distances in structural figures are shown in Å and energies are in kcal/mol.

Molecular dynamics (MD) simulations were performed in the gas phase on the truncated doublet transition states **^{2}I'-TS** (shown in Figure S7) and **^{2}K-TS** (shown in Figure S20). The truncated **^{2}I'-TS** and **^{2}K-TS** were located at the UB3LYP-D3/def2-SVP 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 **^{2}I'-TS** and **^{2}K-TS**, adding zero-point energy for each real normal mode in corresponding transition states, plus a Boltzmann sampling of thermal energy available at 298.15 K with a random phase. The trajectories were propagated backward on **^{2}I'-TS** and forward on **^{2}K-TS** (settings are made on "searchdir" keyword line as shown in Section B), with focus on observing possible radical dissociation or C(sp^2)–C(sp^3) bond formation within the lifetime of Ni(III) intermediate. Parameters of radical dissociation concomitant with generation of Ni(II) intermediate were set as **^{1}G/^{1}G'** (C_{Ph}−C_{tBu} > 3.00 Å and Ni−C_{tBu} > 2.70 Å) for **^{2}K-TS** and **^{1}G/^{1}G'** (C_{Ph}−C_{tBu} > 3.00 Å and Ni−C_{tBu} > 3.50 Å) for **^{2}I'-TS** or product formation as **^{2}P$_B$ + *t*Bu-Ph** (C_{Ph}−C_{tBu} < 1.70 Å and Ni−C_{tBu} > 5.00 Å) based on corresponding distances at the transition states. The classical equations of motion were integrated with a velocity-Verlet algorithm using Singleton's program Progdyn, with the energies and derivatives computed using the UB3LYP-D3/def2-SVP method with Gaussian 09. The step length for integration was 1 fs.

Input parameters on Progdyn

The configuration file progdyn.conf for trajectory initialization for the doublet reduction elimination transition state **^{2}I'-TS** is given below as an example.

```
/#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/def2svp
#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 0
multiplicity 2
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 Ni-trun-TS-RE-r2-g
#*** 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
#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

A1.2 Supplementary Figures

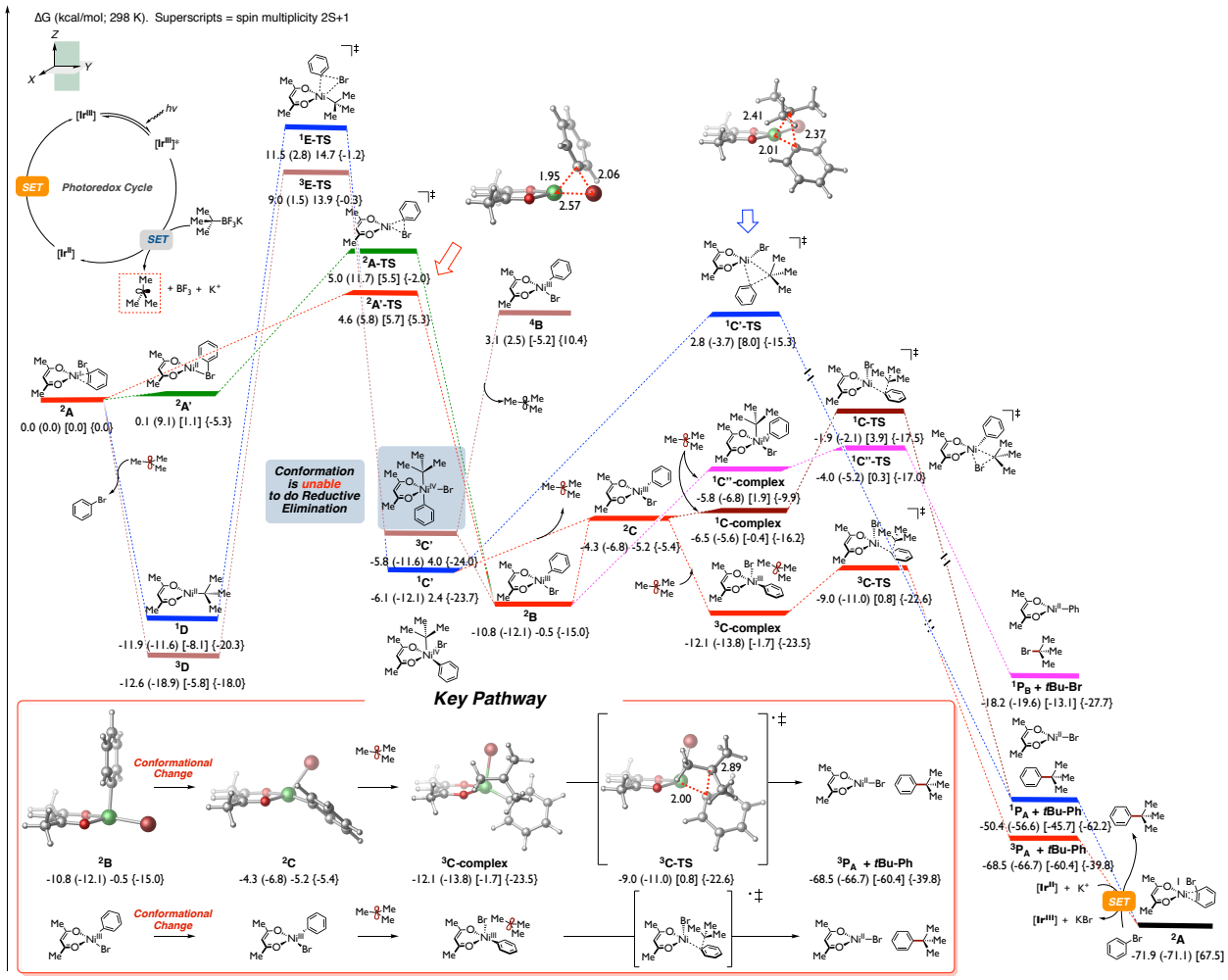


Figure A1.1 Calculated energetics of the Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide using anionic TMHD as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis), UM06/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket), and DLPNO-CCSD(T)/def2-TZVPP-gas//UB3LYP-D3/def2-SVP-CPCM(THF) (in brace) levels of theory. Energetics of the last SET step was calculated in UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis), UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory for better comparison with the Ni-bipyridine system.

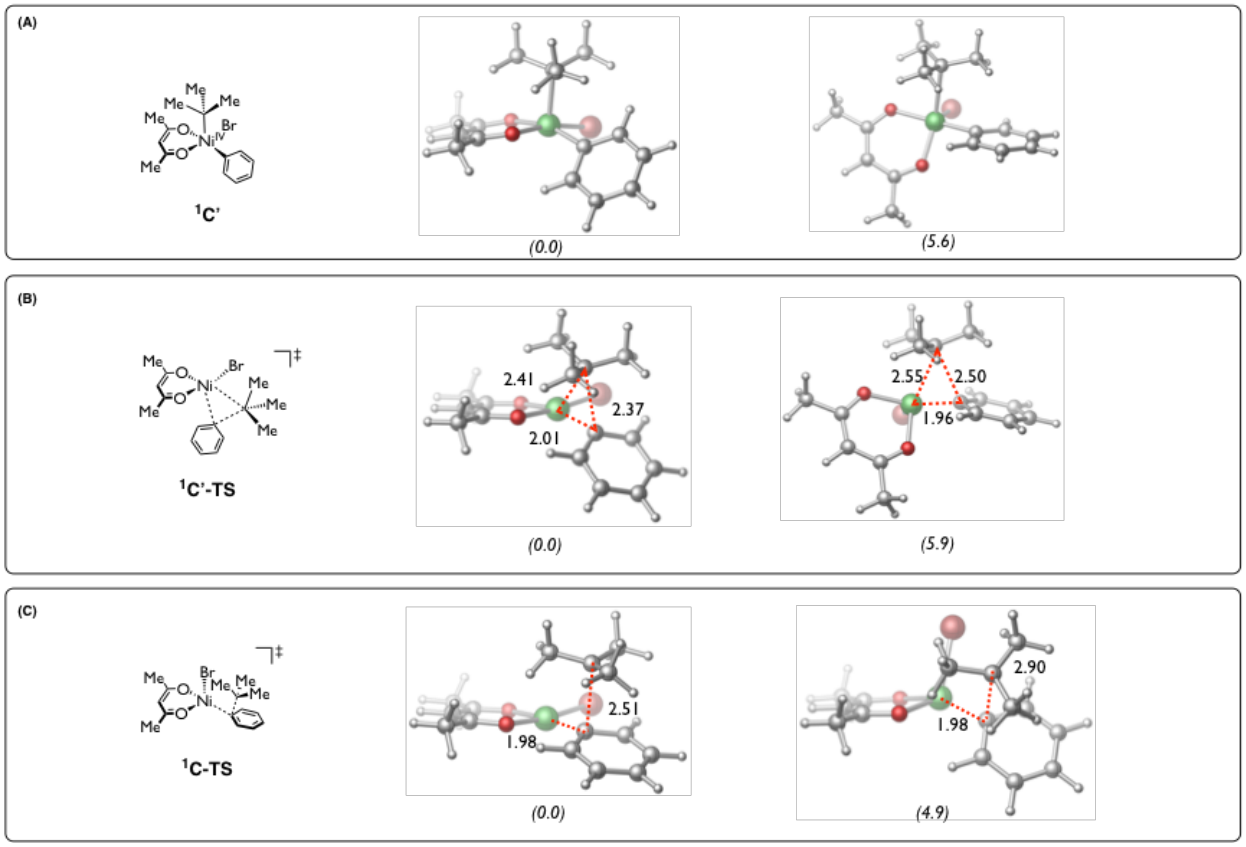


Figure A1.2 Conformational search of key intermediates and transition states of Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide using anionic TMHD as ligand. Relative free energies (kcal/mol) were calculated with respect to corresponding lowest-energy level structure at the UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) level of theory.

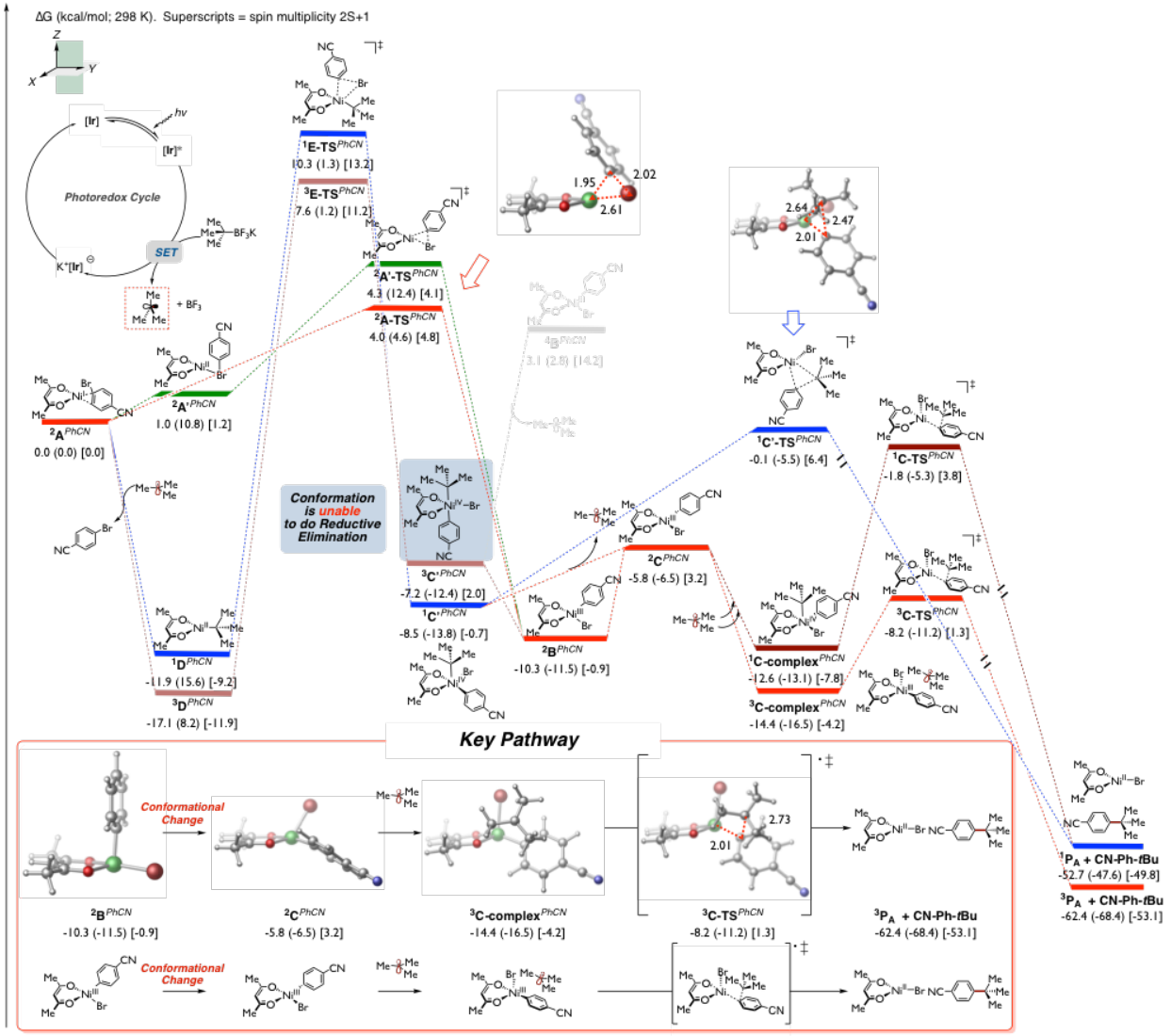


Figure A1.3 Calculated energetics of the Ni-catalyzed cross-coupling between *tert*-butyl radical and 4-bromobenzonitrile using anionic acac as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

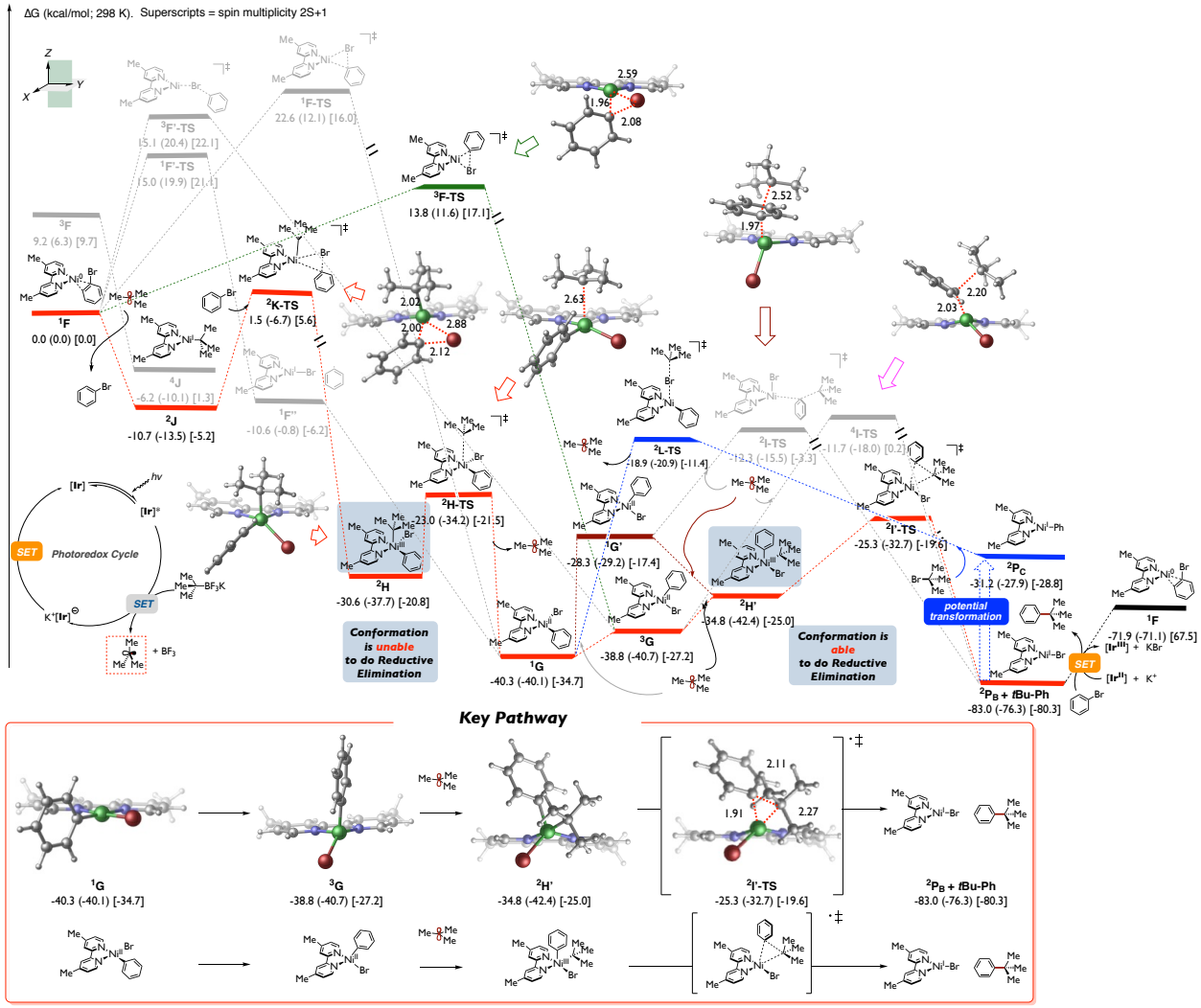


Figure A1.4 Calculated energetics of the Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide using neutral bipyridine as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis), and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

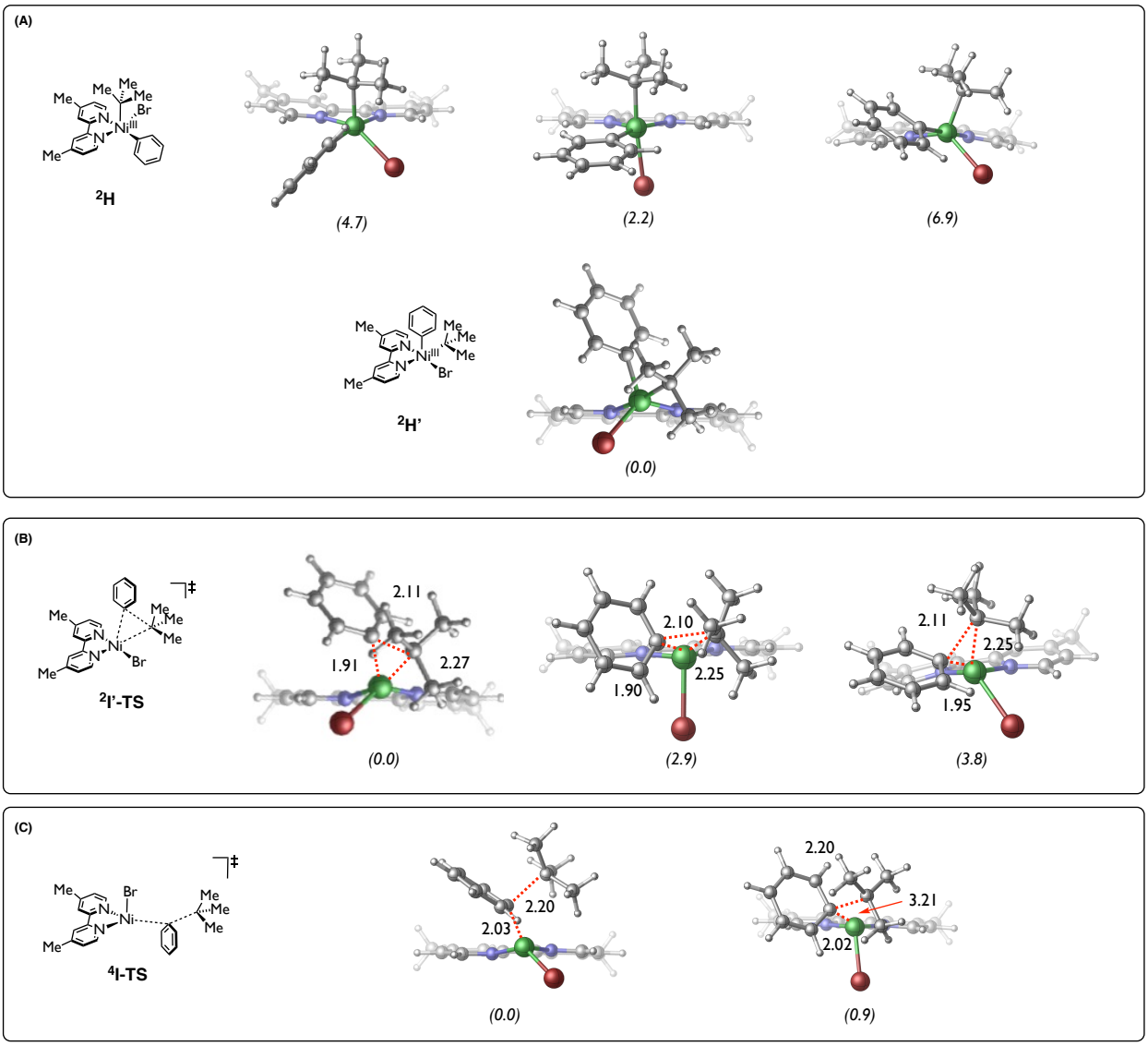


Figure A1.5 Conformational search of key intermediates and transition states of Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide using neutral bipyridine as ligand. Relative free energies (kcal/mol) were calculated with respect to corresponding lowest-energy level structure at the UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) level of theory.

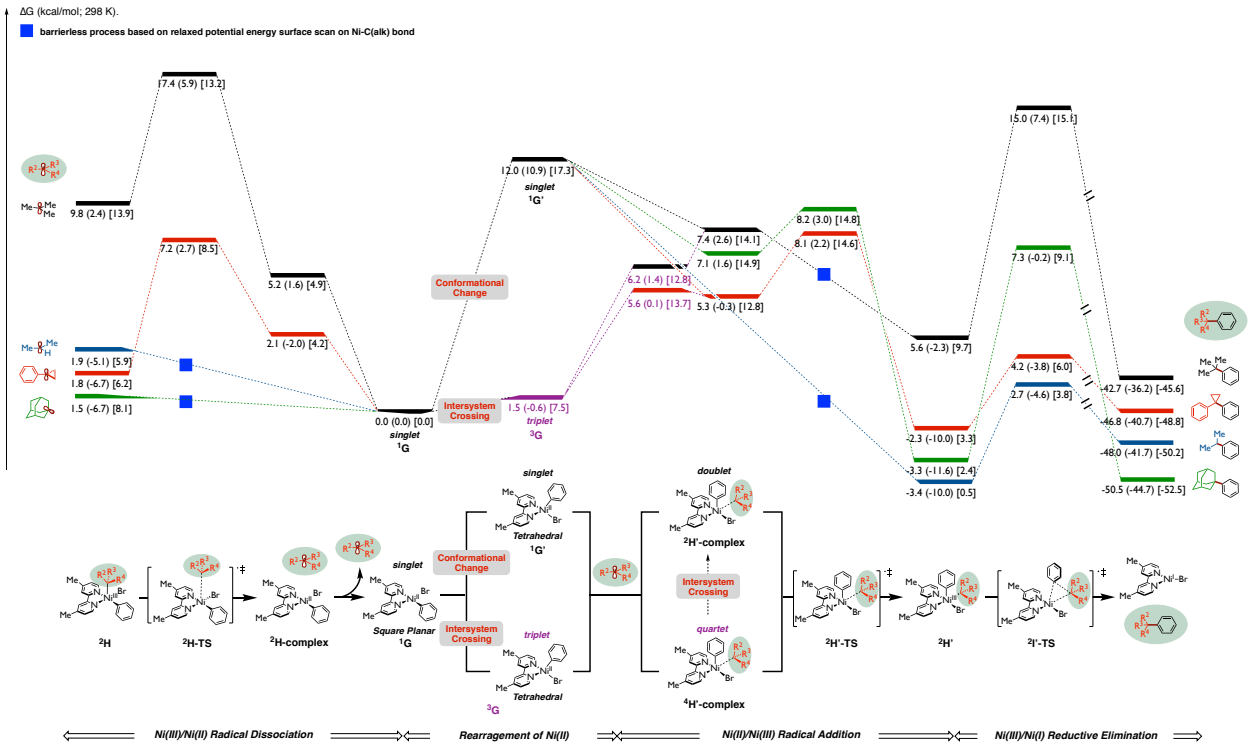


Figure A1.6 Calculated energetics of the key pathway using neutral bipyridine as ligand and *tert*-butyl radical (black), *iso*-propyl radical (blue), 1-phenylcyclopropyl radical (red) and adamantly radical (green) as radical substrates. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis), and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

Starting from *singlet spin square planar* Ni(II) species **^{1}G**, *tert*-butyl radical can undergo radical addition from axial position via **^{2}H-TS** to generate the endergonic Ni(III) intermediate **^{2}H**, which is a reversible process so *tert*-butyl radical is less favorable to be bound to Ni center. Alternatively, **^{1}G** could undergo conformational change or intersystem crossing to generate *singlet spin tetrahedral* Ni(II) species **^{1}G'** and *triplet spin tetrahedral* **^{3}G**, respectively. Upon interaction with *tert*-butyl radical, Ni species can form doublet or quartet (purple energy values) complex, then after barrierless radical addition (blue squares, based on relaxed potential energy surface scan on Ni-C bond) Ni(III) species **^{2}H'** could be formed. More importantly, the barrier of reductive elimination step of *tert*-butyl radical (15.0 kcal/mol with respect to **^{1}G**) is much higher than those

with other alkyl radicals. This might explain the observed failure with *tert*-butyl radical substrate and the success of adamantly and 1-phenylcyclopropyl radicals in experiment.[177]

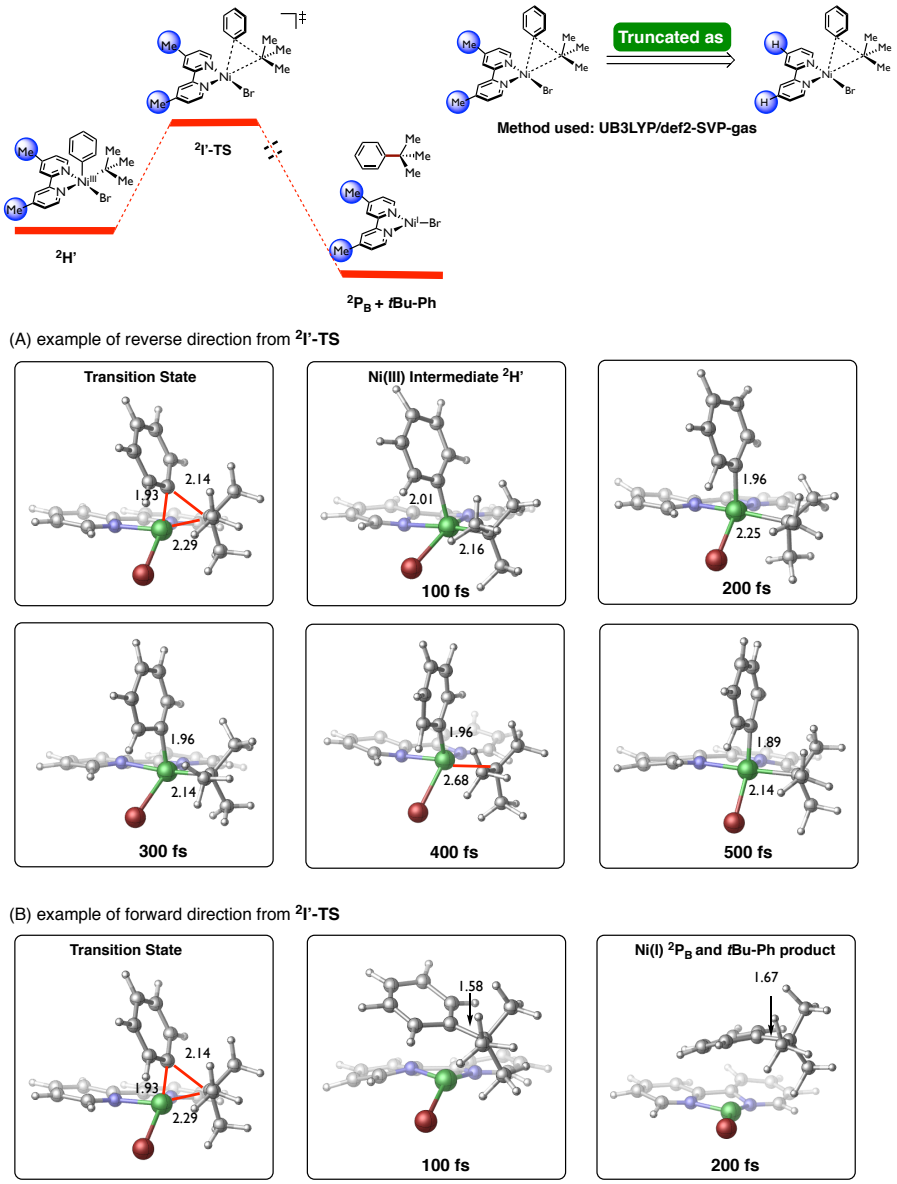


Figure A1.7 Snapshots of representative examples of quasi-classical dynamic calculation of truncated system from reductive elimination transition state **²I'-TS** in both forward and backward directions of Ni-catalyzed cross-coupling between *tert*-butyl radical and phenyl bromide in Ni-bipyridine system.

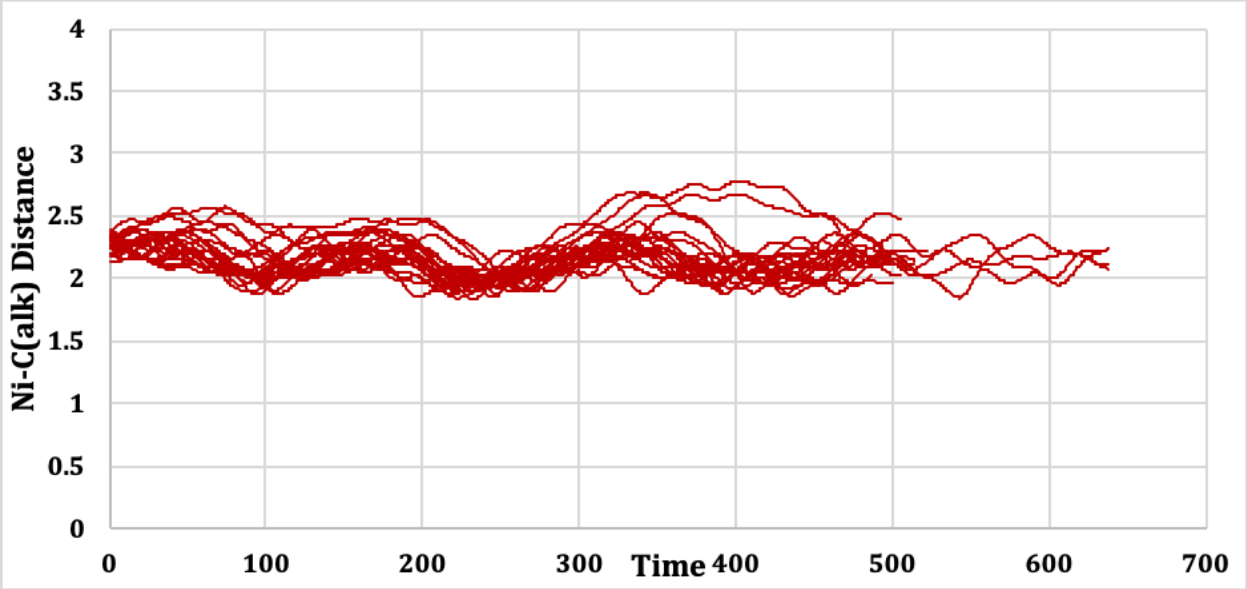


Figure A1.8 Time (fs) plot of trajectories versus Ni-C(alkyl radical) bond length (Å) of truncated system initiated at the reductive elimination transition state **^{2}I'-TS** in the reverse direction.

The red lines represent the results of more than 20 trajectories (ran for 500 to 700 fs) obtained, all of which show that the Ni-C(alk) bond length lies in the range of 1.8 to 2.8 Å. These results suggest that after initiated in the reverse direction at **^{2}I'-TS**, Ni(III) intermediate **^{2}H'** was formed and maintained until the end of trajectory, without the observation of *tert*-butyl radical dissociating from Ni center and generating corresponding Ni(II) intermediate (as shown in **Figure A1.7**). Overall, the results of quasi-classical dynamic calculation is consistent with the proposed pathway that the dissociation of *tert*-butyl radical from Ni(III) intermediate **^{2}H'** is uphill in energy. Also, the radical addition process of *tert*-butyl radical to Ni center occurs on *singlet spin tetrahedral* Ni species **^{1}G'** or *triplet spin tetrahedral* Ni species **^{3}G** rather than *singlet spin square planar* Ni species **^{1}G**, because the former Ni(II) species is either higher in energy level (**^{1}G'**) than Ni(III) intermediate **^{2}H'** while the latter Ni(II) is lower, and the dynamic simulations operate on single-spin state potential energy surface thus cannot reveal the performances of system when spin

state is changed. The exploration in which intermediate does the alkyl radical add to is ongoing in our group.

Table A1.1 Activation Strain-Distortion/Interaction analysis of C(sp^2)–C(sp^3) bond formation step. Relative electronic energy values were computed with respect to separate corresponding phenyl-bromo-Ni-ligand species and *tert*-butyl radical at the UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(THF), and UB3LYP-D3/def2-SVP//UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) levels of theory.

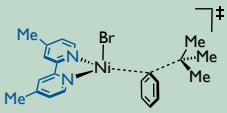
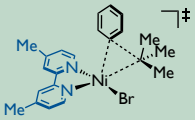
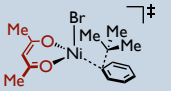
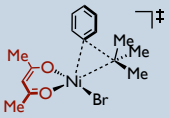
			$\Delta E_{activation}$ (kcal/mol)	$\Delta E_{distortion}$ (kcal/mol)	$\Delta E_{interaction}$ (kcal/mol)
Outer-Sphere		^{2}I-TS	19.1 (16.6)	28.6 (46.0)	-9.6 (-29.4)
		^{4}I-TS	12.2 (5.4)	17.1 (14.8)	-4.9 (-9.5)
Inner-Sphere		^{2}I'-TS	-3.9 (-11.7)	41.0 (39.6)	-44.9 (-51.2)
Outer-Sphere		^{1}C-TS	2.7 (-7.7)	16.0 (16.8)	-14.0 (-24.6)
		^{3}C-TS	-13.3 (-15.6)	18.4 (18.6)	-31.7 (-34.2)
Inner-Sphere		^{1}C'-TS	-13.2 (-18.7)	20.8 (22.0)	-34.0 (-40.6)

Table A1.2 Grey: calculated energetics on inner-sphere reductive elimination step with different alkyl radicals; Green: related analysis on bond dissociation energy of Ni(III) intermediate; Yellow: activation strain-distortion/interaction analysis on reductive elimination transition state (relative electronic energy values was calculated with respect to separate corresponding Ni(II) species and *tert*-butyl radical). All relative energy values were computed with respect to Ni(II) species at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory. BDEs and activation strain-distortion/interaction analysis were computed in the gas phase.

	ΔG (kcal/mol; 298K)			BDE of Ni-C(sp^3) (ΔH; kcal/mol)	$\Delta E_{activation}$ (kcal/mol)	$\Delta E_{distortion}$ (kcal/mol)	$\Delta E_{interaction}$ (kcal/mol)
	^{1}G	^{2}H'	^{2}I'-TS				
		5.6 (-2.3) [9.7]	15.0 (7.4) [15.1]	11.0 (18.8) [7.1]	-3.9 (-11.7) [-3.9]	41.0 (39.6) [44.1]	-44.9 (-51.2) [-48.0]
	0.0 (0.0) [0.0]	-2.3 (-10.0) [3.3]	4.2 (-3.8) [6.0]	18.3 (26.0) [13.2]	-13.9 (-21.9) [-12.2]	37.4 (36.3) [42.5]	-51.2 (-58.2) [-54.7]
		-3.4 (-10.0) [0.5]	2.7 (-4.6) [3.8]	17.9 (24.6) [14.5]	-14.2 (-21.7) [-13.2]	33.1 (31.4) [38.0]	-47.3 (-53.0) [-51.2]
		-3.3 (-11.6) [2.4]	7.3 (-0.2) [9.1]	18.3 (26.6) [12.7]	-8.0 (-15.8) [-6.3]	32.4 (31.4) [37.7]	-40.4 (-47.2) [-44.0]

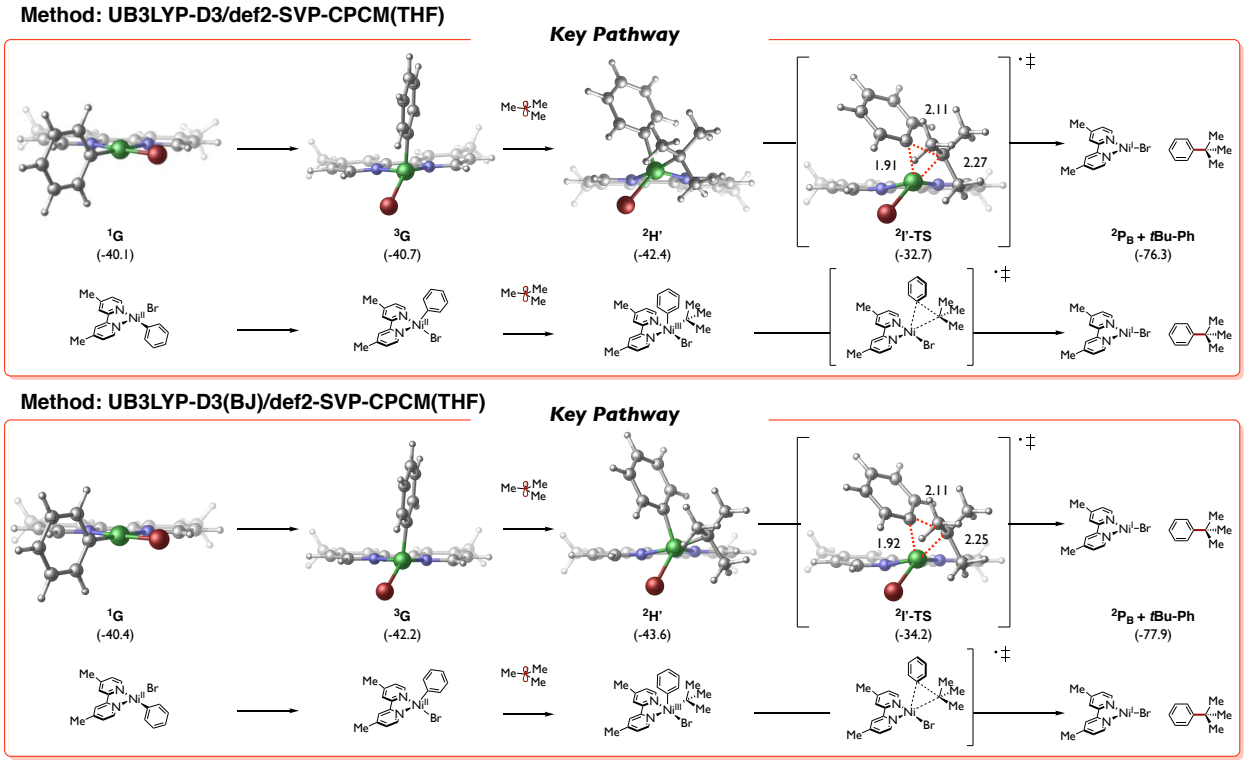


Figure A1.9 Comparison of key pathway in Ni-bipyridine system with original zero damping and Becke-Johnson damping of Grimme's dispersion correction. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) level of theory.

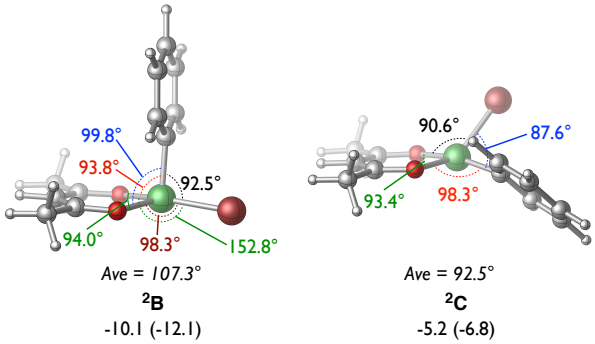


Figure A1.10 Structural parameters of **²B** and **²C**.

We have described "distorted tetrahedral" and "distorted square planar" as defined by the average angle deviations from a true tetrahedral geometry (109°) and square planar (90°). As shown above, the average angle of the "distorted tetrahedral" structure **²B** is 107.3° which is close to the angle of standard tetrahedral structure (109°). Also, the average angle of the "distorted square planar" structure **²C** is 92.5° which is close to the angle of standard square planar structure (90°).

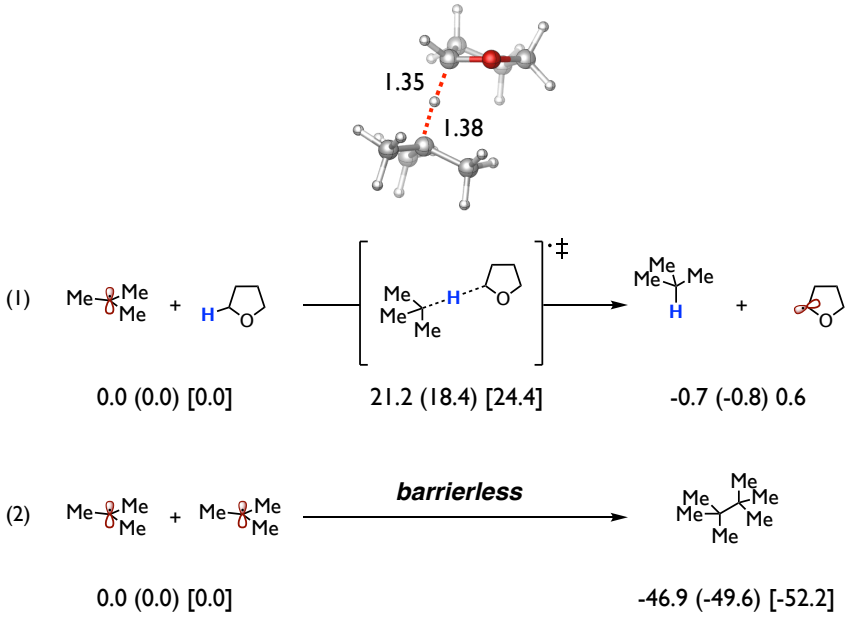


Figure A1.11 Calculated energetics of (1) HAT reaction between *tert*-butyl radical and THF, and (2) dimerization of two tert-butyl radicals. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

We computed the HAT pathways between the presumably formed *t*Bu radical and THF solvent (eq.1) and found that the HAT of *t*Bu• from THF is 0.7 kcal/mol downhill in energy with barrier of 21.1 kcal/mol. In comparison, the barrier of HAT of *t*Bu• from THF is only slightly higher than that of radical addition of *t*Bu• to Ni(II)(bpy) intermediate **^{1}G** (17.3 kcal/mol at **^{2}H-TS**), thus HAT pathway is feasible and stays competitive to the radical addition pathway. This could explain the observed experimental results[177] that both Ar-H (3-15% yield) and THF-Ar were observed in the stoichiometric studies using (bpy)Ni(Ar)(Br) complex and *t*Bu-BF_3K reagent. Moreover, we considered possible dimerization between two *tert*-butyl radicals (eq.2) and found that the dimerization process was barrierless based on relaxed potential energy surface scan on the newly formed C-C bond, resulting in the formation of 2,2-4,4-tetramethylbutane which is 46.9 kcal/mol downhill. This suggests that under higher concentration of *t*Bu radical, as expected, these radicals will likely lead to dimerization instead of undergoing radical addition to Ni(II) intermediate to generate Ni(III) intermediate, which is uphill in energy. Given the efficiency of the system, these calculations support low concentration of *t*Bu radical which lead to the desired cross-coupling product and only minor formation of side products such as HAT from solvent (due to higher barrier) or dimerization (due to low radical concentration).

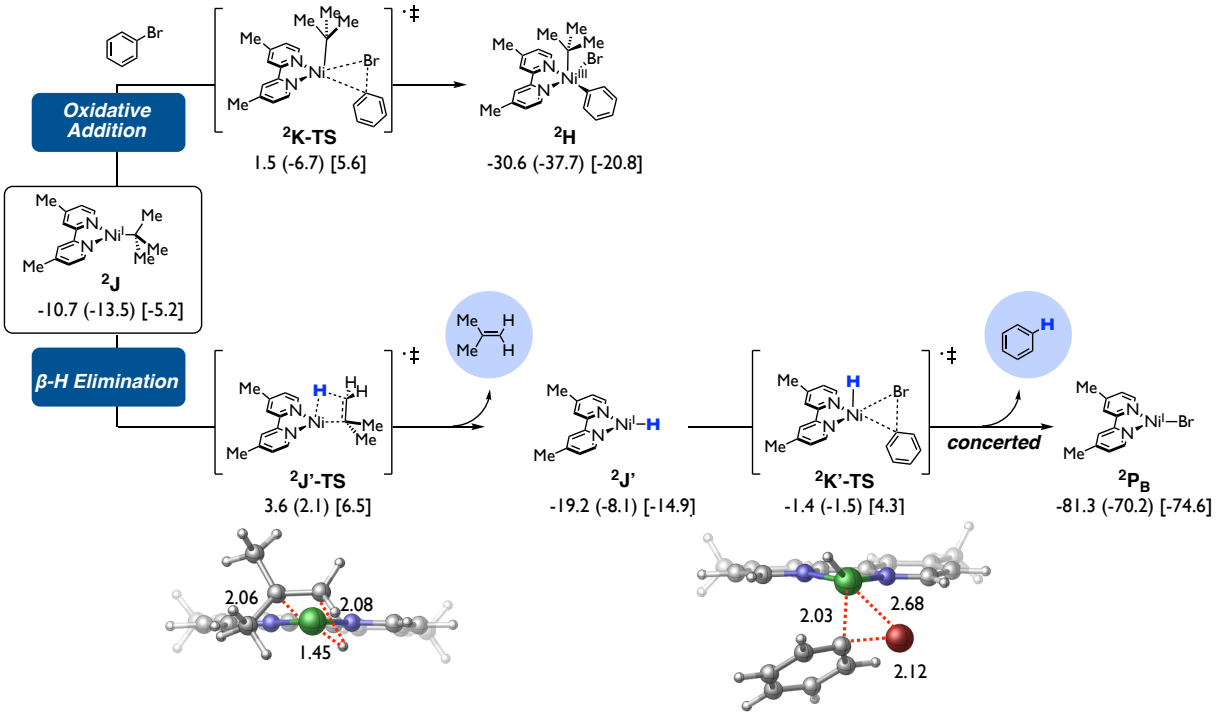


Figure A1.12 Calculated energetics of oxidative addition and β-H elimination pathways from Ni(I)-tBu intermediate **²J**. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

We also performed calculation on possible β-H elimination pathways (*vide infra*) from (bpy)Ni(*t*Bu) intermediate **²J**, and found that oxidative addition to PhBr (via **²K-TS**, with barrier of 12.2 kcal/mol with respect to **²J**) is comparable with the β-H elimination pathway (via **²J'-TS**, with barrier of 14.3 kcal/mol). Moreover, since the difference between barrier of oxidative addition pathway (12.2 kcal/mol) and that of β-H elimination pathway (14.3 kcal/mol) is only 2.1 kcal/mol, the β-H elimination pathway from (bpy)Ni(*t*Bu) intermediate **²J** is a possible side reaction pathway in this reaction system leading to the generation of metal hydride species (bpy)Ni(H) and isobutylene as side products. Unfortunately, isobutylene has a low boiling point (-7.9 ºC) and it is highly volatile thus challenging to assess experimentally. Nonetheless, the newly formed (bpy)Ni(H) species **²J'** can undergo oxidative addition with phenyl bromide (via **²K'-TS**),

followed by concerted Ph-H bond formation (observed via intrinsic reaction coordinate at **^{2}K'-TS**) to generate the experimentally observed side product *benzene* (Ph-H). Taken together, these computational and experimental results provide strong support for the formation of observed side products in experiment (i.e., THF-Ar adduct and Ar-H)[177] due to H atom transfer of *t*Bu radical from THF solvent followed by C-C bond formation and β-H elimination followed by Ar-H bond formation, respectively.

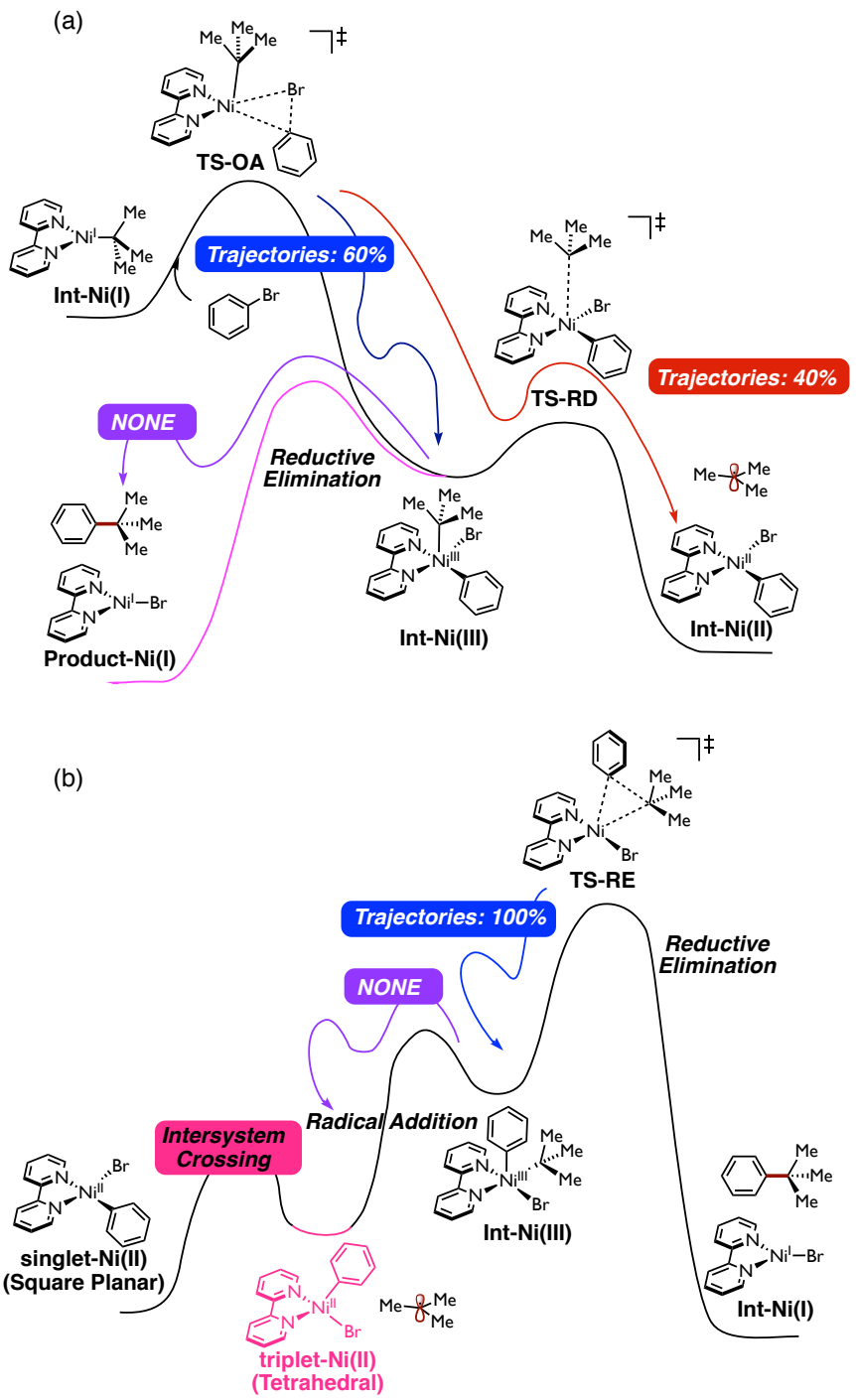


Figure A1.13 Preliminary results of quasi-classical dynamic simulations starting from (a) **^{2}K-TS** in forward direction and (b) **^{2}I'-TS** in reverse direction.

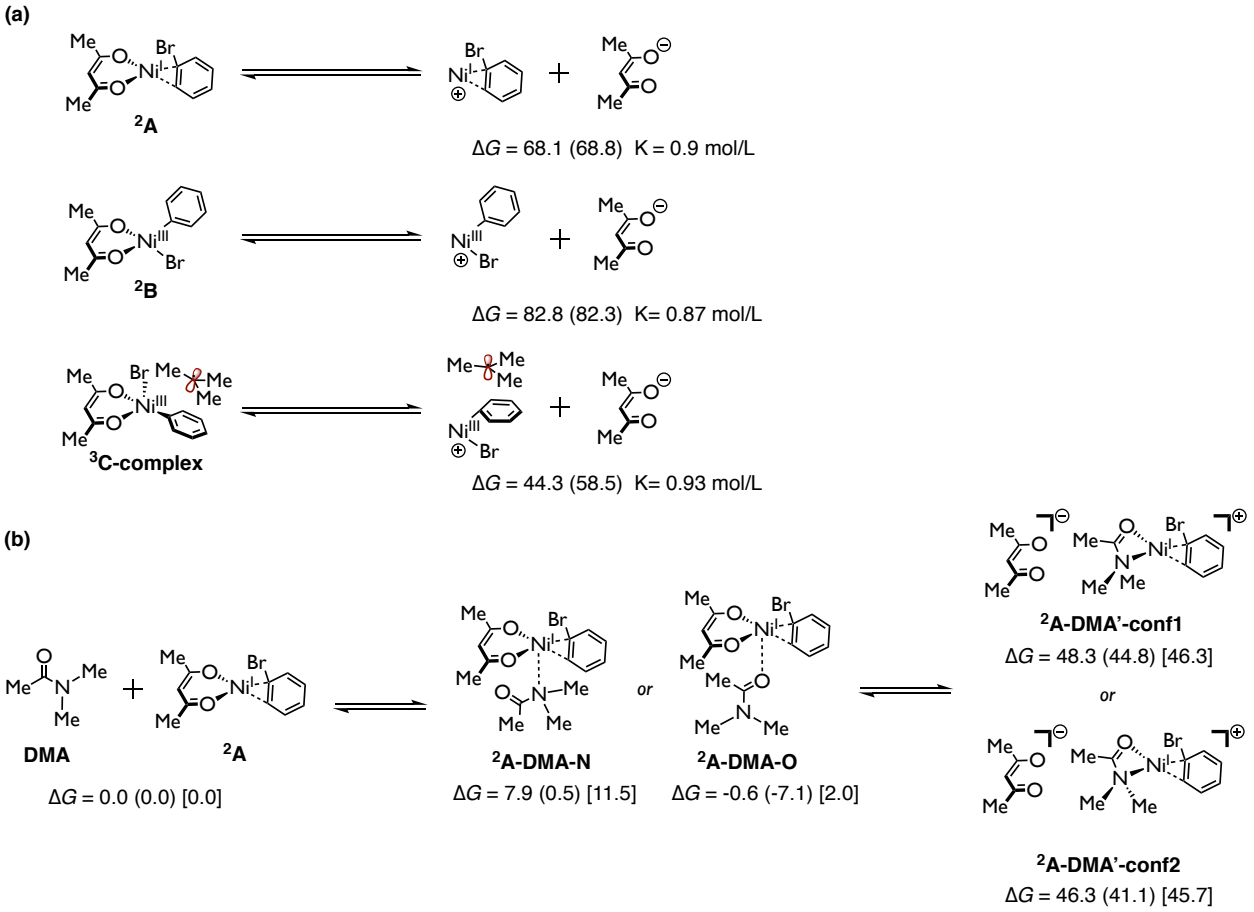


Figure A1.14 Calculated energetics of (a) ligand dissociation from key Ni(acac) species and (b) displacement and coordination of DMA solvent on key Ni(acac) species. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

To assess the likelihood of ligand dissociation, we have performed addition calculations to estimate the energy associated with ligand dissociation (shown above, **Figure A1.14a**), which showed there is an extremely energy uphill if the ligand dissociates from the Ni atom and the equilibrium constant for ligand dissociation is small. As a result, ligand dissociation pathways are unlikely. We also performed computations to gain insight at the propensity of DMA solvent to coordinate to the nickel active species and displace the acac (TMHD) ligand. As shown above (**Figure A1.14b**), the coordination of DMA to the nickel active species (prior to substrate

activation) is energetically disfavored via N-mode coordination, but only weakly (dependent on the method) favorable via O-mode coordination. However, displacement of THMD ligand (here modeled as acac) is found highly unfavorable (> 40 kcal/mol). Based on these results, TMHD ligand is likely to stay coordinated to the Ni center during the whole catalytic process, and the coordination of DMA solvent to Ni center is possible via O-mode but it could not displace TMHD ligand of key Ni catalytic species.

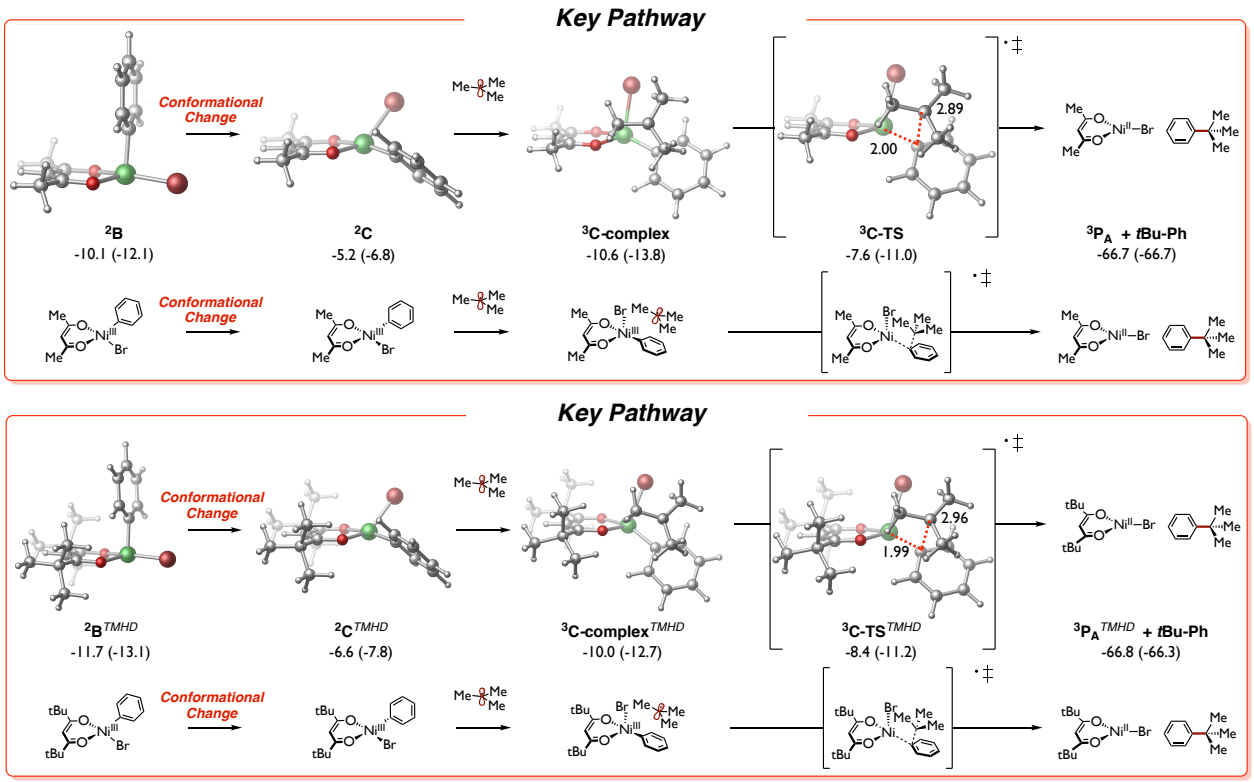


Figure A1.15 Comparison of energetics of the key pathways using truncated and full anionic TMHD as ligands. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) and UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) levels of theory.

We also computed the lowest energy pathway using the full TMHD ligand and found that the results of the full system are consistent with the pathway with truncated ligand (see below). Therefore, using acac ligand as computational model is a reasonable strategy.

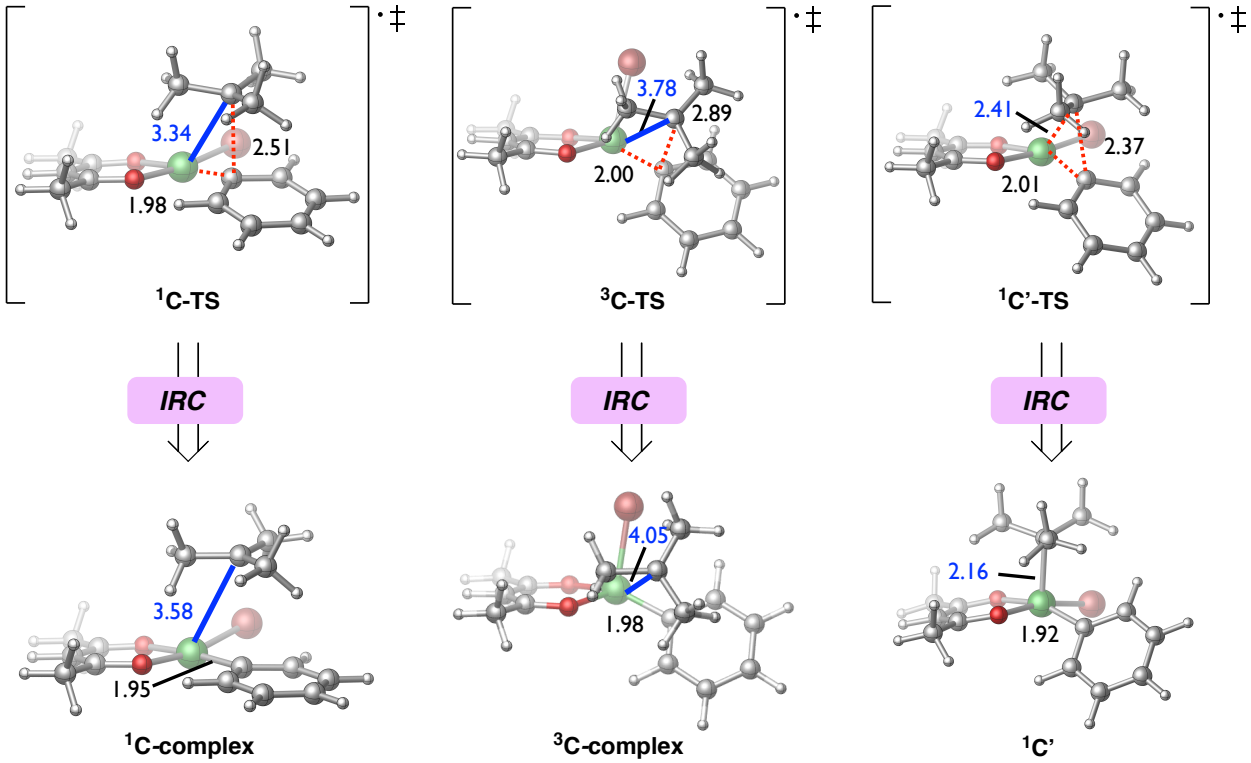


Figure A1.16 Comparison of three transition states of C-C formation in Ni(acac) system and their corresponding intermediates obtained from intrinsic reaction coordinate calculations (Unit: Å).

The distance between the *tert*-butyl and the Ni atom (in blue) in the *outer-sphere* transition states **^{1}C-TS** and **^{3}C-TS** are relative long (3.34 and 3.78 Å, respectively). Thus, based on these distances, there is no Ni-*tert*-butyl interaction in the *outer sphere* transition states. However, for the *inner-sphere* TS **^{1}C'-TS**, the Ni-*t*Bu distance is much shorter, 2.41 Å, than that in the outer-sphere transition states. Moreover, the intrinsic reaction coordinate calculations of **^{1}C-TS**, **^{3}C-TS** and **^{1}C'-TS** showed that the *outer-sphere* transition states **^{1}C-TS** and **^{3}C-TS** lead to Ni•••*t*Bu radical complexes (**^{1}C-complex** and **^{3}C-complex**) rather than Ni-alkyl intermediates (**^{1}C'**) as

determined by examining the corresponding distances between Ni-*t*Bu and the hybridization of the optimized intermediates (from the IRCs), respectively.

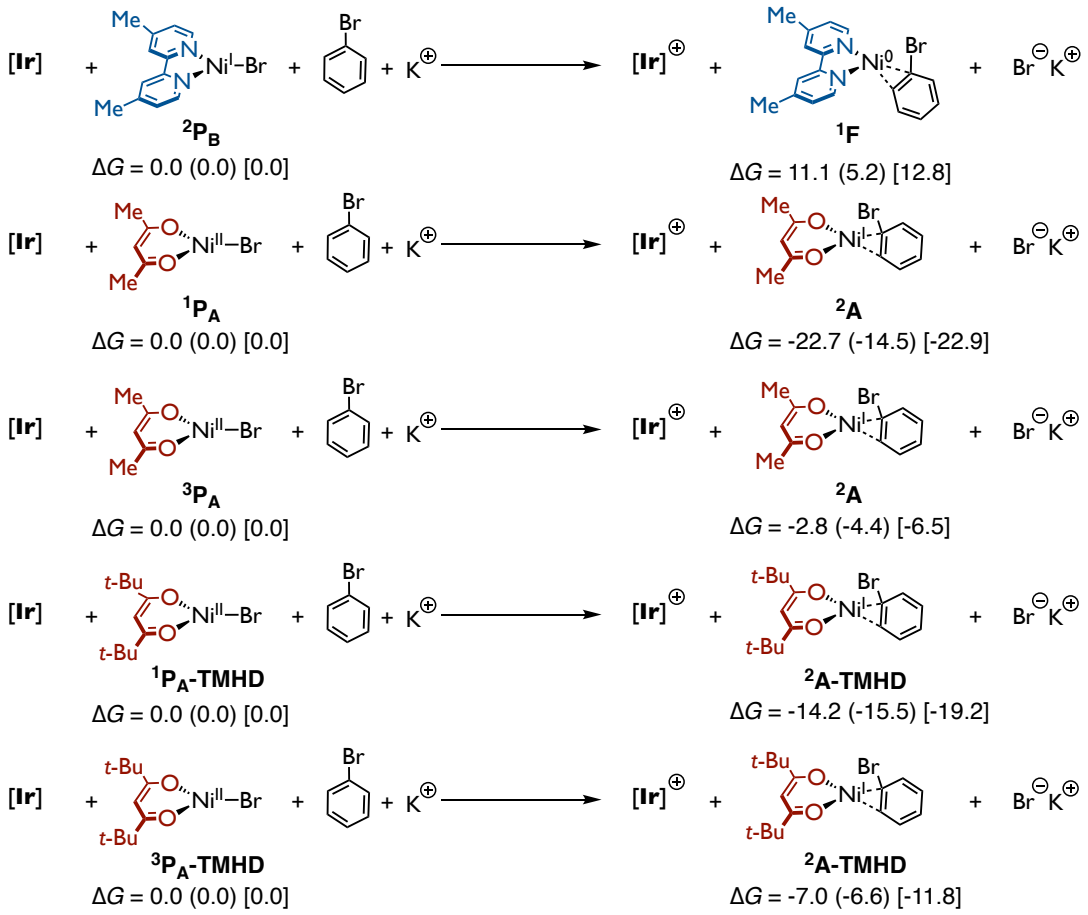


Figure A1.17 Calculation of single electron transfer steps between bromo Ni-ligand species and Ir photocatalyst to regenerate corresponding starting Ni species. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

Based on the calculated thermodynamic data of SET of bromo-Ni-ligand species with reduced Ir(II) photocatalyst , the single electron transfer steps should be not problematic. Specifically, for the Ni(bpy) system, while this process is slightly uphill in energy, based on free energy span model the reaction can still progress with turnover of catalytic cycle since the

following steps from Ni(0) ^{1}**F** have great thermodynamic drive with low barrier. As for Ni(acac) system, the SET steps between (acac)Ni-Br and photocatalyst are downhill in energy for both singlet and triplet spin states of (acac)Ni-Br, thus should be energetically feasible. Calculated results of full Ni-TMHD system are similar with those of the truncated Ni-acac system, both of which are downhill in energy. Therefore, in the absence of any direct experimental evidence (reduction potentials) for any of these mono-ligand bromo Ni species to the best of our knowledge, computations predict that this step should not be problematic for both (acac)Ni(II)-Br and (bpy)Ni(I)-Br to retrieve (acac)Ni(I) complex ^{2}**A** and (bpy)Ni(0) complex ^{1}**F**, respectively.

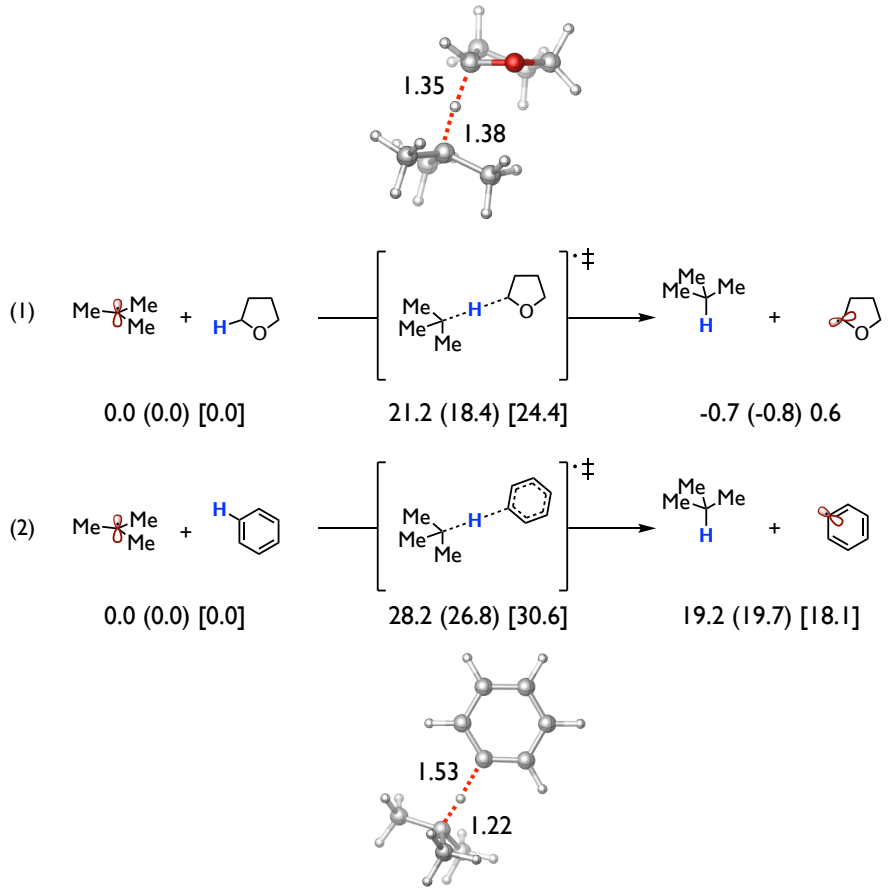


Figure A1.18 Calculated energetics of (1) HAT reaction between *tert*-butyl radical and THF, and (2) benzene. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in

parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

Calculations of HAT reactions between *tert*-butyl radical and different solvent molecules (i.e., THF and benzene) here were intended to show that the mechanism of this type of reaction might differ depending on the nature of solvent, electrophile, nucleophile even though the same *tert*-butyl radical was presumed to exist in the Ni-bipyridine system reported by Fu.

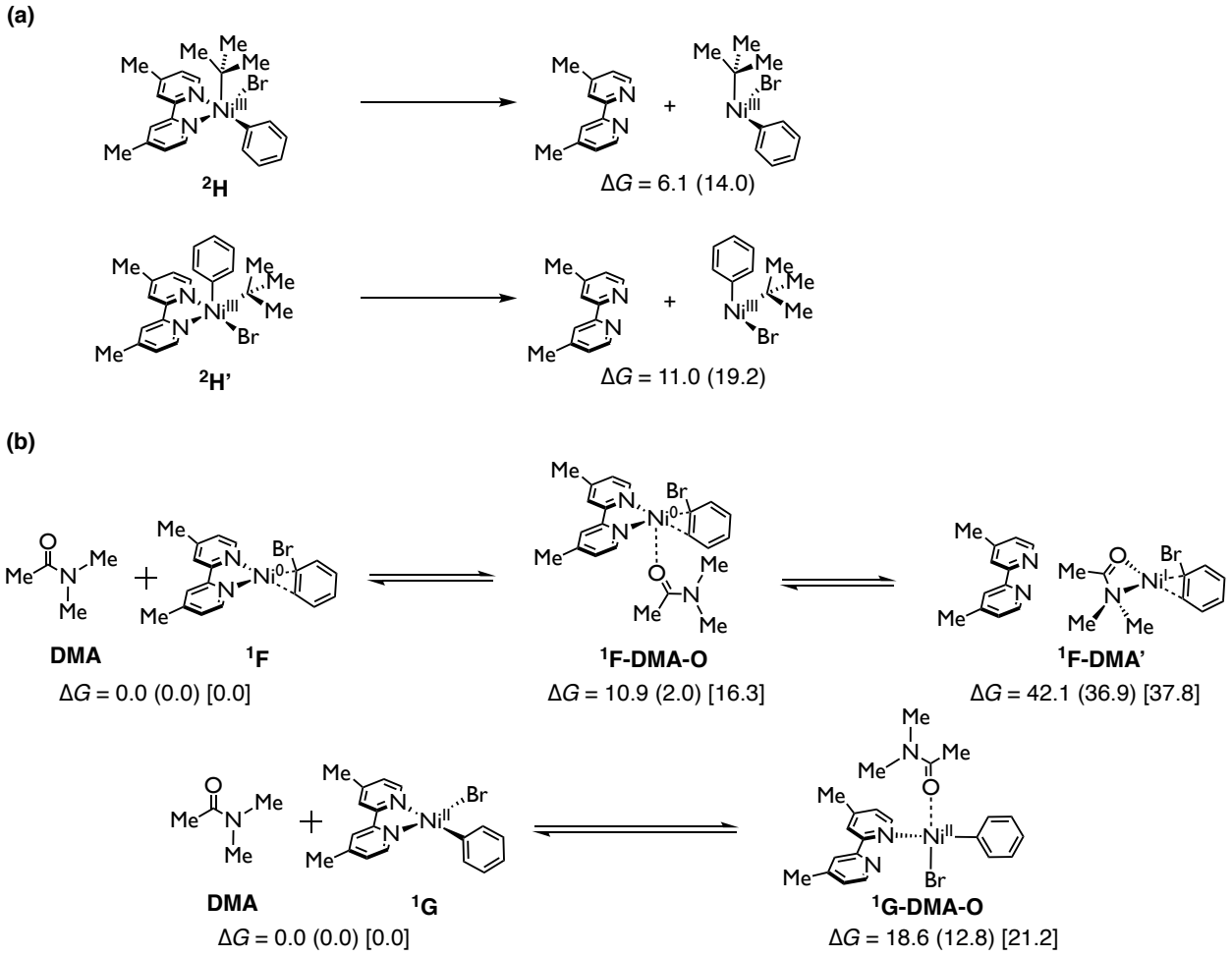


Figure A1.19 Energetics of (a) complete ligand dissociation from key Ni(III) intermediates **²H** and **²H'**, and (b) coordination and displacement with DMA solvent. Relative Gibbs free energy values were computed at the UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

These results show that complete ligand dissociation from Ni(III) intermediates is unlikely to occur since it's uphill in energy level from **[2]H** and **[2]H'** by 6.1 and 11.0 kcal/mol, respectively. Moreover, we explored the tendency of displacement or coordination with DMA solvent for the byp-nickel system, and found that DMA coordination to Ni(0) or Ni(II) is found energetically unfavorable (**[1]F-DMA-O** and **[1]G-DMA-O**) and, like the TMHD ligand, highly unfavorable to cause the dissociation of bipyridine ligand (**[1]F-DMA'**).

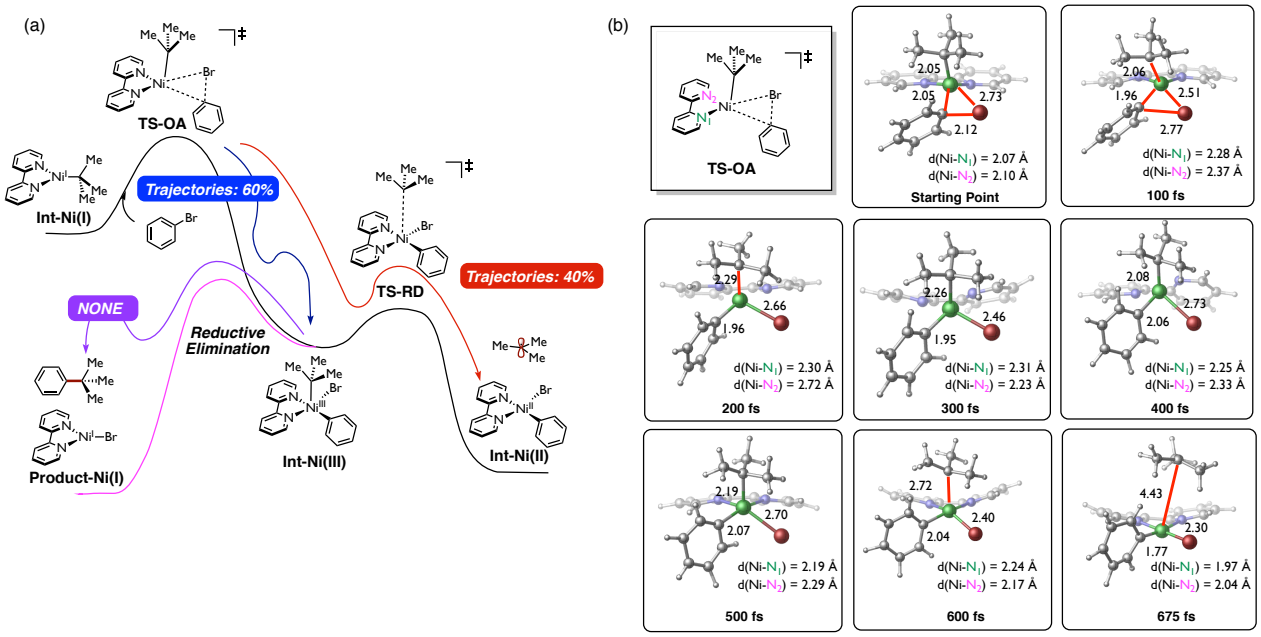


Figure A1.20 (a) Preliminary results of quasi-classical dynamic simulations starting from **[2]K-TS** in forward direction and (b) snapshots of one example trajectory undergoing radical dissociation.

To explore the likelihood of transient ligand dissociation during the reaction, we also performed quasi-classical dynamic calculations which allow us to "see" if ligand dissociation occurs, and if so, at what time step (**Figure A1.20**). Dynamic calculations starting from TS-Oxidative Addition from Ni(I) showed that complete ligand dissociation is unlikely to happen

within the lifetime of Ni(III) intermediate. In addition, although transient decoordination of one of the pyridine ligands was observed during some simulated trajectories (see **Figure A1.20b** for an example trajectory), *the Ni(III) intermediate doesn't undergo any structural rearrangement*. Rather, Ni(III) intermediate either stayed the same conformation until the end of simulation (60% of trajectories) or underwent radical dissociation of *t*Bu radical from axial position of Ni center (40% of trajectories).

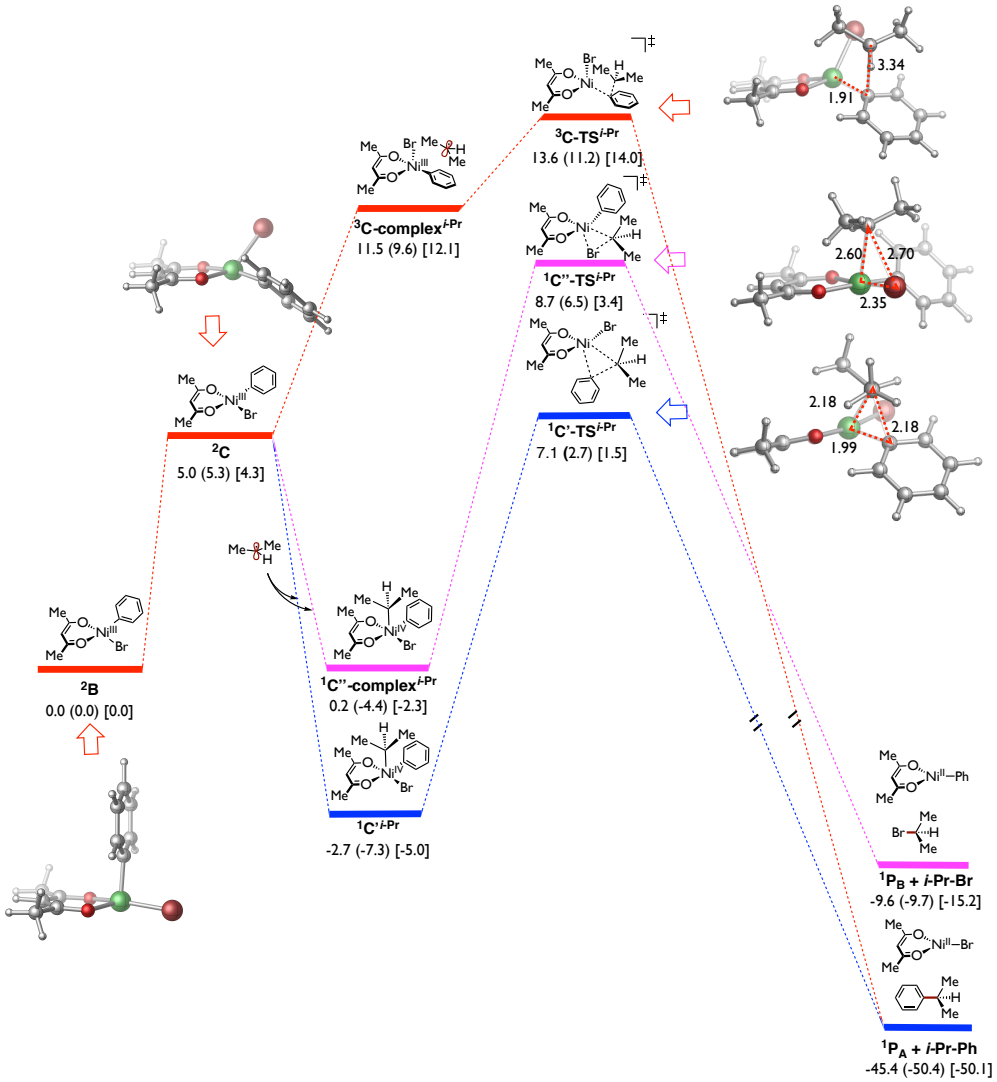


Figure A1.21 Calculated energetics of the Ni-catalyzed cross-coupling between *iso*-propyl radical and phenyl bromide using anionic acac as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-

D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

We performed computations to investigate the effect of secondary radical in the reaction pathway and found that the favored pathway is via inner-sphere C-C bond formation with overall barriers for C-C bond formation of ~9 kcal/mol. Thus, the cross-coupling of secondary alkyl radical is also applicable in Ni-TMHD system, which is shown in the experiment results done by collaborator. Presumably, the less sterically hindered secondary alkyl radical (in contrast to the tertiary alkyl radical) does not pay a penalty to form the LNi-alkyl-Ar-Br species and can quickly undergo inner sphere C-C bond formation. Thus, from these results, we hypothesize that for acac/TMHD-Ni systems, sterics more than electronics influence the nature of the C–C bond formation and whether inner- or outer-sphere $C(sp^2)$–$C(sp^3)$ is operative.

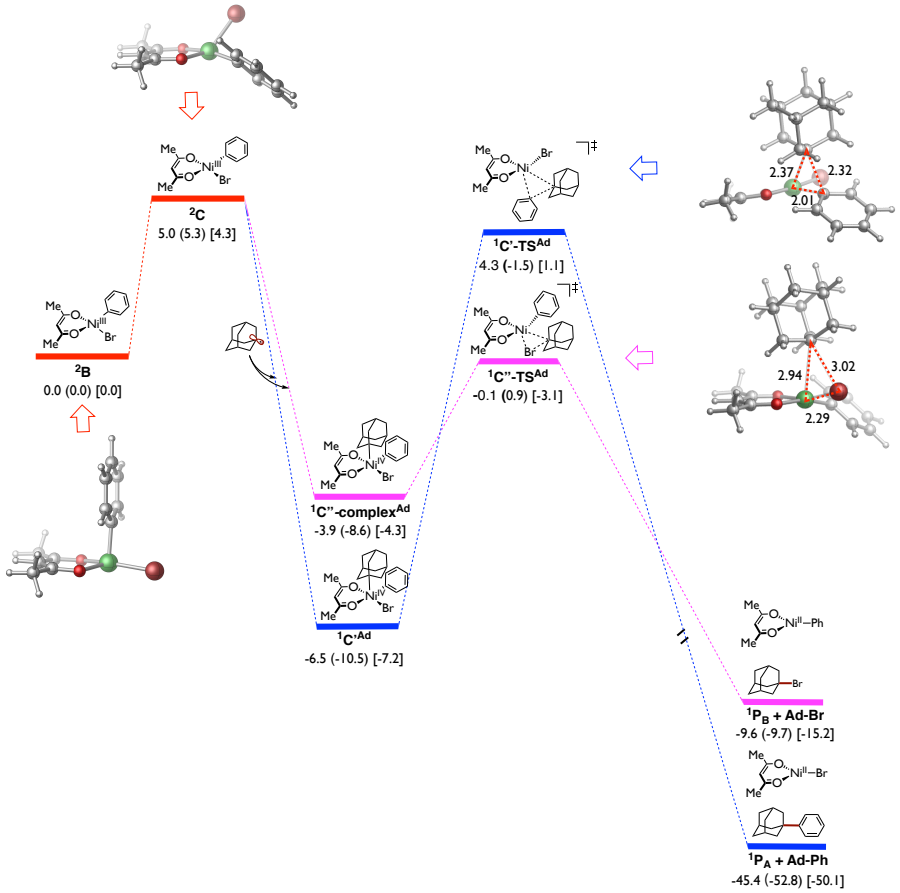


Figure A1.22 Calculated energetics of the Ni-catalyzed cross-coupling between adamantyl radical and phenyl bromide using anionic acac as ligand. Free energies (kcal/mol) were computed at the UB3LYP-D3/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF), UB3LYP-D3/def2-SVP-CPCM(THF) (in parenthesis) and UM06/def2-TZVPP-CPCM(DMA)//UB3LYP-D3/def2-SVP-CPCM(THF) (in bracket) levels of theory.

We performed computations to investigate the effect of cyclic tertiary radical in the reaction pathway, showing that, if the cyclic radical were to engage with the nickel in the cross-coupling cycle, formation of 1-bromoadamantane via inner-sphere C-Br bond formation is favored over C-C bond formation. However, since this step is reversible with only 5.7 kcal/mol in thermodynamic drive with low barrier of 3.8 kcal/mol, the acac-Ni species is likely to also undergo other pathways in this system. Presumably, the sterically hindered cyclic adamantyl radical (compared with the acyclic tertiary radical and acyclic secondary radical) needs to pay a penalty

to undergo inner-sphere C-C bond formation to form the desired product 1-phenyladamantane. As a result, we assume that sterics plays an important role in the C-C bond formation step and have a significant effect on the final product. Compared with the experimental results (done by collaborator) where no cross-coupling product was observed and aryl bromide was recovered, our calculations suggest that *if the aryl halide substrate were activated*, the reactions of adamantyl radical should be feasible to form many possible products, including 1-bromoadamantane and phenyladamantane. While regarding the failure of activating aryl bromide substrate in this system, more exploration of its properties in the Ni-TMHD system is ongoing in our group.

A1.3 Coordinates and Energies

Figure A1.4
***tert*-Butyl radical**
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.115524 (Hartree/Particle)
Thermal correction to Energy= 0.121853
Thermal correction to Enthalpy= 0.122797
Thermal correction to Gibbs Free Energy= 0.086138
Sum of electronic and zero-point Energies= -157.575218
Sum of electronic and thermal Energies= -157.568888
Sum of electronic and thermal Enthalpies= -157.567944
Sum of electronic and thermal Free Energies= -157.604604

C	0.05439000	1.47296400	1.28749000
H	1.15371300	1.47939600	1.19271400
H	-0.30833600	2.51095700	1.19567200
H	-0.16750400	1.15507600	2.33125000
C	-2.04795000	0.72978000	0.00109100
H	-2.34155300	1.79222600	-0.04829300
H	-2.34037500	0.24384600	-0.94544000
H	-2.67577200	0.26835000	0.79647700
C	0.05291600	-0.75676200	0.00135100
H	-0.30729100	-1.19427100	-0.94544200
H	1.15254900	-0.68014400	-0.04738600
H	-0.17378700	-1.50250000	0.79647000
C	-0.58858200	0.56453700	0.28731600

$\Delta G_{solvation}^{UM06}$= -0.00051217
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.86998506
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.72008051
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.49166663063

***t*Bu–Ph**
Zero-point correction= 0.212567 (Hartree/Particle)
Thermal correction to Energy= 0.222196
Thermal correction to Enthalpy= 0.223140
Thermal correction to Gibbs Free Energy= 0.178263
Sum of electronic and zero-point Energies= -389.034497
Sum of electronic and thermal Energies= -389.024869
Sum of electronic and thermal Enthalpies= -389.023924
Sum of electronic and thermal Free Energies= -389.068801

C	-2.58176900	1.21472200	0.38690900
C	-1.22824900	1.17869200	-0.00409700
C	-0.63158200	2.39658000	-0.37075900
C	-1.35282800	3.59764200	-0.34863500
C	-2.69310700	3.61187300	0.04204300
C	-3.30571500	2.40859500	0.41120700
H	-3.08621700	0.29102200	0.68019000
H	0.41272100	2.42820900	-0.68195400
H	-0.85703000	4.52750500	-0.64054300
H	-3.25607900	4.54860800	0.05950800
H	-4.35445400	2.39895700	0.72043100
C	-0.47089600	-0.16262400	-0.01661400
C	-0.47838100	-0.76833300	1.40543100

H	0.05896700	-1.73089600	1.41423100
H	0.01717500	-0.09334900	2.12156900
H	-1.50102700	-0.95357000	1.76740000
C	0.99279300	-0.00337300	-0.46382900
H	1.49247000	-0.98475200	-0.45386700
H	1.06693700	0.39712100	-1.48696000
H	1.55563000	0.66298200	0.20845000
C	-1.17186700	-1.13447600	-0.99315200
H	-2.21471300	-1.32907300	-0.69996500
H	-1.17865300	-0.72448000	-2.01584700
H	-0.64427600	-2.10218800	-1.01578600

$\Delta G_{solvation}^{UM06}$= -0.00210233
UB3LYP-D3/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -389.32908106
UM06/def2-TZVPP-CPCM(DMA)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -389.32942074
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -388.77305156643

***t*Bu-Br**
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.121383 (Hartree/Particle)
Thermal correction to Energy= 0.127998
Thermal correction to Enthalpy= 0.128942
Thermal correction to Gibbs Free Energy= 0.090831
Sum of electronic and zero-point Energies= -2731.509375
Sum of electronic and thermal Energies= -2731.502760
Sum of electronic and thermal Enthalpies= -2731.501816
Sum of electronic and thermal Free Energies= -2731.539927

C	-0.80126600	0.79228800	-0.05867000
C	-2.32358400	0.83072300	0.00721800
H	-2.69950800	1.86412100	0.00978500
H	-2.72789300	0.31834600	-0.88296400
H	-2.70045000	0.31407300	0.90179900
C	-0.25779100	-0.63025600	0.00764600
H	-0.60744900	-1.18347300	-0.88130800
H	0.84182700	-0.64079900	0.00849400
H	-0.61779200	-1.15675100	0.90345100
C	-0.25801100	1.56088200	-1.25757100
H	-0.62018200	2.59917700	-1.26690400
H	0.84159800	1.56916000	-1.26547000
H	-0.60583300	1.06605800	-2.18093300
Br	-0.11938200	1.75722800	1.61166300

$\Delta G_{solvation}^{UM06}$= -0.00339442shang
UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2732.12476199
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2731.85678123
DLPNO-CCSD(T)/def2-TZVPP-gas// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2730.27021223902

^{1}F
UB3LYP-D3/def2-SVP-CPCM(THF)
$\langle S^2 \rangle$ = 0.0000
Zero-point correction= 0.303924 (Hartree/Particle)
Thermal correction to Energy= 0.325242
Thermal correction to Enthalpy= 0.326187
Thermal correction to Gibbs Free Energy= 0.250047
Sum of electronic and zero-point Energies= -4886.916607
Sum of electronic and thermal Energies= -4886.895289
Sum of electronic and thermal Enthalpies= -4886.894345
Sum of electronic and thermal Free Energies= -4886.970485

C	-2.35713200	0.66818000	1.26433000
C	-2.03043400	-0.65370700	0.71070300
C	-2.62076800	-1.02021400	-0.55416500
C	-3.44410600	-0.14832400	-1.22864300
C	-3.81708500	1.11177900	-0.66154400
C	-3.31437600	1.48551300	0.56283800
Br	-1.96632800	-2.28793700	2.02852200
H	-2.38920200	-2.00165300	-0.97713300
H	-2.27581600	0.83379700	2.34714300
H	-3.66010700	2.41098000	1.03589400
H	-4.52466100	1.75435400	-1.19237200
H	-3.83293100	-0.43097800	-2.21173200
C	2.21375300	0.23800000	0.02640300
C	1.28434400	-1.89145700	0.08627200
C	2.50108900	-2.47921900	-0.24527300
C	3.63211900	-1.67205600	-0.45328500
C	3.46510300	-0.28824000	-0.30866900
C	1.93080300	1.68321100	0.20974400
C	0.27895400	3.23495100	0.72077800
C	1.17039700	4.29550300	0.59312500
C	2.51051000	4.03996100	0.25709500
C	2.87800700	2.70142300	0.06452300
H	0.38679600	-2.48706000	0.26939100
H	2.56598100	-3.56530600	-0.34084200
H	4.31685000	0.37601000	-0.45956400
H	-0.77124200	3.39503000	0.97473900
H	0.82053000	5.31726600	0.75559100
H	3.90785100	2.45862100	-0.19952300
N	1.13741300	-0.56421400	0.21612900
N	0.64473000	1.95767100	0.53838200
Ni	-0.50805500	0.38037200	0.64864600
C	3.49880600	5.16258500	0.09922700
H	4.52387400	4.78948200	-0.03455000
H	3.24147300	5.78012500	-0.77752400
H	3.47932900	5.82800300	0.97684100
C	4.96407200	-2.27782300	-0.80119200
H	5.70898400	-1.51094000	-1.05612000
H	5.35276300	-2.86437800	0.04800500
H	4.86880100	-2.97073500	-1.65217600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.748303
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.625241

^{3}F

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.303037 (Hartree/Particle)
Thermal correction to Energy= 0.324280
Thermal correction to Enthalpy= 0.325224
Thermal correction to Gibbs Free Energy= 0.249695
Sum of electronic and zero-point Energies= -4886.907048
Sum of electronic and thermal Energies= -4886.885805
Sum of electronic and thermal Enthalpies= -4886.884861
Sum of electronic and thermal Free Energies= -4886.960390

C	-2.86004700	0.53399500	1.63679200
C	-2.15805200	-0.57910400	1.08878500
C	-2.26351900	-0.85908500	-0.30596100
C	-3.10501400	-0.04467300	-1.10984200
C	-3.79390400	1.02973300	-0.56253900
C	-3.64814000	1.32896700	0.81157400
Br	-1.52628800	-1.94341300	2.30708200
H	-1.85251500	-1.78191100	-0.71809400
H	-2.77869900	0.74475100	2.70382100
H	-4.16773000	2.18873400	1.24078100
H	-4.43714500	1.64913600	-1.19054800
H	-3.21198200	-0.28990300	-2.16894500
C	2.15628700	0.25623200	-0.12325500
C	1.20467500	-1.89164300	-0.22112200
C	2.43029100	-2.49963900	-0.42579900
C	3.60169000	-1.68391100	-0.48870600
C	3.44226400	-0.31924600	-0.33446200
C	1.90132600	1.65745700	0.05116200
C	0.24662700	3.29745600	0.41826600
C	1.16875300	4.32630100	0.40858600
C	2.55027900	4.01179700	0.20563700
C	2.88970500	2.68307500	0.03207200
H	0.29296100	-2.49250900	-0.15567100
H	2.49366400	-3.58438700	-0.53297200
H	4.31863800	0.33053900	-0.37358800
H	-0.81895300	3.49727300	0.57204000
H	0.84330100	5.35821500	0.55466200
H	3.93614900	2.41393200	-0.12380200
N	1.03958100	-0.56588900	-0.07685900
N	0.57121700	2.00171800	0.24642200
Ni	-0.64075000	0.46304200	0.21118700
C	3.57627900	5.11229600	0.18684700
H	4.59281000	4.72480500	0.02373200
H	3.35484800	5.84380100	-0.60967300
H	3.57029400	5.67354700	1.13742000
C	4.94888900	-2.31570000	-0.71341400
H	5.75680500	-1.56926700	-0.72674000
H	5.17458600	-3.05339200	0.07598500
H	4.97190800	-2.86455500	-1.67084600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7324304
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.61024

***tert*-butyl radical**

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.115524 (Hartree/Particle)
Thermal correction to Energy= 0.121853
Thermal correction to Enthalpy= 0.122797
Thermal correction to Gibbs Free Energy= 0.086138
Sum of electronic and zero-point Energies= -157.575218
Sum of electronic and thermal Energies= -157.568888
Sum of electronic and thermal Enthalpies= -157.567944
Sum of electronic and thermal Free Energies= -157.604604

C	-1.40592600	-5.80885900	-0.81665200
C	-0.76293300	-4.90023200	-1.81663000
H	0.33639100	-4.89385900	-1.72186500
H	-0.98485100	-5.21787700	-2.86045900
H	-1.12562200	-3.86224700	-1.72457600
C	-2.86529500	-5.64365300	-0.53040600
H	-3.49311600	-6.10490200	-1.32589700
H	-3.15773800	-6.12978300	0.41601800
H	-3.15888000	-4.58121200	-0.48079900
C	-0.76445100	-7.13022500	-0.53094900
H	0.33518400	-7.05363400	-0.48219000
H	-1.12467000	-7.56791800	0.41575500
H	-0.99116000	-7.87580100	-1.32621900

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-157.7200251
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-157.8699418

^{1}F'

UB3LYP-D3/def2-SVP-CPCM(THF)
$\langle S^2 \rangle$ = 1.0136 (before annihilation, 0.1453 after)
Zero-point correction= 0.303179 (Hartree/Particle)
Thermal correction to Energy= 0.324700
Thermal correction to Enthalpy= 0.325644
Thermal correction to Gibbs Free Energy= 0.249331
Sum of electronic and zero-point Energies= -4886.889735
Sum of electronic and thermal Energies= -4886.868214
Sum of electronic and thermal Enthalpies= -4886.867270
Sum of electronic and thermal Free Energies= -4886.943582

Ni	0.45097900	0.75422500	-0.51615600
C	-2.61923300	1.79943100	0.69437800
C	-3.80753400	2.52186400	0.78846000
C	-2.19830900	0.91052900	1.68156500
C	-4.60388600	2.33902600	1.92544600
H	-4.11043300	3.21117600	-0.00201500
C	-3.00841600	0.74202800	2.80967800
H	-1.26345000	0.35964700	1.56075100
C	-4.20732800	1.45287100	2.93326100
H	-5.53949000	2.89587200	2.01842400
H	-2.69559000	0.04769500	3.59335200
H	-4.83495500	1.31567000	3.81678000

Br	-1.50765300	2.03093300	-0.89197600
N	2.28718000	0.21033200	-0.31399000
C	4.84792900	-0.93207900	0.03142900
C	3.39401500	0.97541600	-0.30108000
C	2.41655000	-1.16425800	-0.14525500
C	3.71534600	-1.72516400	0.02368700
C	4.67452600	0.47726100	-0.13626800
N	0.03521700	-1.16120900	-0.33288500
C	-0.13784100	-3.96464000	-0.05814400
C	-1.15006500	-1.78968900	-0.37876300
C	1.19027000	-1.91125100	-0.16131900
C	1.08842900	-3.32614300	-0.02063400
C	-1.30380400	-3.15959400	-0.24831900
H	3.22394300	2.04850100	-0.43475300
H	3.81785500	-2.80464900	0.15126000
H	5.53174800	1.15357700	-0.13713000
H	-2.01951200	-1.13964800	-0.52399200
H	1.99565600	-3.91758100	0.11796900
H	-2.29792000	-3.60929800	-0.28986200
C	-0.27003300	-5.45646000	0.09238600
H	0.70641800	-5.94504900	0.22688500
H	-0.90393100	-5.71038000	0.95979200
H	-0.75831100	-5.90086800	-0.79227800
C	6.22827000	-1.50473400	0.20983000
H	6.72258100	-1.07366300	1.09787100
H	6.20833200	-2.59852100	0.32607300
H	6.87116100	-1.26235900	-0.65425100

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7258715
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6064849

^{1}F-TS
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.301918 (Hartree/Particle)
Thermal correction to Energy= 0.322858
Thermal correction to Enthalpy= 0.323802
Thermal correction to Gibbs Free Energy= 0.249700
Sum of electronic and zero-point Energies= -4886.898920
Sum of electronic and thermal Energies= -4886.877980
Sum of electronic and thermal Enthalpies= -4886.877036
Sum of electronic and thermal Free Energies= -4886.951138

C	-2.70242500	-0.07554900	1.35175300
C	-2.48593000	-0.39023000	-0.01498100
C	-3.05621300	0.39728800	-1.04546700
C	-3.73353300	1.55588600	-0.69934200
C	-3.89777500	1.92626000	0.65600600
C	-3.38781700	1.11697300	1.66513800
Br	-2.12202100	-2.41383100	-0.41069800
H	-2.92249600	0.10757100	-2.08902100
H	-2.45280700	-0.78360900	2.14542300
H	-3.54905800	1.37642100	2.71467400
H	-4.44490500	2.83755500	0.90673400
H	-4.13919000	2.19419300	-1.48866800
C	2.19635700	-0.18511600	0.13256200
C	1.61021300	-2.43581700	0.48578500
C	2.91959700	-2.85802600	0.37086400
C	3.94211800	-1.89307300	0.11678500
C	3.55615000	-0.56848700	-0.00168500
C	1.69785800	1.16386500	0.02495300
C	-0.22368200	2.51283400	0.03841500
C	0.51265500	3.67144500	-0.13362700
C	1.93122600	3.58101900	-0.23607400
C	2.50121600	2.32069200	-0.14974900
H	0.79904300	-3.14721000	0.66887500
H	3.16380100	-3.91739100	0.47412500
H	4.30957700	0.19363200	-0.20966200
H	-1.31199400	2.54355600	0.12135900
H	0.00621600	4.63712200	-0.19221500
H	3.58624200	2.21663100	-0.20901400
N	1.23237700	-1.14498000	0.38190200
N	0.32544800	1.28692800	0.10394600
Ni	-0.59521100	-0.44560400	0.41120500
C	2.75756800	4.82441400	-0.42441900
H	3.83290500	4.59969700	-0.47785000
H	2.46931800	5.35042400	-1.35077400
H	2.59448200	5.53480400	0.40408600
C	5.37543700	-2.32903300	-0.02113200
H	6.04717400	-1.47871200	-0.20990800
H	5.72017300	-2.84371400	0.89234900
H	5.49120200	-3.04913900	-0.84959000

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7224721
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.5888467

^{3}F-TS
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.302378 (Hartree/Particle)
Thermal correction to Energy= 0.323155
Thermal correction to Enthalpy= 0.324099
Thermal correction to Gibbs Free Energy= 0.249623
Sum of electronic and zero-point Energies= -4886.899261
Sum of electronic and thermal Energies= -4886.878484
Sum of electronic and thermal Enthalpies= -4886.877540
Sum of electronic and thermal Free Energies= -4886.952015

C	-2.98196100	0.53763500	1.38884700
C	-2.33565200	-0.52608900	0.72079200
C	-2.36186400	-0.63350000	-0.68707300
C	-2.91143900	0.41192200	-1.42107900
C	-3.48624400	1.52278900	-0.77458900
C	-3.52523800	1.57702300	0.61953700
Br	-2.08238700	-2.26280700	1.84526800
H	-1.90111900	-1.49363900	-1.17414800
H	-3.04337300	0.55394600	2.47831900
H	-3.99362100	2.42496800	1.12564600
H	-3.91880800	2.33250400	-1.36618300
H	-2.89098200	0.36639800	-2.51298700
C	2.05129500	-0.07640600	0.27065900
C	1.46030100	-2.33969800	0.54765700

C	2.64594000	-2.78631300	-0.00664700
C	3.60420100	-1.82406500	-0.45249700
C	3.28789500	-0.48615500	-0.30556800
C	1.64408500	1.28764500	0.46008000
C	-0.06051900	2.71784700	1.23765500
C	0.65030600	3.85620700	0.90591100
C	1.94513700	3.71219100	0.31631600
C	2.41633100	2.43014600	0.10215400
H	0.70141500	-3.04605900	0.89799400
H	2.84014600	-3.85685000	-0.09874500
H	3.99931200	0.27131700	-0.63996600
H	-1.05796400	2.78637800	1.68256700
H	0.22330000	4.84404900	1.09008300
H	3.39904400	2.29004700	-0.35189200
N	1.14828700	-1.03991000	0.69664600
N	0.39751300	1.46825400	1.04211400
Ni	-0.52639600	-0.24001900	1.41846100
C	2.74293800	4.93376200	-0.05191900
H	3.71690200	4.67299800	-0.49169400
H	2.19380200	5.55869000	-0.77748000
H	2.92340600	5.56765700	0.83347900
C	4.90367700	-2.28019500	-1.05894700
H	5.54204100	-1.43300400	-1.35015000
H	5.46934000	-2.91019800	-0.35082700
H	4.72425000	-2.89977300	-1.95472800

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7206594
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6028485

^{1}F'-TS
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.302070 (Hartree/Particle)
Thermal correction to Energy= 0.323321
Thermal correction to Enthalpy= 0.324265
Thermal correction to Gibbs Free Energy= 0.248135
Sum of electronic and zero-point Energies= -4886.884886
Sum of electronic and thermal Energies= -4886.863635
Sum of electronic and thermal Enthalpies= -4886.862690
Sum of electronic and thermal Free Energies= -4886.938820

Ni	-3.25440100	1.69922200	-0.86461000
C	-6.35073000	2.74589100	0.53308000
C	-7.53839400	3.44711300	0.67417300
C	-5.86220800	1.86132000	1.48043900
C	-8.28028700	3.24455700	1.84917500
H	-7.88972100	4.13539600	-0.10011600
C	-6.61321900	1.66746500	2.64876800
H	-4.91949200	1.33067400	1.30643200
C	-7.81837600	2.35839500	2.83071200
H	-9.22162300	3.78253300	1.99505000
H	-6.25559300	0.97493500	3.41641200
H	-8.40158400	2.20507500	3.74213700
Br	-5.14157500	2.96186900	-1.30211900
N	-1.43673700	1.14855000	-0.56103500
C	1.13037600	0.04417700	-0.13811000
C	-0.33715600	1.93142800	-0.52312200
C	-1.28515500	-0.21011700	-0.37455300
C	0.00054600	-0.76171700	-0.17187300
C	0.93910900	1.44332600	-0.31648700
N	-3.65142800	-0.21949300	-0.60653600
C	-3.85403800	-3.00901400	-0.27941300
C	-4.84620800	-0.83417400	-0.65249500
C	-2.52059100	-0.97139200	-0.40358000
C	-2.61976500	-2.37340400	-0.23952300
C	-5.00368800	-2.20043400	-0.49558900
H	-0.51503800	3.00012000	-0.67276100
H	0.10638300	-1.83949400	-0.03613000
H	1.78764300	2.13053100	-0.29576000
H	-5.70475700	-0.17691700	-0.81941800
H	-1.71623100	-2.96410700	-0.07912700
H	-6.00041000	-2.64452600	-0.53793000
C	-3.99416700	-4.49675500	-0.10296000
H	-3.02112100	-4.98599000	0.04915400
H	-4.63647800	-4.72965900	0.76334700
H	-4.47599200	-4.95299000	-0.98434100
C	2.51010400	-0.51465700	0.07923900
H	2.97467100	-0.07668900	0.97929200
H	2.49559500	-1.60786000	0.19844700
H	3.17260700	-0.26945500	-0.76839500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.712787
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.5994182

^{3}F'-TS
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.301975 (Hartree/Particle)
Thermal correction to Energy= 0.323268
Thermal correction to Enthalpy= 0.324212
Thermal correction to Gibbs Free Energy= 0.246893
Sum of electronic and zero-point Energies= -4886.882832
Sum of electronic and thermal Energies= -4886.861540
Sum of electronic and thermal Enthalpies= -4886.860596
Sum of electronic and thermal Free Energies= -4886.937914

Ni	-3.25263800	1.70106100	-0.95983300
C	-6.35184300	2.70762400	0.47578100
C	-7.55100900	3.38369900	0.63666300
C	-5.83505700	1.82269900	1.40707900
C	-8.27458100	3.15564700	1.81877700
H	-7.92568500	4.07211900	-0.12667200
C	-6.56771500	1.60345900	2.58285800
H	-4.88479500	1.31169300	1.21578400
C	-7.78363000	2.26932300	2.78604100
H	-9.22429000	3.67396400	1.98147500
H	-6.18755400	0.91068700	3.33952800
H	-8.35277500	2.09594900	3.70278900
Br	-5.16984200	2.93988300	-1.39971200
N	-1.44440100	1.16785800	-0.57589000
C	1.12337200	0.07844800	-0.12970900
C	-0.34815200	1.95332000	-0.55288900

C	-1.28934600	-0.18483900	-0.37268100
C	-0.00578600	-0.73140600	-0.15506900
C	0.93004300	1.47088600	-0.33441100
N	-3.64223100	-0.21697000	-0.71040900
C	-3.86427200	-2.97683700	-0.19545900
C	-4.83578800	-0.83350300	-0.75824100
C	-2.52536900	-0.95129400	-0.40433400
C	-2.63166100	-2.33606400	-0.14348800
C	-5.00027300	-2.18742000	-0.51776000
H	-0.52837500	3.01905900	-0.71892100
H	0.10223800	-1.80749000	-0.00874000
H	1.77655600	2.16077100	-0.32147800
H	-5.68585400	-0.18916700	-1.00093400
H	-1.73827800	-2.90972000	0.10926100
H	-5.99455300	-2.63537700	-0.57555400
C	-4.01310800	-4.44828300	0.08160900
H	-3.04713800	-4.92357100	0.30576000
H	-4.68840300	-4.61997400	0.93698100
H	-4.46063000	-4.96689600	-0.78309200
C	2.50309700	-0.47512700	0.10090000
H	2.48847200	-1.56499400	0.24673500
H	3.16503000	-0.25058400	-0.75271500
H	2.96709300	-0.01490200	0.98984600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.710583
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.5980175

^{1}G
UB3LYP-D3/def2-SVP-CPCM(THF)
$<S^2> = 0.0000$
Zero-point correction= 0.306236
(Hartree/Particle)
Thermal correction to Energy= 0.327471
Thermal correction to Enthalpy= 0.328416
Thermal correction to Gibbs Free Energy= 0.251298
Sum of electronic and zero-point Energies= -4886.979456
Sum of electronic and thermal Energies= -4886.958220
Sum of electronic and thermal Enthalpies= -4886.957276
Sum of electronic and thermal Free Energies= -4887.034393

Ni	-4.62164100	0.37276900	-0.35551800
C	-6.48961200	0.30741100	-0.60607900
C	-7.09110200	0.71952100	-1.80860200
C	-7.32438700	-0.22393800	0.39359000
C	-8.47025500	0.58409600	-2.01712600
H	-6.47263100	1.15269500	-2.60117700
C	-8.70484800	-0.36076100	0.19395800
H	-6.89063800	-0.54663600	1.34577600
C	-9.28439000	0.04067100	-1.01568600
H	-8.91247300	0.90753700	-2.96479400
H	-9.33112800	-0.78186000	0.98683500
H	-10.36102100	-0.06552000	-1.17536300
Br	-4.86562300	2.59801700	0.38673300
C	-2.08305200	-0.93380400	-0.43222200
C	-0.71910400	-1.20423500	-0.28347300
C	0.14074900	-0.22825800	0.23592100
C	-0.43238600	1.00444300	0.58288700
C	-1.79853600	1.20493800	0.40952800
C	-3.06402100	-1.89823600	-0.97117700
C	-2.72086900	-3.17719700	-1.42003300
C	-3.69785200	-4.04180700	-1.92546000
C	-5.01382400	-3.55700200	-1.95217400
C	-5.29150600	-2.27595300	-1.49150600
H	-0.31683100	-2.17600900	-0.56937000
H	0.18079400	1.81192400	0.98842400
H	-2.28181300	2.14944200	0.66877300
H	-1.68270700	-3.50593000	-1.37942800
H	-5.83107600	-4.17356900	-2.33189100
H	-6.30644800	-1.88304700	-1.50502500
N	-2.61180200	0.26140400	-0.08511500
N	-4.34639000	-1.44945200	-1.00598000
C	1.60662000	-0.49444200	0.43630000
H	1.81183200	-0.69302500	1.50204700
H	1.94610500	-1.36673200	-0.14000000
H	2.21068100	0.37926600	0.14824900
C	-3.36195400	-5.41711900	-2.42902400
H	-3.53113800	-5.47644100	-3.51705900
H	-2.31471700	-5.68322400	-2.22918800
H	-4.01304700	-6.17284000	-1.96195100

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.8048777
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6907597

^{3}G
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.305000
(Hartree/Particle)
Thermal correction to Energy= 0.326820
Thermal correction to Enthalpy= 0.327764
Thermal correction to Gibbs Free Energy= 0.248330
Sum of electronic and zero-point Energies= -4886.978664
Sum of electronic and thermal Energies= -4886.956844
Sum of electronic and thermal Enthalpies= -4886.955900
Sum of electronic and thermal Free Energies= -4887.035334

C	-1.73044200	0.93421700	-0.63476400
C	-1.87312800	0.01418300	0.42272300
C	-3.09150000	-0.69213400	0.48577300
C	-4.11710000	-0.48980600	-0.44888000
C	-3.94577100	0.43216300	-1.48845600
C	-2.74396600	1.14515500	-1.57994400
Br	-0.88450500	-2.21177200	3.23222000
H	-3.23786100	-1.42479400	1.28704600
H	-0.80136700	1.50807000	-0.73169700
H	-2.59751400	1.86676900	-2.39048300
H	-4.74106900	0.59286600	-2.22222600
H	-5.05158000	-1.05493100	-0.36868500
C	2.01065800	0.06705500	0.27402200
C	1.37737300	-2.16886900	0.19169000
C	2.45861300	-2.49492100	-0.62011900
C	3.36180300	-1.48973000	-1.00624600
C	3.11900900	-0.19089800	-0.54028200

C	1.66580800	1.40468700	0.82149200
C	0.17929400	2.58600300	2.15870500
C	0.84043600	3.78607700	1.92081700
C	1.97024400	3.79875800	1.08551300
C	2.37512800	2.57640700	0.53376900
H	0.65416600	-2.91549900	0.52937300
H	2.59867200	-3.52731600	-0.94686900
H	3.80224600	0.61390500	-0.81193400
H	-0.71171300	2.54155000	2.79011400
H	0.47461800	4.70615700	2.38100800
H	3.24287400	2.54531600	-0.12525700
N	1.16153900	-0.92126200	0.62231300
N	0.58416900	1.42588700	1.62949600
Ni	-0.43901900	-0.35359100	1.74233300
C	2.69511000	5.08093000	0.78436100
H	3.65064800	4.90126000	0.27232000
H	2.07555700	5.72408100	0.13705800
H	2.88953100	5.64723300	1.70840800
C	4.53562400	-1.80355900	-1.89196600
H	5.22460800	-0.95168800	-1.97632800
H	5.09354100	-2.67194100	-1.50816100
H	4.18856300	-2.06632300	-2.90518900

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7899161
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6853609

^{1}G'
UB3LYP-D3/def2-SVP-CPCM(THF)
$\langle S^2 \rangle$ = 0.9508 (before annihilation, 0.0349 after)
Zero-point correction= 0.304833 (Hartree/Particle)
Thermal correction to Energy= 0.326760
Thermal correction to Enthalpy= 0.327704
Thermal correction to Gibbs Free Energy= 0.247505
Sum of electronic and zero-point Energies= -4886.959643
Sum of electronic and thermal Energies= -4886.937717
Sum of electronic and thermal Enthalpies= -4886.936773
Sum of electronic and thermal Free Energies= -4887.016971

Ni	1.09190800	0.85609700	-1.70045300
C	2.38443500	0.71457900	-0.24778600
C	4.32361600	0.52823400	1.82293400
C	2.00852900	0.65376700	1.10673000
C	3.76251500	0.67514900	-0.53491700
C	4.72335100	0.58681800	0.48277100
C	2.95825500	0.55992200	2.13304300
H	0.94689300	0.67949200	1.37739800
H	4.09105500	0.70806600	-1.57887300
H	5.78794100	0.56005200	0.22846600
H	2.63351000	0.51232000	3.17757600
N	-0.25402700	2.12891000	-0.78486400
C	-2.03722900	3.59640700	0.80378900
C	-0.08589800	3.44506300	-0.61045800
C	-1.28901800	1.50693000	-0.18117900
C	-2.19373900	2.21728500	0.61705300
C	-0.94786200	4.21283200	0.16501000
N	-0.34638900	-0.47557600	-1.12802500
C	-2.39020200	-2.15220500	-0.22052400
C	-0.31543500	-1.78422300	-1.40004300
C	-1.36863100	0.04049700	-0.41723000
C	-2.40540200	-0.77721600	0.04796700
C	-1.30952600	-2.65450600	-0.96577900
H	0.77765700	3.88987600	-1.11133800
H	-3.01999300	1.69972700	1.10459300
H	-0.76936800	5.28462200	0.27348500
H	0.53822100	-2.12410100	-1.99223700
H	-3.23277300	-0.34994300	0.61481500
H	-1.24475100	-3.71689000	-1.20969400
Br	1.96750300	0.21137900	-3.84444000
H	5.06948400	0.45680800	2.61980200
C	-3.48105700	-3.06467300	0.26779900
H	-3.89910200	-3.65146300	-0.56545100
H	-3.07828400	-3.78603900	0.99785100
H	-4.29730700	-2.50768600	0.74835000
C	-2.98421500	4.39357400	1.65712600
H	-3.78647000	3.76897300	2.07386900
H	-2.44347800	4.86833200	2.49191800
H	-3.44307200	5.20520200	1.06971000

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4887.7735251
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4888.6678698

^{1}F'' (Ni-bromo species)
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.214708 (Hartree/Particle)
Thermal correction to Energy= 0.230876
Thermal correction to Enthalpy= 0.231820
Thermal correction to Gibbs Free Energy= 0.166322
Sum of electronic and zero-point Energies= -4655.579462
Sum of electronic and thermal Energies= -4655.563294
Sum of electronic and thermal Enthalpies= -4655.562349
Sum of electronic and thermal Free Energies= -4655.627848

Ni	-3.99183200	1.30009300	-1.54653000
C	-1.87359800	-0.39708200	-0.83451100
C	-0.60463100	-0.81497600	-0.41773600
C	0.38038200	0.12429500	-0.09164500
C	0.02971800	1.48282700	-0.20377800
C	-1.24637600	1.83242200	-0.62458000
C	-2.97912600	-1.31121800	-1.19958100
C	-2.90514100	-2.70937500	-1.17420400
C	-4.01531200	-3.47922700	-1.54213400
C	-5.17917400	-2.78948900	-1.92940000
C	-5.18373000	-1.39947400	-1.93172800
H	-0.37768600	-1.87943400	-0.34653600
H	0.75171100	2.26661600	0.03582700
H	-1.54668200	2.87837300	-0.72245500
H	-1.98301600	-3.20525100	-0.86858000
H	-6.07708900	-3.33486700	-2.22820500
H	-6.06484300	-0.82279400	-2.22618200
N	-2.18757800	0.92199600	-0.93709400

N	-4.11313300	-0.67488700	-1.57617200
C	1.75486100	-0.28579000	0.36089600
H	1.95781900	0.09097300	1.37696900
H	1.87445700	-1.37835300	0.36807700
H	2.52660300	0.14347000	-0.29878000
C	-3.97959500	-4.98297800	-1.52479800
H	-2.98906900	-5.36658100	-1.24261000
H	-4.71990400	-5.37924000	-0.81035300
H	-4.24149600	-5.38984900	-2.51492300
Br	-5.83964900	2.56755300	-2.20535500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4656.2756634
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4656.9610627

^{1}F'' (phenyl radical)
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.087289 (Hartree/Particle)
Thermal correction to Energy= 0.091650
Thermal correction to Enthalpy= 0.092595
Thermal correction to Gibbs Free Energy= 0.059244
Sum of electronic and zero-point Energies= -231.315888
Sum of electronic and thermal Energies= -231.311527
Sum of electronic and thermal Enthalpies= -231.310583
Sum of electronic and thermal Free Energies= -231.343933

C	-0.29103800	0.26151900	0.00004900
C	1.08781900	0.18926900	0.00053500
C	1.78056300	1.41499000	-0.00004200
C	1.07310400	2.62406400	-0.00104400
C	-0.32767200	2.63227200	-0.00149100
C	-1.04299800	1.41956500	-0.00093600
H	1.62938100	-0.76109600	0.00131300
H	2.87438700	1.41756800	0.00029600
H	1.61954800	3.57046000	-0.00149000
H	-0.87218400	3.58094900	-0.00227600
H	-2.13682400	1.41357900	-0.00127400

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-231.4580093
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-231.6566083

^{2}J
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.331279 (Hartree/Particle)
Thermal correction to Energy= 0.351894
Thermal correction to Enthalpy= 0.352838
Thermal correction to Gibbs Free Energy= 0.280022
Sum of electronic and zero-point Energies= -2239.242341
Sum of electronic and thermal Energies= -2239.221726
Sum of electronic and thermal Enthalpies= -2239.220782
Sum of electronic and thermal Free Energies= -2239.293598

Ni	-4.10779300	1.25373400	-1.32019600
C	-5.28347400	2.10080600	0.03079000
C	-5.03401900	1.38406500	1.35564100
H	-5.25906000	0.30620400	1.28131900
H	-3.98154200	1.47642200	1.67430500
H	-5.66375000	1.79496700	2.17789100
C	-6.74299800	1.93257600	-0.39703800
H	-6.94980400	2.42389700	-1.36397600
H	-7.01521500	0.86793600	-0.50344000
H	-7.44565000	2.37383100	0.34714100
C	-4.92890800	3.58415100	0.15262900
H	-3.87438700	3.72864900	0.44643000
H	-5.08315600	4.12523800	-0.79738700
H	-5.55196400	4.09679500	0.92164600
C	-1.89191700	-0.41456100	-0.88502500
C	-0.61814100	-0.81574800	-0.41270300
C	0.35899600	0.12005500	-0.11030600
C	0.02631300	1.49591800	-0.28126800
C	-1.23753900	1.83555500	-0.71914600
C	-2.96893100	-1.31088500	-1.24418800
C	-2.91389500	-2.72433300	-1.16927600
C	-3.99501600	-3.50287200	-1.55282100
C	-5.16206000	-2.82501300	-2.01248100
C	-5.17490100	-1.44531200	-2.04011900
H	-0.40127800	-1.87823200	-0.28847900
H	0.75671600	2.27789200	-0.06274800
H	-1.53394200	2.88224600	-0.83746600
H	-2.00592900	-3.20789700	-0.80444100
H	-6.04307800	-3.38544700	-2.33253800
H	-6.06335400	-0.89367900	-2.36210800
N	-2.18708600	0.92479600	-1.02438100
N	-4.11948700	-0.68522600	-1.67555800
C	1.72370800	-0.27320800	0.38598300
H	1.91667200	0.15250000	1.38561100
H	1.83814000	-1.36510800	0.45040600
H	2.51186200	0.11755900	-0.28004500
C	-3.96763700	-5.00572600	-1.48791700
H	-2.99793700	-5.38363700	-1.13244600
H	-4.75292300	-5.38446500	-0.81138900
H	-4.16727900	-5.44621100	-2.47965200

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2239.8687984
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2240.5868708

^{4}J
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.331122 (Hartree/Particle)
Thermal correction to Energy= 0.351753
Thermal correction to Enthalpy= 0.352697
Thermal correction to Gibbs Free Energy= 0.279075
Sum of electronic and zero-point Energies= -2239.236155
Sum of electronic and thermal Energies= -2239.215524

Sum of electronic and thermal Enthalpies= -2239.214580
Sum of electronic and thermal Free Energies= -2239.288203

Ni	-4.11364400	1.25171300	-1.35136700
C	-5.30943000	2.15278900	-0.05189500
C	-5.12379100	1.41771900	1.27095000
H	-5.39083100	0.35173000	1.17915700
H	-4.07610200	1.46491900	1.61216600
H	-5.75620800	1.85139700	2.07662700
C	-6.75210500	2.03935200	-0.54491100
H	-6.89621400	2.53596100	-1.51987700
H	-7.06181300	0.98624900	-0.65716300
H	-7.46358700	2.51074500	0.16894000
C	-4.88469300	3.61585700	0.07013500
H	-3.83618700	3.70884700	0.40156800
H	-4.98128000	4.15545000	-0.88780900
H	-5.50788100	4.15995300	0.81427700
C	-1.91951800	-0.43473700	-0.77691700
C	-0.59133900	-0.83128600	-0.44384100
C	0.37256900	0.10003800	-0.10652300
C	-0.00177800	1.48126100	-0.10583800
C	-1.29654900	1.81858100	-0.45309700
C	-2.98536800	-1.32921200	-1.12487800
C	-2.87841100	-2.74941200	-1.18917800
C	-3.96492000	-3.53686600	-1.52063800
C	-5.20546100	-2.88212200	-1.80354600
C	-5.25574700	-1.50197000	-1.74635900
H	-0.33246100	-1.89167700	-0.45113800
H	0.71715700	2.25835400	0.16045200
H	-1.61984100	2.86445500	-0.47338200
H	-1.92065000	-3.22417300	-0.96819200
H	-6.09774700	-3.45525900	-2.06244500
H	-6.18319900	-0.96266000	-1.96463600
N	-2.23720000	0.91623900	-0.78353100
N	-4.20098500	-0.73186300	-1.42625700
C	1.77899500	-0.29547500	0.25316800
H	2.03975500	0.05842200	1.26556500
H	1.92119900	-1.38575800	0.22253200
H	2.50625700	0.16658900	-0.43672600
C	-3.87769300	-5.03726600	-1.58960400
H	-2.86973500	-5.40369900	-1.34554800
H	-4.59329800	-5.50453600	-0.89112100
H	-4.14191300	-5.40041900	-2.59786800

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2239.8575927
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2240.5786207

^{2}K-TS
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.422956 (Hartree/Particle)
Thermal correction to Energy= 0.450436
Thermal correction to Enthalpy= 0.451380
Thermal correction to Gibbs Free Energy= 0.361910
Sum of electronic and zero-point Energies= -5044.524684
Sum of electronic and thermal Energies= -5044.497204
Sum of electronic and thermal Enthalpies= -5044.496260
Sum of electronic and thermal Free Energies= -5044.585730

Ni	-0.56887500	-0.10884500	0.03179700
C	-2.00773300	0.73061800	-1.07367400
C	-1.81809100	3.47023400	-1.69584400
C	-2.92075100	1.65519000	-0.50062400
C	-1.11674800	1.17633300	-2.09208400
C	-1.00348100	2.54641200	-2.35490100
C	-2.78829100	3.00870100	-0.78061000
H	-3.67843900	1.30166500	0.19970900
H	-0.51865100	0.45366200	-2.64898900
H	-0.27773300	2.88665100	-3.09898500
H	-3.44890000	3.72264300	-0.28033800
N	0.96824900	1.25462800	0.18035100
C	3.21273000	2.93003500	0.37307900
C	0.83008500	2.54873000	0.50132000
C	2.20297300	0.76608600	-0.07367600
C	3.34015400	1.58115100	0.02500900
C	1.91223300	3.41398800	0.60596400
N	1.02235400	-1.20962300	-0.72080700
C	3.36186200	-2.72388100	-1.08916100
C	0.95766700	-2.48795200	-1.12680000
C	2.23627000	-0.65439000	-0.49338800
C	3.41657000	-1.39275300	-0.66507600
C	2.08643100	-3.27123000	-1.32808200
H	-0.19249800	2.89070500	0.66852000
H	4.32833000	1.17240700	-0.18817700
H	1.74447000	4.46123100	0.86657200
H	-0.04933300	-2.87875200	-1.29817400
H	4.38455800	-0.93335800	-0.46190100
H	1.97710300	-4.30344700	-1.66790300
Br	-2.75469400	-1.21241800	-1.48193200
C	-1.25942500	-0.30913100	1.91997700
H	-1.73267300	4.53737400	-1.91319300
C	4.60421000	-3.55062400	-1.27741800
H	5.51773900	-2.95597000	-1.13619400
H	4.62398100	-4.38736500	-0.55940500
H	4.62857200	-3.99435000	-2.28578400
C	4.40757900	3.83624900	0.49373300
H	4.53584500	4.16752900	1.53775800
H	5.33438400	3.33736200	0.17694300
H	4.27328200	4.74427900	-0.11569700
C	-0.10593600	-1.08166100	2.57143300
H	-0.28871200	-1.26294300	3.65582700
H	0.04439400	-2.07046200	2.10401900
H	0.85066700	-0.53464100	2.49801600
C	-2.54257900	-1.12746400	2.00560400
H	-3.39265400	-0.61222000	1.52877500
H	-2.44129500	-2.10488300	1.50598200
H	-2.83192800	-1.32398200	3.06326500
C	-1.44613300	1.02819800	2.62310500
H	-0.50872100	1.60684200	2.65959400
H	-2.20175500	1.65594800	2.12145600
H	-1.78013400	0.89735600	3.67747900

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.4850601
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5185177

^{2}H

UB3LYP-D3/def2-SVP-CPCM(THF)

Zero-point correction= 0.427053 (Hartree/Particle)

Thermal correction to Energy= 0.454642

Thermal correction to Enthalpy= 0.455586

Thermal correction to Gibbs Free Energy= 0.366581

Sum of electronic and zero-point Energies= -5044.574659

Sum of electronic and thermal Energies= -5044.547070

Sum of electronic and thermal Enthalpies= -5044.546126

Sum of electronic and thermal Free Energies= -5044.635131

Ni	-0.56337000	-0.04631900	0.09841600
C	-1.85804600	1.35728300	-0.24505500
C	-3.52873200	3.40894600	-1.28522000
C	-3.21390200	1.44004700	0.10238600
C	-1.36915700	2.30647500	-1.16099100
C	-2.18768500	3.32555400	-1.66969900
C	-4.04026600	2.45236000	-0.40091300
H	-3.65663600	0.70026200	0.77209900
H	-0.33487500	2.25428800	-1.51272900
H	-1.77097400	4.05105900	-2.37504500
H	-5.09288800	2.48722500	-0.10395600
N	1.18278400	1.17021700	0.40025100
C	3.58866200	2.49028000	1.00364600
C	1.18840300	2.46208000	0.75018400
C	2.35080400	0.49932700	0.36745100
C	3.56597200	1.13467400	0.65549500
C	2.35389800	3.15589100	1.05841300
N	0.98567200	-1.44060000	0.01814400
C	3.18735400	-3.15570700	-0.31343600
C	0.81036500	-2.75503700	-0.17462800
C	2.24156800	-0.95071800	0.06963400
C	3.35492100	-1.78141500	-0.10891200
C	1.87055000	-3.64127200	-0.32900300
H	0.21530000	2.95470900	0.77867800
H	4.50024400	0.57419700	0.62972700
H	2.29688100	4.20930500	1.34012000
H	-0.22492700	-3.09449300	-0.22423700
H	4.36042800	-1.36177600	-0.09062700
H	1.66697900	-4.70462200	-0.47039500
Br	-1.71056300	-1.32864000	-1.79047600
C	-1.01599900	-0.24129500	2.08666000
H	-4.17092500	4.20206200	-1.67755800
C	4.35962500	-4.07147500	-0.52983600
H	5.30517400	-3.60717500	-0.21595500
H	4.22852600	-5.01710600	0.01787800
H	4.44652500	-4.32663800	-1.59967900
C	4.87320000	3.21007200	1.30667700
H	4.79438000	3.77049200	2.25134900
H	5.72470600	2.51890000	1.37659300
H	5.09240900	3.94510400	0.51426800
C	0.22707200	-0.77930600	2.79634400
H	-0.00940400	-0.91046400	3.87057900
H	0.55316300	-1.75566600	2.41804000
H	1.07501900	-0.08110100	2.74214300
C	-2.10117100	-1.30721300	2.02841900
H	-2.99088000	-0.97953000	1.47438100
H	-1.73718700	-2.23009000	1.55095900
H	-2.42666400	-1.57395900	3.05447600
C	-1.45739800	1.03009500	2.80018200
H	-0.67484600	1.80304400	2.75646200
H	-2.38075100	1.46045700	2.39947000
H	-1.63209800	0.80641000	3.87152200

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)

HF=-5045.5318625

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)

HF=-5046.574292

^{2}H-TS

UB3LYP-D3/def2-SVP-CPCM(THF)

Zero-point correction= 0.425172 (Hartree/Particle)

Thermal correction to Energy= 0.452637

Thermal correction to Enthalpy= 0.453581

Thermal correction to Gibbs Free Energy= 0.364426

Sum of electronic and zero-point Energies= -5044.568901

Sum of electronic and thermal Energies= -5044.541436

Sum of electronic and thermal Enthalpies= -5044.540492

Sum of electronic and thermal Free Energies= -5044.629648

Ni	-0.46974300	0.02068700	-0.41675500
C	-1.67999300	1.47643000	-0.71360400
C	-3.33826900	3.67087900	-1.45007500
C	-2.93718800	1.67823500	-0.11874800
C	-1.29229400	2.39258900	-1.71215700
C	-2.10400800	3.47523700	-2.07868300
C	-3.75171000	2.76341500	-0.46731700
H	-3.30482800	0.96789700	0.62514800
H	-0.32764400	2.26819500	-2.21592700
H	-1.76874500	4.16777600	-2.85720600
H	-4.72066300	2.89393800	0.02480100
N	1.12230200	1.19482600	0.05908800
C	3.44215700	2.57769300	0.86492300
C	1.07213100	2.49079000	0.40411800
C	2.31387300	0.55519600	0.12799900
C	3.48031900	1.22225200	0.51855700
C	2.19097300	3.20998100	0.80897500
N	1.02820200	-1.38687300	-0.39265100
C	3.26845500	-3.08892800	-0.43383200
C	0.88870200	-2.70292700	-0.60348100
C	2.26766600	-0.89109600	-0.17997300
C	3.39905200	-1.71348400	-0.20709000
C	1.96801900	-3.58059600	-0.62304700
H	0.09083200	2.95996400	0.35015300
H	4.42582100	0.68308600	0.57120700
H	2.08068200	4.26147400	1.08174800
H	-0.13439700	-3.04380200	-0.77330200
H	4.38996300	-1.28850400	-0.04812700
H	1.79076100	-4.64487400	-0.79103100
Br	-2.06051700	-1.42111000	-1.56489200
C	-0.76489300	-0.35275700	2.17087200
H	-3.97441700	4.51618300	-1.72696000
C	4.46631600	-3.99507300	-0.49511200
H	5.33972900	-3.55120300	0.00358500

H	4.25037000	-4.97063000	-0.03427000
H	4.74108900	-4.18581400	-1.54668100
C	4.68127100	3.32656200	1.26822300
H	4.47905600	3.99892200	2.11576100
H	5.49923900	2.64542300	1.54252400
H	5.03122800	3.95568200	0.43210800
C	0.50842700	-0.98541500	2.66028000
H	0.42913300	-1.17567500	3.75235700
H	0.71453000	-1.95213600	2.17918200
H	1.38256900	-0.32989800	2.52195900
C	-1.93737800	-1.28175200	2.04413200
H	-2.79048300	-0.81209200	1.53520400
H	-1.67886300	-2.18943100	1.47926000
H	-2.28243400	-1.59901300	3.05304200
C	-1.03843600	1.00820600	2.74490500
H	-0.15733500	1.66519500	2.67936800
H	-1.88232000	1.51224100	2.25590000
H	-1.28787500	0.91589500	3.82446800

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5308871
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5693344

^{2}H'

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.427088 (Hartree/Particle)
Thermal correction to Energy= 0.454746
Thermal correction to Enthalpy= 0.455691
Thermal correction to Gibbs Free Energy= 0.366759
Sum of electronic and zero-point Energies= -5044.582270
Sum of electronic and thermal Energies= -5044.554611
Sum of electronic and thermal Enthalpies= -5044.553667
Sum of electronic and thermal Free Energies= -5044.642599

C	2.72335600	0.70789700	0.18970800
C	3.75298800	-0.41261300	0.27880000
C	2.97297200	1.55139000	-1.06760500
H	3.70918900	-1.07763500	-0.59404700
H	3.61723800	-1.01751200	1.18615500
H	3.11295700	0.91777900	-1.95212800
H	2.16471200	2.26014100	-1.30123400
C	-1.70961900	1.57648700	-0.04686300
C	-2.65033500	2.60378800	0.11017800
C	-2.24023100	3.93516500	0.23146300
C	-0.85950600	4.17639400	0.18311300
C	0.01525300	3.10655200	0.02942200
C	-2.10728300	0.15486800	-0.20310600
C	-3.43402400	-0.28925800	-0.10788500
C	-3.73664600	-1.64641600	-0.26159800
C	-2.66328500	-2.51620700	-0.51343200
C	-1.37323800	-2.00530300	-0.59468700
H	-3.71474700	2.37279300	0.12957800
H	-0.46145000	5.18998600	0.26278000
H	1.08852400	3.28660900	-0.00950700
H	-4.23973900	0.41575000	0.09379700
H	-2.82910800	-3.58791500	-0.64141200
H	-0.51253300	-2.64608700	-0.79182700
N	-0.38202400	1.83068500	-0.07700800
N	-1.10205500	-0.70319200	-0.44673700
Br	1.50064300	-1.34350900	-2.30830600
Ni	0.86324300	0.01931200	-0.25483600
C	0.82842000	-0.73700000	1.51091600
C	0.23013700	-0.08929800	2.59837300
C	1.21218600	-2.07747200	1.64691200
C	0.02519700	-0.76720800	3.80788300
H	-0.07727800	0.95631400	2.50930000
C	1.00946900	-2.75990800	2.85462700
H	1.67143400	-2.59586100	0.79964700
H	-0.44213800	-0.24725900	4.64978200
H	1.31577900	-3.80640300	2.94602500
C	0.41579000	-2.10526800	3.94016600
H	0.25773600	-2.63455900	4.88374000
C	-3.22289900	5.06030200	0.39531800
H	-3.13734000	5.77041300	-0.44331400
H	-4.25907000	4.69732800	0.43832600
H	-3.01158100	5.62624400	1.31685800
C	-5.14604400	-2.16100000	-0.16329600
H	-5.45402400	-2.62397900	-1.11504700
H	-5.22023800	-2.94123900	0.61121900
H	-5.85899800	-1.36057200	0.07871800
H	4.76852300	0.02874600	0.32310300
H	3.89106400	2.15487300	-0.92408400
C	2.77608100	1.55777200	1.45779800
H	1.92937700	2.24961100	1.55717100
H	2.78584400	0.93211000	2.36012000
H	3.70125000	2.16594700	1.45988300

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5387051
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5811753

^{2}I'-TS

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.426807 (Hartree/Particle)
Thermal correction to Energy= 0.453769
Thermal correction to Enthalpy= 0.454713
Thermal correction to Gibbs Free Energy= 0.366959
Sum of electronic and zero-point Energies= -5044.567409
Sum of electronic and thermal Energies= -5044.540447
Sum of electronic and thermal Enthalpies= -5044.539502
Sum of electronic and thermal Free Energies= -5044.627257

C	2.47756700	0.52963500	0.50619500
C	3.59074200	-0.50541300	0.62937500
C	2.69296100	1.27633000	-0.83597600
H	3.50650100	-1.27055700	-0.15537000
H	3.59625100	-0.99952600	1.61104300
H	2.89116500	0.58777800	-1.66519700
H	1.87756200	1.94478300	-1.14710300
C	-2.00954800	1.50230600	-0.13993600
C	-2.94484600	2.52885500	0.05036000
C	-2.53057300	3.85937000	0.16696800

C	-1.15101300	4.10093700	0.08094300
C	-0.28187800	3.03329200	-0.11364300
C	-2.40652900	0.07676900	-0.26387500
C	-3.70782000	-0.38689300	-0.02447700
C	-4.00335400	-1.74934200	-0.14650300
C	-2.94968800	-2.60226100	-0.51360000
C	-1.68261200	-2.07229100	-0.73146100
H	-4.00836400	2.29638700	0.09838000
H	-0.75091100	5.11370200	0.16189500
H	0.79136600	3.21327800	-0.18329100
H	-4.49584300	0.30491700	0.27245700
H	-3.11289100	-3.67649700	-0.62411400
H	-0.83301300	-2.69688500	-1.01558600
N	-0.68378500	1.75827400	-0.22123600
N	-1.41708500	-0.76567600	-0.61231500
Br	1.40168200	-1.60311700	-2.29320600
Ni	0.51705700	-0.02284900	-0.48947000
C	0.89376300	-0.62924200	1.28296600
C	0.15210500	-0.03739800	2.32491800
C	1.14006200	-2.01494600	1.35357400
C	-0.36135300	-0.80750500	3.37237100
H	-0.05846300	1.03243100	2.30102800
C	0.62738700	-2.78433700	2.40279400
H	1.69961200	-2.49969600	0.55288600
H	-0.95334000	-0.32388900	4.15510200
H	0.81577700	-3.86192800	2.42004200
C	-0.12792600	-2.18770600	3.41948900
H	-0.52755500	-2.78946600	4.23983300
C	-3.50767800	4.98413300	0.36577100
H	-3.45621400	5.69224200	-0.47742700
H	-4.54096600	4.61980500	0.44926900
H	-3.26263800	5.55310700	1.27705300
C	-5.38404000	-2.28838400	0.10891100
H	-5.77387800	-2.79393300	-0.78952600
H	-5.36298100	-3.03958400	0.91507700
H	-6.08872000	-1.49437900	0.39309300
H	4.56567300	0.00058500	0.50057000
H	3.58393500	1.92378900	-0.71775000
C	2.55206500	1.54057900	1.64884500
H	1.72780400	2.26708000	1.62507400
H	2.54372100	1.05494100	2.63426500
H	3.49408500	2.11235900	1.56275600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5303702
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5662454

^{2}I-TS

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.422563 (Hartree/Particle)
Thermal correction to Energy= 0.451102
Thermal correction to Enthalpy= 0.452046
Thermal correction to Gibbs Free Energy= 0.358259
Sum of electronic and zero-point Energies= -5044.535437
Sum of electronic and thermal Energies= -5044.506898
Sum of electronic and thermal Enthalpies= -5044.505954
Sum of electronic and thermal Free Energies= -5044.599741

Ni	1.15698000	0.80313900	-0.58477500
C	2.32848100	0.33814200	0.92428500
C	5.11920600	0.20086500	1.49479100
C	3.04155200	1.45126300	1.43037300
C	3.07877700	-0.84127500	0.69778300
C	4.44572700	-0.91665100	0.98020600
C	4.40990400	1.38942900	1.71551000
H	2.50862100	2.39036600	1.62008700
H	2.57443100	-1.73002300	0.30029100
H	4.99329200	-1.84687500	0.79755300
H	4.92832600	2.26924700	2.11004400
N	-0.40671000	1.93537300	0.04765400
C	-2.69659900	3.26224200	0.96611900
C	-0.33012700	3.19445800	0.49328600
C	-1.60084200	1.30443100	0.03778200
C	-2.75851900	1.94552700	0.49241800
C	-1.43981300	3.89018500	0.96037900
N	-0.34382800	-0.53554700	-0.82382800
C	-2.55499400	-2.24308600	-1.00356100
C	-0.20010200	-1.78530500	-1.27722900
C	-1.56646500	-0.09342900	-0.46128400
C	-2.68807300	-0.92631400	-0.54461700
C	-1.26934200	-2.66854900	-1.37809500
H	0.66285300	3.65020900	0.47535400
H	-3.71494700	1.42282200	0.48486800
H	-1.32455100	4.91485400	1.31930300
H	0.81230000	-2.07394900	-1.57021900
H	-3.67063500	-0.55699600	-0.25052300
H	-1.10182100	-3.68134400	-1.74991400
Br	2.04109800	1.26858800	-2.81423400
C	0.90892800	-0.32085900	2.89960800
C	2.06565600	-0.62608100	3.80419000
C	0.14137600	0.92248900	3.22797600
H	2.70749700	0.25543600	3.95657700
H	2.69217600	-1.43948000	3.40736200
H	0.79502900	1.81017100	3.24348300
H	-0.67731400	1.10772600	2.52043400
H	6.18789400	0.14581000	1.71989400
C	-3.73205600	-3.17533400	-1.08137800
H	-3.75552200	-3.69814800	-2.05004800
H	-3.65572600	-3.94915500	-0.29912400
H	-4.68451900	-2.64474300	-0.94359900
C	-3.92289200	3.98596800	1.44833600
H	-4.78181200	3.30884900	1.55526400
H	-3.73480200	4.47411400	2.41718100
H	-4.20010800	4.78067500	0.73558800
C	0.14094900	-1.50531600	2.39991100
H	-0.66437500	-1.21879700	1.71091100
H	0.79774500	-2.22523500	1.88452900
H	-0.33165900	-2.05264400	3.24444900
H	-0.31389900	0.84612700	4.23935000
H	1.69877500	-0.94589100	4.80346700

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.4957062
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5367812

^{4}I-TS

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.423090 (Hartree/Particle)
Thermal correction to Energy= 0.450907
Thermal correction to Enthalpy= 0.451851
Thermal correction to Gibbs Free Energy= 0.361396
Sum of electronic and zero-point Energies= -5044.542031
Sum of electronic and thermal Energies= -5044.514215
Sum of electronic and thermal Enthalpies= -5044.513270
Sum of electronic and thermal Free Energies= -5044.603726

Ni	1.00135600	1.42580000	0.04129900
C	2.02000000	0.07814700	1.17453600
C	3.93315500	-2.07728400	1.15319100
C	3.43288500	0.29828400	1.02085000
C	1.63092500	-1.30446900	1.21498900
C	2.55286200	-2.34444500	1.23634800
C	4.35898900	-0.74276500	1.03278300
H	3.79393400	1.32489200	0.90185400
H	0.56512100	-1.55255200	1.24828500
H	2.20252300	-3.38075100	1.29090300
H	5.42643100	-0.52063300	0.92890300
N	-0.89401700	2.03940500	0.51380700
C	-3.56934600	2.63784800	1.09908700
C	-1.21167500	3.15802500	1.18217100
C	-1.87998700	1.21421900	0.09068800
C	-3.22327800	1.48924400	0.38009700
C	-2.52195100	3.49173000	1.49550500
N	-0.09733200	0.04534000	-0.98052000
C	-1.72321000	-2.06579300	-1.84944700
C	0.42587200	-0.97644000	-1.67241200
C	-1.41869300	0.04577700	-0.68977000
C	-2.24981100	-0.99990400	-1.11028500
C	-0.34489300	-2.03680300	-2.13142800
H	-0.37158200	3.79948600	1.45667900
H	-4.00678500	0.81553400	0.03241500
H	-2.72889600	4.41386500	2.04218700
H	1.50289900	-0.93420300	-1.84772000
H	-3.31006400	-0.99346900	-0.85626500
H	0.12601800	-2.84155600	-2.69960600
Br	2.10369000	3.55939100	-0.38470900
C	1.60926300	0.73058300	3.23513900
C	2.54956500	-0.10886100	4.05616600
C	1.93791500	2.19806400	3.21829800
H	3.60092400	0.08623000	3.79444600
H	2.35480700	-1.18411500	3.92224600
H	2.99142400	2.37533000	2.95440400
H	1.32098100	2.75065800	2.49722400
H	4.65885800	-2.89498300	1.15903700
C	-2.58235200	-3.20804900	-2.31633900
H	-3.63844800	-3.06244600	-2.04961600
H	-2.51152600	-3.32503800	-3.40984200
H	-2.23976200	-4.15626900	-1.87026900
C	-4.99807700	2.96615500	1.43148300
H	-5.69656700	2.22517400	1.01846500
H	-5.13933800	3.00560100	2.52409000
H	-5.26879600	3.95941000	1.03818500
C	0.15182100	0.40560400	3.42019600
H	-0.46414900	0.87526500	2.64206100
H	-0.02996500	-0.67959200	3.39789400
H	-0.20509700	0.78000400	4.40156300
H	1.76418400	2.64050000	4.22078000
H	2.42471500	0.12233500	5.13414200

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.4932847
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5389644

^{2}L-TS

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.422923 (Hartree/Particle)
Thermal correction to Energy= 0.451544
Thermal correction to Enthalpy= 0.452488
Thermal correction to Gibbs Free Energy= 0.356259
Sum of electronic and zero-point Energies= -5044.541704
Sum of electronic and thermal Energies= -5044.513083
Sum of electronic and thermal Enthalpies= -5044.512138
Sum of electronic and thermal Free Energies= -5044.608368

Ni	-0.42182000	0.28394900	0.52338800
C	-1.80483100	1.59839400	0.08222800
C	-3.75127500	3.55126000	-0.71046800
C	-3.11085500	1.62512200	0.62313500
C	-1.52534800	2.60154000	-0.87716700
C	-2.46877300	3.56119400	-1.27153000
C	-4.06879200	2.57418800	0.24189900
H	-3.38188200	0.88078600	1.38049600
H	-0.52897400	2.64102100	-1.33505300
H	-2.20361700	4.31984100	-2.01585000
H	-5.06786900	2.55682500	0.69094200
N	1.38089900	1.24846600	0.65316400
C	3.94018900	2.39158400	0.67012700
C	1.53603800	2.56455300	0.83111200
C	2.47049700	0.46895700	0.48739400
C	3.75881600	1.01414900	0.48322500
C	2.78796100	3.17384400	0.85031300
N	0.86296800	-1.29176100	0.35058000
C	2.78615500	-3.31968700	0.11769000
C	0.49414600	-2.57644000	0.27451100
C	2.17591600	-0.98024300	0.33754200
C	3.15617800	-1.97280700	0.21740800
C	1.41223400	-3.61388500	0.15535900
H	0.61307200	3.13688900	0.95197000
H	4.62822500	0.37261300	0.33671800
H	2.86288300	4.25292500	1.00057900
H	-0.58091200	-2.76685800	0.32347700
H	4.21293800	-1.70438900	0.20897700
H	1.05973000	-4.64567000	0.09425500
C	-1.70339200	-1.51724700	4.95922900
H	-4.49368300	4.29747100	-1.00910500
C	3.80773700	-4.41465600	-0.01957800
H	4.83431000	-4.02383000	0.01188900
H	3.69193600	-5.15735300	0.78619000
H	3.67032500	-4.95176500	-0.97237900
C	5.31233900	3.00659900	0.70318300

H	5.61477600	3.20019900	1.74652000
H	6.06663800	2.34633500	0.25205200
H	5.32697200	3.97333400	0.17749400
C	-3.17908900	-1.74559500	4.77101000
H	-3.72436000	-0.79764000	4.64426200
H	-3.38258300	-2.38384100	3.89725400
H	-3.59803200	-2.25610000	5.66316200
C	-0.85347500	-2.75976100	4.94519400
H	0.22032000	-2.51700700	4.94208600
H	-1.05765300	-3.36614900	5.85213700
H	-1.07002500	-3.38925900	4.06831700
C	-1.33700500	-0.49842700	6.00492700
H	-1.58017900	-0.89104400	7.01440800
H	-0.26032500	-0.26896400	5.98909400
H	-1.89570700	0.44068200	5.87117300
Br	-1.07018600	-0.42224200	2.89432600

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5045.5065849
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-5046.5454233

^2P_B
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.214708 (Hartree/Particle)
Thermal correction to Energy= 0.230876
Thermal correction to Enthalpy= 0.231820
Thermal correction to Gibbs Free Energy= 0.166322
Sum of electronic and zero-point Energies= -4655.579462
Sum of electronic and thermal Energies= -4655.563294
Sum of electronic and thermal Enthalpies= -4655.562349
Sum of electronic and thermal Free Energies= -4655.627848

Ni	-3.99183200	1.30009300	-1.54653000
C	-1.87359800	-0.39708200	-0.83451100
C	-0.60463100	-0.81497600	-0.41773600
C	0.38038200	0.12429500	-0.09164500
C	0.02971800	1.48282700	-0.20377800
C	-1.24637600	1.83242200	-0.62458000
C	-2.97912600	-1.31121800	-1.19958100
C	-2.90514100	-2.70937500	-1.17420400
C	-4.01531200	-3.47922700	-1.54213400
C	-5.17917400	-2.78948900	-1.92940000
C	-5.18373000	-1.39947400	-1.93172800
H	-0.37768600	-1.87943400	-0.34653600
H	0.75171100	2.26661600	0.03582700
H	-1.54668200	2.87837300	-0.72245500
H	-1.98301600	-3.20525100	-0.86858000
H	-6.07708900	-3.33486700	-2.22820500
H	-6.06484300	-0.82279400	-2.22618200
N	-2.18757800	0.92199600	-0.93709400
N	-4.11313300	-0.67488700	-1.57617200
C	1.75486100	-0.28579000	0.36089600
H	1.95781900	0.09097300	1.37696900
H	1.87445700	-1.37835300	0.36807700
H	2.52660300	0.14347000	-0.29878000
C	-3.97959500	-4.98297800	-1.52479800
H	-2.98906900	-5.36658100	-1.24261000
H	-4.71990400	-5.37924000	-0.81035300
H	-4.24149600	-5.38984900	-2.51492300
Br	-5.83964900	2.56755300	-2.20535500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4656.2756634
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-4656.9610627

***t*Bu-Ph**
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.212552 (Hartree/Particle)
Thermal correction to Energy= 0.222172
Thermal correction to Enthalpy= 0.223116
Thermal correction to Gibbs Free Energy= 0.178247
Sum of electronic and zero-point Energies= -389.034504
Sum of electronic and thermal Energies= -389.024885
Sum of electronic and thermal Enthalpies= -389.023940
Sum of electronic and thermal Free Energies= -389.068810

C	0.04421000	1.70961600	1.14572500
C	1.44490300	1.73358100	1.12055900
C	2.12656700	2.88889000	0.73341700
C	1.38993500	4.02254300	0.37071900
C	-0.00591100	3.99264800	0.39798600
C	-0.71318100	2.83690300	0.78576000
H	-0.45028400	0.78804600	1.45338500
H	2.00284900	0.83794100	1.40728300
H	3.21924500	2.90824800	0.71359200
H	1.90528600	4.93693000	0.06433300
H	-0.55299400	4.89314100	0.10924100
C	-2.25333700	2.84939200	0.79950700
C	-2.74935100	3.94948800	1.76551900
H	-2.40180400	4.94892000	1.46299200
H	-3.85134000	3.97127700	1.78683700
H	-2.39094800	3.76208800	2.79042100
C	-2.84401600	1.50472700	1.25836000
H	-3.94379100	1.56138300	1.25324000
H	-2.55073000	0.67977000	0.59043900
H	-2.52933600	1.24749100	2.28192300
C	-2.77455500	3.14452300	-0.62558100
H	-3.87683800	3.15946900	-0.63495500
H	-2.42445300	4.11964200	-0.99703000
H	-2.43723000	2.37132500	-1.33443100

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-389.3290308
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-389.6748001

^2P_C
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.303134 (Hartree/Particle)
Thermal correction to Energy= 0.322860

Thermal correction to Enthalpy= 0.323805
Thermal correction to Gibbs Free Energy= 0.250611
Sum of electronic and zero-point Energies= -2313.026966
Sum of electronic and thermal Energies= -2313.007240
Sum of electronic and thermal Enthalpies= -2313.006296
Sum of electronic and thermal Free Energies= -2313.079489

Ni	-3.96398300	1.44675100	-1.21509900
C	-1.83575500	-0.36900700	-0.73179300
C	-0.55130400	-0.83036800	-0.42006200
C	0.43164200	0.05760500	0.03112800
C	0.06264200	1.41025300	0.15257000
C	-1.22735300	1.80375600	-0.17808400
C	-2.94328000	-1.23262600	-1.20069300
C	-2.85927000	-2.62301000	-1.34872800
C	-3.97607300	-3.35335800	-1.77274900
C	-5.15577000	-2.63260900	-2.03077500
C	-5.16546600	-1.25120500	-1.86635600
H	-0.31078600	-1.88864300	-0.52848300
H	0.78098300	2.15531600	0.50175800
H	-1.53996000	2.84781500	-0.09948800
H	-1.92710500	-3.14475700	-1.12852900
H	-6.06285900	-3.14566800	-2.35800600
H	-6.06078500	-0.65514500	-2.05962300
N	-2.16615900	0.94343400	-0.61445400
N	-4.08728100	-0.56287300	-1.46861500
C	1.82261900	-0.39985100	0.37491200
H	2.05670900	-0.17550000	1.42863300
H	1.94941500	-1.48000600	0.21584000
H	2.56967500	0.13060300	-0.23804800
C	-3.92851700	-4.84679700	-1.94782400
H	-2.95001600	-5.26161200	-1.66768600
H	-4.70238900	-5.33564400	-1.33408100
H	-4.13207500	-5.11973300	-2.99640100
C	-5.53228400	2.36315800	-1.90331200
C	-6.16411500	3.46923000	-1.27984400
C	-6.13057200	1.95132100	-3.12227500
C	-7.29512300	4.10503900	-1.81103500
H	-5.75841000	3.85373800	-0.33612700
C	-7.25947700	2.57286700	-3.67293800
H	-5.69267000	1.10759400	-3.66945300
C	-7.85243900	3.65805100	-3.01549200
H	-7.74560100	4.95361600	-1.28450500
H	-7.67970900	2.21192800	-4.61812500
H	-8.73512500	4.14906300	-3.43623300

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2313.662927
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2314.4257224

***t*Bu-Br**
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.121249 (Hartree/Particle)
Thermal correction to Energy= 0.127905
Thermal correction to Enthalpy= 0.128849
Thermal correction to Gibbs Free Energy= 0.090653
Sum of electronic and zero-point Energies= -2731.509462
Sum of electronic and thermal Energies= -2731.502806
Sum of electronic and thermal Enthalpies= -2731.501862
Sum of electronic and thermal Free Energies= -2731.540058

Br	0.66845300	-3.32582400	-0.02012300
C	-0.35404100	-1.55353000	-0.02192100
C	0.09890600	-0.79012700	-1.26110700
H	-0.13485200	-1.34337700	-2.18230000
H	-0.43396200	0.17601100	-1.29443400
H	1.17917200	-0.58596100	-1.23527900
C	-1.83589000	-1.90706100	-0.07308600
H	-2.13789300	-2.49998800	0.80239100
H	-2.42204700	-0.97172100	-0.07532100
H	-2.08349000	-2.47031100	-0.98450400
C	0.02110100	-0.83233800	1.26757900
H	-0.51694000	0.13087300	1.30189300
H	-0.26517900	-1.41745400	2.15359400
H	1.10013000	-0.62515900	1.31345500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2731.8563155
UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2732.1242505

Table A1.2
1-adamantyl radical
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.121249 (Hartree/Particle)
Thermal correction to Energy= 0.127905
Thermal correction to Enthalpy= 0.128849
Thermal correction to Gibbs Free Energy= 0.090653
Sum of electronic and zero-point Energies= -2731.509462
Sum of electronic and thermal Energies= -2731.502806
Sum of electronic and thermal Enthalpies= -2731.501862
Sum of electronic and thermal Free Energies= -2731.540058

Br	0.66845300	-3.32582400	-0.02012300
C	-0.35404100	-1.55353000	-0.02192100
C	0.09890600	-0.79012700	-1.26110700
H	-0.13485200	-1.34337700	-2.18230000
H	-0.43396200	0.17601100	-1.29443400
H	1.17917200	-0.58596100	-1.23527900
C	-1.83589000	-1.90706100	-0.07308600
H	-2.13789300	-2.49998800	0.80239100
H	-2.42204700	-0.97172100	-0.07532100
H	-2.08349000	-2.47031100	-0.98450400
C	0.02110100	-0.83233800	1.26757900
H	-0.51694000	0.13087300	1.30189300
H	-0.26517900	-1.41745400	2.15359400
H	1.10013000	-0.62515900	1.31345500

UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2731.8563155

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF=-2732.1242505

Figure A1.9 (with Becke-Johnson damping)

[1]G

UB3LYP-D3BJ/def2-SVP-CPCM(THF)
Zero-point correction= 0.306461 (Hartree/Particle)
Thermal correction to Energy= 0.326798
Thermal correction to Enthalpy= 0.327742
Thermal correction to Gibbs Free Energy= 0.253612
Sum of electronic and zero-point Energies= -4887.034664
Sum of electronic and thermal Energies= -4887.014327
Sum of electronic and thermal Enthalpies= -4887.013383
Sum of electronic and thermal Free Energies= -4887.087513

Ni	-4.61455800	0.39141800	-0.38378100
C	-6.47995100	0.32752600	-0.64642700
C	-7.06929100	0.72563800	-1.85950000
C	-7.32573900	-0.19722300	0.34733000
C	-8.44464000	0.58283800	-2.08288600
H	-6.44788200	1.15381400	-2.65241400
C	-8.70232500	-0.34109800	0.13197000
H	-6.90771400	-0.51094000	1.30937600
C	-9.26861600	0.04583400	-1.08749400
H	-8.87587500	0.89543900	-3.03877400
H	-9.33600100	-0.75704500	0.92114600
H	-10.34235900	-0.06639400	-1.25931300
Br	-4.83954100	2.61489600	0.34890300
C	-2.08006400	-0.92116800	-0.45758300
C	-0.71658600	-1.19386200	-0.31567800
C	0.14713300	-0.21566200	0.18983700
C	-0.42098800	1.02026200	0.53406200
C	-1.78653700	1.22356800	0.36804800
C	-3.06510700	-1.88765800	-0.98117200
C	-2.72565700	-3.17109000	-1.41575200
C	-3.70626600	-4.03929000	-1.90596700
C	-5.02125000	-3.55308100	-1.93323700
C	-5.29618900	-2.26681600	-1.48742800
H	-0.31865600	-2.16867700	-0.59552600
H	0.19699500	1.82707600	0.93279300
H	-2.26735000	2.17027400	0.62492300
H	-1.68801300	-3.50015800	-1.37533500
H	-5.84024600	-4.17312400	-2.30241600
H	-6.31123600	-1.87427200	-1.50210400
N	-2.60198000	0.27710900	-0.11591900
N	-4.34663200	-1.43785100	-1.01661200
C	1.61663500	-0.47344500	0.36269600
H	1.89776400	-0.40195800	1.42590300
H	1.90088100	-1.46896700	-0.00428500
H	2.20936800	0.28185300	-0.17712700
C	-3.37343200	-5.42157500	-2.38792100
H	-3.59867400	-5.51805300	-3.46249700
H	-2.31286900	-5.66220400	-2.23393200
H	-3.98429000	-6.17334000	-1.86370600

[3]G

UB3LYP-D3BJ/def2-SVP-CPCM(THF)
Zero-point correction= 0.305082 (Hartree/Particle)
Thermal correction to Energy= 0.327019
Thermal correction to Enthalpy= 0.327963
Thermal correction to Gibbs Free Energy= 0.246939
Sum of electronic and zero-point Energies= -4887.032375
Sum of electronic and thermal Energies= -4887.010439
Sum of electronic and thermal Enthalpies= -4887.009494
Sum of electronic and thermal Free Energies= -4887.090519

C	-1.67439600	0.90308300	-0.64637300
C	-1.84605600	0.00921700	0.42800600
C	-3.07766900	-0.67227900	0.49143500
C	-4.08768700	-0.47102500	-0.45923300
C	-3.88787800	0.42453000	-1.51520600
C	-2.67264600	1.11236300	-1.60688000
Br	-0.90109600	-2.16723900	3.30580200
H	-3.25387400	-1.38515300	1.30419200
H	-0.73615300	1.46023800	-0.75016000
H	-2.50304800	1.81374400	-2.43003000
H	-4.67130500	0.58428500	-2.26125500
H	-5.03298000	-1.01689000	-0.37771600
C	1.99355600	0.06542900	0.28566900
C	1.37074100	-2.17251900	0.20732800
C	2.44074900	-2.48947000	-0.62142100
C	3.33200200	-1.47888000	-1.01880900
C	3.08937000	-0.18348100	-0.54637800
C	1.65209400	1.39945800	0.83712100
C	0.17967400	2.57976100	2.18952000
C	0.83585100	3.77934100	1.94024000
C	1.95525000	3.79245000	1.09192400
C	2.35588900	2.57050500	0.53879900
H	0.65892000	-2.92818700	0.54830100
H	2.58098600	-3.51968000	-0.95371900
H	3.76239000	0.62605000	-0.82761700
H	-0.70242300	2.53971100	2.83335800
H	0.47388300	4.69967200	2.40212200
H	3.21583000	2.53874300	-0.12966200
N	1.15583200	-0.92758900	0.64512400
N	0.58069100	1.41995500	1.65742100
Ni	-0.43284100	-0.35400600	1.76916300
C	2.67656200	5.07255000	0.78089400
H	3.61042600	4.89040300	0.23203700
H	2.03937000	5.72984800	0.16640500
H	2.91062900	5.62385500	1.70458600
C	4.49472400	-1.78212000	-1.92015900
H	5.15539700	-0.91255100	-2.03768400
H	5.08551300	-2.62309900	-1.52506400
H	4.13702000	-2.08132800	-2.91901300

[2]H'

UB3LYP-D3BJ/def2-SVP-CPCM(THF)
Zero-point correction= 0.426844 (Hartree/Particle)
Thermal correction to Energy= 0.454721
Thermal correction to Enthalpy= 0.455665
Thermal correction to Gibbs Free Energy= 0.365748
Sum of electronic and zero-point Energies= -5044.644159

Sum of electronic and thermal Energies= -5044.616282
Sum of electronic and thermal Enthalpies= -5044.615338
Sum of electronic and thermal Free Energies= -5044.705255

C	2.71091400	0.70133000	0.17596900
C	3.72349900	-0.43154200	0.28402500
C	2.98998400	1.53526600	-1.08049000
H	3.67687400	-1.10725700	-0.58063800
H	3.57774000	-1.02143400	1.19949200
H	3.15682700	0.89559100	-1.95584100
H	2.18550900	2.23884300	-1.34152700
C	-1.69402700	1.55618600	-0.04726500
C	-2.63173800	2.57677800	0.15141200
C	-2.22064200	3.90684800	0.27641200
C	-0.84314500	4.15306100	0.18713200
C	0.03023000	3.08910500	-0.00498100
C	-2.09021700	0.13838900	-0.21383300
C	-3.41303500	-0.30945800	-0.10707200
C	-3.71271400	-1.66483200	-0.27611500
C	-2.64112400	-2.52694500	-0.55775500
C	-1.35382900	-2.01254400	-0.65025000
H	-3.69370500	2.34105200	0.20160700
H	-0.44643100	5.16687700	0.26539300
H	1.10083200	3.27379300	-0.07558200
H	-4.21723300	0.39093900	0.11374100
H	-2.80673000	-3.59632400	-0.70153300
H	-0.49597000	-2.64747600	-0.87629200
N	-0.36945900	1.81503100	-0.11266300
N	-1.08673700	-0.71263200	-0.48381700
Br	1.50821600	-1.31897800	-2.33001600
Ni	0.85259800	0.02307700	-0.28079500
C	0.79730100	-0.69864000	1.49793900
C	0.19519200	-0.03263100	2.57163300
C	1.17579900	-2.03728600	1.66018800
C	-0.01918000	-0.68997200	3.79003700
H	-0.10878200	1.01265000	2.47201700
C	0.96369600	-2.69875500	2.87698900
H	1.63990400	-2.57691200	0.82945200
H	-0.48937000	-0.15415600	4.61983500
H	1.26665300	-3.74406700	2.98682800
C	0.36551400	-2.02585000	3.94750800
H	0.19984000	-2.53889000	4.89826300
C	-3.20164200	5.02385800	0.48646100
H	-3.13626200	5.75429200	-0.33587700
H	-4.23415500	4.65350500	0.54162900
H	-2.97452000	5.56770700	1.41724000
C	-5.11835800	-2.18248600	-0.16317700
H	-5.43728700	-2.64475300	-1.11124400
H	-5.18275500	-2.96280500	0.61179300
H	-5.82734500	-1.38202800	0.08820300
H	4.74437300	-0.00292000	0.32699200
H	3.90056500	2.14439200	-0.91590400
C	2.76897100	1.55791900	1.43739900
H	1.95083600	2.28612000	1.51619100
H	2.74202400	0.94099800	2.34489300
H	3.71643100	2.13055100	1.44891200

^{2}I'-TS
UB3LYP-D3BJ/def2-SVP-CPCM(THF)

Zero-point correction= 0.426726 (Hartree/Particle)
Thermal correction to Energy= 0.453765
Thermal correction to Enthalpy= 0.454709
Thermal correction to Gibbs Free Energy= 0.366635
Sum of electronic and zero-point Energies= -5044.630260
Sum of electronic and thermal Energies= -5044.603220
Sum of electronic and thermal Enthalpies= -5044.602276
Sum of electronic and thermal Free Energies= -5044.690350

C	2.44567300	0.53879700	0.51789700
C	3.55988700	-0.48320800	0.69515100
C	2.69124800	1.26143600	-0.82820000
H	3.51406200	-1.25983000	-0.08110200
H	3.53199200	-0.96353900	1.68286000
H	2.97872300	0.55874900	-1.61770900
H	1.84801100	1.85518400	-1.21171100
C	-1.97392900	1.50906500	-0.14440500
C	-2.90744400	2.53108100	0.06641500
C	-2.49476400	3.86306000	0.16272800
C	-1.11973300	4.10986300	0.03412600
C	-0.25100100	3.04575600	-0.17615500
C	-2.36794500	0.08522200	-0.26140900
C	-3.65266100	-0.38646800	0.03509500
C	-3.94659600	-1.74822600	-0.09126900
C	-2.90999100	-2.58957500	-0.52593500
C	-1.65662000	-2.05212900	-0.79547800
H	-3.96773700	2.29311700	0.14331500
H	-0.72282900	5.12494000	0.09412100
H	0.81856500	3.23114600	-0.27955900
H	-4.42648800	0.29800700	0.38125300
H	-3.07541100	-3.66202900	-0.64685900
H	-0.81926500	-2.66854200	-1.13014400
N	-0.65260300	1.76954400	-0.26060600
N	-1.39242000	-0.74687800	-0.66659600
Br	1.43767500	-1.57408300	-2.31924700
Ni	0.52937800	0.00131100	-0.52962500
C	0.85280700	-0.63865600	1.24830300
C	0.09354700	-0.06193700	2.28413400
C	1.10655300	-2.02232200	1.30784000
C	-0.43862000	-0.84744200	3.31019100
H	-0.11698500	1.00807500	2.27819200
C	0.57567900	-2.80689800	2.33566600
H	1.68758200	-2.49660000	0.51628400
H	-1.04554100	-0.37555300	4.08810000
H	0.76942900	-3.88326900	2.34387300
C	-0.20357300	-2.22681000	3.34286400
H	-0.61848600	-2.84046300	4.14613200
C	-3.47141200	4.98238300	0.38274900
H	-3.43766600	5.69516600	-0.45690500
H	-4.50023900	4.61061200	0.48136200
H	-3.21471500	5.54710100	1.29320600
C	-5.30712300	-2.29630900	0.23476800
H	-5.71999000	-2.85009600	-0.62328000
H	-5.24523600	-3.00657000	1.07528700
H	-6.01222800	-1.49930600	0.50773000
H	4.53399100	0.03065800	0.59548900
H	3.52402500	1.97625100	-0.68136900
C	2.46599700	1.56065500	1.64871200

H	1.63202800	2.27372300	1.59353400
H	2.43495200	1.08311300	2.63716600
H	3.40078300	2.14669100	1.58526300

Figure A1.11
TS-HAT (*t*Bu with THF)
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.229357 (Hartree/Particle)
Thermal correction to Energy= 0.240955
Thermal correction to Enthalpy= 0.241899
Thermal correction to Gibbs Free Energy= 0.191011
Sum of electronic and zero-point Energies= -389.737578
Sum of electronic and thermal Energies= -389.725980
Sum of electronic and thermal Enthalpies= -389.725036
Sum of electronic and thermal Free Energies= -389.775924

C	-1.44189600	-5.62124800	-0.67071100
C	-0.61480900	-5.32477500	-1.90511300
H	0.42581800	-5.67253000	-1.79015200
H	-1.03222900	-5.82984500	-2.79962000
H	-0.58926400	-4.24371200	-2.12344100
C	-2.83311600	-5.02126000	-0.70209400
H	-3.44082800	-5.45479900	-1.52205400
H	-3.37638700	-5.20671800	0.23949800
H	-2.79434600	-3.93056700	-0.85593700
C	-1.39181600	-7.06756400	-0.22146500
H	-0.35337000	-7.42058800	-0.10399400
H	-1.91094600	-7.21344800	0.74069000
H	-1.88170500	-7.73489100	-0.95970900
H	-0.81877200	-4.90191300	0.32518700
C	-0.33452700	-4.09984500	1.30392300
O	-1.24547200	-3.04426000	1.45253600
C	-0.33630300	-4.89587900	2.59470000
H	0.63069200	-3.73694500	0.91889100
C	-2.10155200	-3.29099300	2.57721000
C	-1.79547200	-4.71958900	3.04322000
H	0.35604400	-4.45544600	3.33635100
H	-0.04777600	-5.94793800	2.44839100
H	-1.87162600	-2.55110400	3.36634100
H	-3.15091700	-3.14936800	2.27110800
H	-1.94582300	-4.85268400	4.12428800
H	-2.44122600	-5.44128100	2.51794600

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -390.4090221
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -390.0778207

***t*Bu–*t*Bu**
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.243588 (Hartree/Particle)
Thermal correction to Energy= 0.253800
Thermal correction to Enthalpy= 0.254744
Thermal correction to Gibbs Free Energy= 0.210503
Sum of electronic and zero-point Energies= -315.255129
Sum of electronic and thermal Energies= -315.244917
Sum of electronic and thermal Enthalpies= -315.243973
Sum of electronic and thermal Free Energies= -315.288214

C	-2.41708000	-0.14457300	0.06622800
C	-0.88402500	-0.24743600	-0.08529400
H	-2.74165800	0.88150100	0.29535000
H	-2.94544800	-0.47308000	-0.84217800
H	-2.75610000	-0.78736300	0.89495100
C	-0.51590700	-1.74621100	-0.13042400
C	-0.24575200	0.35513700	1.18492900
H	0.55546200	-1.90306300	-0.32988500
H	-0.74310900	-2.21871100	0.83915500
H	-1.08705800	-2.28817800	-0.89894500
H	-0.70779400	-0.08687200	2.08277100
H	0.83422400	0.15250100	1.24049600
H	-0.39027400	1.44511100	1.24399800
C	-0.38354500	0.50698200	-1.39515200
C	-1.02342000	1.90725400	-1.51033200
C	1.14931300	0.69016800	-1.38276200
C	-0.75168200	-0.28406100	-2.66911300
H	-2.10296400	1.85183000	-1.71534600
H	-0.88128800	2.50327700	-0.59565000
H	-0.56103700	2.46448200	-2.34135800
H	1.67895000	-0.26049400	-1.21503400
H	1.48707500	1.08812900	-2.35358700
H	1.47371500	1.40115000	-0.60831800
H	-0.52342700	0.31783100	-3.56385600
H	-0.18082000	-1.22083700	-2.75183900
H	-1.82331800	-0.53448200	-2.70559900

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -315.8529126
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -315.5614974

Figure A1.12
^{2}J'-TS
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.328127 (Hartree/Particle)
Thermal correction to Energy= 0.347968
Thermal correction to Enthalpy= 0.348913
Thermal correction to Gibbs Free Energy= 0.279623
Sum of electronic and zero-point Energies= -2239.220375
Sum of electronic and thermal Energies= -2239.200534
Sum of electronic and thermal Enthalpies= -2239.199590
Sum of electronic and thermal Free Energies= -2239.268880

Ni	-4.61321300	0.86810700	-0.83470900
C	-5.09920600	2.52182300	0.29792100
C	-4.55216600	2.36939500	1.70282700
H	-4.74404000	1.36415800	2.10736000
H	-3.46927900	2.55485400	1.75648600
H	-5.03615100	3.10331500	2.37489000
C	-6.24127500	1.79571800	-0.07944700

H	-5.62378300	0.94464700	-1.87805000
H	-6.68945700	1.07302700	0.61440600
H	-6.94016700	2.20648100	-0.81286700
C	-4.78498200	3.83112300	-0.39198000
H	-3.70030100	4.01587900	-0.45027500
H	-5.18660100	3.85527800	-1.41595400
H	-5.21989000	4.68057300	0.16788600
C	-2.20522700	-0.58647000	-0.60403900
C	-0.85255000	-0.89231600	-0.31440800
C	0.03915300	0.09547400	0.07013200
C	-0.46446300	1.42555500	0.15669300
C	-1.79703900	1.66488700	-0.11083000
C	-3.17470400	-1.53453700	-1.08989400
C	-2.90900100	-2.88733300	-1.42387700
C	-3.92227300	-3.72644200	-1.85676900
C	-5.23232100	-3.17313400	-1.96101900
C	-5.42983800	-1.83926700	-1.66462100
H	-0.50950600	-1.92534500	-0.39587200
H	0.19020400	2.25523600	0.43172100
H	-2.19733800	2.67733000	-0.04657800
H	-1.88994200	-3.26940700	-1.34127500
H	-6.07577700	-3.79000100	-2.27829500
H	-6.41337500	-1.37414400	-1.76261000
N	-2.67878000	0.70624200	-0.47133900
N	-4.44404300	-1.02209100	-1.23617000
C	1.48007800	-0.19579000	0.38774600
H	1.72097600	0.09427000	1.42487200
H	1.72000200	-1.26210300	0.26533200
H	2.15178000	0.38656200	-0.26590500
C	-3.67659100	-5.16537400	-2.22023400
H	-4.31313100	-5.83586200	-1.61799400
H	-3.93272000	-5.35359100	-3.27696500
H	-2.62705600	-5.45514600	-2.06506800

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2240.5636168
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2239.8498736

^{2}J'

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.218542 (Hartree/Particle)
Thermal correction to Energy= 0.233345
Thermal correction to Enthalpy= 0.234289
Thermal correction to Gibbs Free Energy= 0.174716
Sum of electronic and zero-point Energies= -2082.200898
Sum of electronic and thermal Energies= -2082.186094
Sum of electronic and thermal Enthalpies= -2082.185150
Sum of electronic and thermal Free Energies= -2082.244723

Ni	-4.14128400	1.35473100	-1.69261700
H	-5.44683100	2.14366100	-2.15615700
C	-1.98417500	-0.28633800	-0.86820800
C	-0.70498300	-0.64872200	-0.42793000
C	0.27134100	0.32654400	-0.20166200
C	-0.09836300	1.66595300	-0.43842900
C	-1.38204500	1.95976800	-0.87425400
C	-3.07986300	-1.24022000	-1.13348300
C	-2.98621500	-2.63051500	-0.98125800
C	-4.08889600	-3.44510900	-1.26067400
C	-5.26798000	-2.80868900	-1.69242600
C	-5.29004200	-1.42466400	-1.82069600
H	-0.46479800	-1.69941600	-0.25909600
H	0.61651500	2.47707900	-0.28247700
H	-1.69463300	2.98938000	-1.06507000
H	-2.05320000	-3.08385600	-0.64411100
H	-6.16263600	-3.39015800	-1.92588200
H	-6.18629700	-0.89328500	-2.15166600
N	-2.31931600	1.01465600	-1.08971900
N	-4.22769500	-0.65399600	-1.54992000
C	1.65392700	-0.02271100	0.27689900
H	1.84919000	0.42643700	1.26505500
H	1.79507800	-1.10967900	0.36065200
H	2.41867300	0.37455100	-0.41046400
C	-4.02947500	-4.94106600	-1.11192900
H	-3.05325800	-5.27716600	-0.73493400
H	-4.81014400	-5.29435300	-0.41873800
H	-4.21487300	-5.43465100	-2.08017100

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2083.2746658
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2082.7071176

1,1-dimethylethene

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.107040 (Hartree/Particle)
Thermal correction to Energy= 0.112322
Thermal correction to Enthalpy= 0.113267
Thermal correction to Gibbs Free Energy= 0.079765
Sum of electronic and zero-point Energies= -157.012996
Sum of electronic and thermal Energies= -157.007713
Sum of electronic and thermal Enthalpies= -157.006769
Sum of electronic and thermal Free Energies= -157.040270

C	-5.45780700	2.07262200	0.23723400
C	-5.52946100	0.85899400	1.12932400
H	-6.18072200	0.07439500	0.71608900
H	-4.52384500	0.42950900	1.28546300
H	-5.90716300	1.13242700	2.13066000
C	-6.12859400	2.15207900	-0.92172300
H	-6.76266200	1.33174500	-1.27263500
H	-6.06610800	3.04018900	-1.55848800
C	-4.57879200	3.19055500	0.73860400
H	-3.54036500	2.83933200	0.87450700
H	-4.56607400	4.05129000	0.05348300
H	-4.91872000	3.53998000	1.72977100

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.3001298
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -157.1516226

^{2}K'-TS
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.309716 (Hartree/Particle)
Thermal correction to Energy= 0.331219
Thermal correction to Enthalpy= 0.332163
Thermal correction to Gibbs Free Energy= 0.255765
Sum of electronic and zero-point Energies= -4887.483265
Sum of electronic and thermal Energies= -4887.461762
Sum of electronic and thermal Enthalpies= -4887.460818
Sum of electronic and thermal Free Energies= -4887.537216

Ni	-0.79917400	-0.18317200	0.37337300
C	-1.59750800	0.64027300	-1.29816000
C	-0.96341900	3.22629700	-2.16800300
C	-2.36114100	1.73785700	-0.84662200
C	-0.61544700	0.82411200	-2.29669300
C	-0.27976900	2.11796100	-2.69156100
C	-2.01349800	3.02495500	-1.26137200
H	-3.17246700	1.57386600	-0.13808600
H	-0.08267700	-0.03906500	-2.69625000
H	0.52534700	2.26263500	-3.41731900
H	-2.56944300	3.88025800	-0.86738400
N	0.73831700	1.17004400	0.61386500
C	2.88889900	2.96658200	0.63201800
C	0.57718400	2.41769300	1.06391300
C	1.94612800	0.78038200	0.15858700
C	3.03910900	1.65625900	0.16120700
C	1.61503200	3.34445000	1.08820000
N	0.80701100	-1.25157900	-0.39748800
C	3.15053000	-2.56636100	-1.22288500
C	0.76597600	-2.51433900	-0.84472100
C	1.99870400	-0.61427200	-0.34700400
C	3.17962600	-1.24773700	-0.75376000
C	1.89886900	-3.20297600	-1.26433900
H	-0.42788700	2.66934600	1.41062100
H	4.00894200	1.32914000	-0.21439100
H	1.43146900	4.35481000	1.45993100
H	-0.22342900	-2.97575700	-0.87505900
H	4.13164700	-0.71891900	-0.70211900
H	1.80530400	-4.23033100	-1.62269200
Br	-2.58780400	-1.23666900	-1.32829200
H	-0.69604400	4.23708700	-2.48470300
C	4.40185400	-3.28332100	-1.64903900
H	4.66136500	-4.06629700	-0.91677400
H	4.25605200	-3.78560800	-2.61812300
H	5.25751200	-2.59854300	-1.73256300
C	4.04019800	3.93441300	0.65931400
H	3.75413400	4.89726400	0.20758700
H	4.33939300	4.14378400	1.69999600
H	4.91734100	3.54304800	0.12497400
H	-1.77995400	0.05875200	1.64063100

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4889.1966238
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4888.3092754

Ph–H
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.100501 (Hartree/Particle)
Thermal correction to Energy= 0.104869
Thermal correction to Enthalpy= 0.105813
Thermal correction to Gibbs Free Energy= 0.073041
Sum of electronic and zero-point Energies= -231.991414
Sum of electronic and thermal Energies= -231.987046
Sum of electronic and thermal Enthalpies= -231.986102
Sum of electronic and thermal Free Energies= -232.018875

C	-1.78619400	0.38638600	-1.50220400
C	-1.08232300	3.09483000	-1.40580500
C	-2.51675000	1.27142400	-0.70025300
C	-0.70376700	0.85565300	-2.25604600
C	-0.35185200	2.20986100	-2.20777100
C	-2.16479500	2.62562500	-0.65210600
H	-3.36188700	0.90503200	-0.11142400
H	-0.13344100	0.16460300	-2.88246100
H	0.49324200	2.57637100	-2.79661600
H	-2.73519400	3.31669300	-0.02575100
H	-0.80755600	4.15235000	-1.36828900
H	-2.06099000	-0.67106600	-1.53988700

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -232.3465283
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -232.1429457

Figure A1.14
DMA
UB3LYP-D3/def2-SVP-CPCM(THF)
$\langle S^2 \rangle = 0.0000$
Zero-point correction= 0.129574 (Hartree/Particle)
Thermal correction to Energy= 0.137214
Thermal correction to Enthalpy= 0.138159
Thermal correction to Gibbs Free Energy= 0.097818
Sum of electronic and zero-point Energies= -287.506478
Sum of electronic and thermal Energies= -287.498838
Sum of electronic and thermal Enthalpies= -287.497894
Sum of electronic and thermal Free Energies= -287.538234

C	-2.77549400	1.10576800	0.17344400
O	-3.37576400	0.04098600	0.30285000
N	-1.42066200	1.15712500	-0.02483700
C	-3.53169900	2.42604000	0.23195600
H	-3.17999200	3.06144900	1.05983000
H	-3.42570500	3.00001200	-0.70177600
H	-4.59143000	2.19194000	0.38873300
C	-0.64344600	2.37040000	-0.20318800
H	-1.25639800	3.26981200	-0.09049600
H	0.17034500	2.41803800	0.54165400
H	-0.18014800	2.39406000	-1.20606400

C	-0.65581000	-0.07661500	-0.10272300
H	-1.32981400	-0.92785900	0.04169300
H	-0.16180500	-0.16647800	-1.08632700
H	0.12810200	-0.09653400	0.67449200

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -287.968183
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -287.7556375

Figure A1.17
[Ir(II)]
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.456088 (Hartree/Particle)
Thermal correction to Energy= 0.496055
Thermal correction to Enthalpy= 0.496999
Thermal correction to Gibbs Free Energy= 0.378449
Sum of electronic and zero-point Energies= -2626.184144
Sum of electronic and thermal Energies= -2626.144177
Sum of electronic and thermal Enthalpies= -2626.143232
Sum of electronic and thermal Free Energies= -2626.261783

Ir	-0.38361500	0.77402400	0.05316900
C	2.34735200	1.55708000	1.07420000
C	2.41755700	1.29983400	-1.28265800
C	3.73792100	1.88540800	1.05493200
C	1.54618300	1.50257900	2.25738700
C	3.76397300	1.61776800	-1.34905400
H	1.85216300	1.05616000	-2.18579600
C	4.43596300	1.91595000	-0.13134000
H	4.24922400	2.11309300	1.99056100
C	2.02866400	1.78209300	3.57294900
H	4.27848300	1.63319400	-2.31040600
H	5.49928800	2.16794500	-0.13425200
C	-0.59876000	1.08108500	3.17806200
C	1.18832500	1.70340600	4.66064600
H	3.07308700	2.06117100	3.71419800
C	-0.17324600	1.33815200	4.47076900
H	-1.63515300	0.80142300	2.97206200
H	1.56779800	1.92063400	5.66211800
H	-0.87109400	1.26044100	5.30511000
C	-1.20298700	-1.96383800	0.73819500
C	1.11681300	-1.82859300	0.34511200
C	-1.07689600	-3.34293800	0.99669600
C	-2.43196900	-1.17336500	0.77340100
C	1.28877300	-3.18376500	0.59613000
H	1.95705500	-1.18870400	0.07846900
C	0.16627400	-3.95482400	0.92500200
H	-1.95872600	-3.92382500	1.24996100
C	-2.28624200	0.21283100	0.45110000
C	-3.71127200	-1.66010700	1.10138600
H	0.26512200	-5.02467200	1.11845200
C	-3.42294200	1.03566800	0.46870100
C	-4.83725100	-0.84913300	1.12405700
C	-4.66164900	0.49780900	0.80247100
H	-3.36520800	2.09860200	0.22890800
H	-5.81457800	-1.25438600	1.38393400
C	-0.76136600	0.59493300	-1.92704200
C	-1.08185900	1.82964800	-2.57472800
C	-0.70798800	-0.57879600	-2.69448400
C	-1.32492000	1.82253700	-3.96108600
C	-1.12033100	3.00700200	-1.70896600
C	-0.95672700	-0.52336500	-4.06206400
H	-0.47155300	-1.54613700	-2.24825800
C	-1.26781200	0.66511300	-4.72473000
C	-1.42632300	4.32796300	-2.09075400
H	-1.45934100	0.69105800	-5.79690900
C	-0.81789200	3.72327200	0.51586400
C	-1.42840100	5.34401800	-1.14574900
H	-1.66027100	4.54557000	-3.12862000
C	-1.11862300	5.03850900	0.18583900
H	-1.66255400	6.36897900	-1.43944600
N	1.71837900	1.25851900	-0.13231300
N	0.20508800	1.16057400	2.10042000
N	-0.08694600	-1.23930600	0.40954300
N	-0.82238600	2.74098200	-0.39775800
C	2.66020500	-3.80107100	0.55323200
F	3.14500300	-4.01512800	1.79241600
F	3.54522900	-3.02117500	-0.09014500
F	2.63996800	-4.99550400	-0.06605700
F	-3.88932800	-2.95793500	1.41527800
F	-5.73932900	1.29702900	0.81882300
F	-1.62428200	2.96511100	-4.60875900
F	-0.89844900	-1.65281300	-4.78414100
H	-0.56136900	3.43599300	1.53475600
C	-1.15339100	6.10205200	1.24945300
F	-0.61759400	7.25480300	0.80869300
F	-0.48167500	5.73342700	2.35350300
F	-2.41670600	6.38074700	1.62781400

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2629.5151152
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2627.9322792

[Ir(III)]$^+$
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.459873 (Hartree/Particle)
Thermal correction to Energy= 0.499499
Thermal correction to Enthalpy= 0.500443
Thermal correction to Gibbs Free Energy= 0.383450
Sum of electronic and zero-point Energies= -2626.063035
Sum of electronic and thermal Energies= -2626.023409
Sum of electronic and thermal Enthalpies= -2626.022465
Sum of electronic and thermal Free Energies= -2626.139458

Ir	-0.36720300	0.77952700	0.06402700
C	2.38652400	1.58502300	1.06698800
C	2.42805500	1.35755700	-1.25950400
C	3.73997300	1.94563400	1.07249400
C	1.56470700	1.49006000	2.29981200
C	3.77401700	1.71107200	-1.32161800
H	1.86155100	1.11139000	-2.15945200
C	4.43993800	2.00930000	-0.13187700

H	4.24890400	2.17751000	2.00668500
C	2.07363700	1.73195000	3.58207600
H	4.28084200	1.74808300	-2.28671300
H	5.49488900	2.28997700	-0.13730600
C	-0.54779900	1.03770800	3.19369300
C	1.23267100	1.61942200	4.68865100
H	3.11804600	2.00575800	3.72187300
C	-0.10296800	1.26420200	4.49413000
H	-1.58236600	0.75935700	2.98495900
H	1.62051500	1.80683600	5.69171500
H	-0.79616300	1.16232700	5.33004100
C	-1.21972100	-1.95400300	0.73314100
C	1.10163800	-1.85646100	0.34063800
C	-1.11821500	-3.33733900	0.97548300
C	-2.43541000	-1.14432500	0.77199500
C	1.25013700	-3.21667800	0.57522400
H	1.95744300	-1.23755900	0.07567900
C	0.11416200	-3.97017800	0.89631400
H	-2.01018300	-3.90644400	1.21964200
C	-2.27236700	0.23887500	0.45318600
C	-3.72190900	-1.61132400	1.10260600
H	0.19325500	-5.04396300	1.07620300
C	-3.39069500	1.08218300	0.47576200
C	-4.83382600	-0.78149000	1.12989900
C	-4.63836000	0.56239400	0.81197100
H	-3.32047300	2.14392000	0.23766600
H	-5.81688700	-1.17171500	1.39127000
C	-0.74495800	0.58128800	-1.90904100
C	-1.07074200	1.80607900	-2.56857000
C	-0.67417000	-0.60085500	-2.65716800
C	-1.30553300	1.78075600	-3.95663300
C	-1.12303600	2.99278100	-1.71722400
C	-0.91559400	-0.56296500	-4.02840200
H	-0.43349300	-1.56155800	-2.20088300
C	-1.23351300	0.61441100	-4.70518000
C	-1.45072100	4.30320700	-2.11465900
H	-1.41910400	0.62615600	-5.77867700
C	-0.83773400	3.74010900	0.49917100
C	-1.47314600	5.32942900	-1.18093400
H	-1.68875200	4.50473300	-3.15477800
C	-1.16335400	5.04493300	0.15494100
H	-1.72632500	6.34619300	-1.48708800
N	1.75547400	1.29387500	-0.09938000
N	0.26119100	1.15194300	2.12847300
N	-0.09061500	-1.24482100	0.41597400
N	-0.81828700	2.74747400	-0.40373300
C	2.61267600	-3.85661200	0.52181200
F	3.10234800	-4.07120500	1.75753400
F	3.50139300	-3.08854900	-0.13119600
F	2.56742400	-5.04948500	-0.09414100
F	-3.91702700	-2.90403800	1.41404900
F	-5.69845700	1.37943900	0.83251100
F	-1.60903600	2.91184300	-4.61605200
F	-0.84204900	-1.69891000	-4.73266500
H	-0.58538500	3.47760800	1.52538800
C	-1.22539400	6.11997400	1.20806100
F	-0.68430200	7.26779300	0.76615200
F	-0.57444400	5.76211400	2.32835200
F	-2.49680900	6.39308100	1.55489100

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2629.3946502
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -2627.8122578

K^+
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015176
Sum of electronic and zero-point Energies= -599.792231
Sum of electronic and thermal Energies= -599.790815
Sum of electronic and thermal Enthalpies= -599.789871
Sum of electronic and thermal Free Energies= -599.807407

K	0.67977500	1.81953700	-2.01383600

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -599.8697705
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -599.8424387

KBr
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.000291 (Hartree/Particle)
Thermal correction to Energy= 0.003334
Thermal correction to Enthalpy= 0.004279
Thermal correction to Gibbs Free Energy= -0.024774
Sum of electronic and zero-point Energies= -3173.856696
Sum of electronic and thermal Energies= -3173.853653
Sum of electronic and thermal Enthalpies= -3173.852709
Sum of electronic and thermal Free Energies= -3173.881762

K	-0.27573900	1.80647700	-1.00469500
Br	-3.38333800	1.80647700	-1.00469500

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -3174.256792
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -3174.1001508

Figure A1.18
TS-HAT (*t*Bu from Ph–H)
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.213786 (Hartree/Particle)
Thermal correction to Energy= 0.225178
Thermal correction to Enthalpy= 0.226122
Thermal correction to Gibbs Free Energy= 0.173602
Sum of electronic and zero-point Energies= -389.540592

Sum of electronic and thermal Energies= -389.529200
Sum of electronic and thermal Enthalpies= -389.528256
Sum of electronic and thermal Free Energies= -389.580776

C	-1.32452900	-5.70999100	-0.64601400
C	-0.12003600	-5.86266600	-1.56424400
H	0.68500100	-6.43887600	-1.07969700
H	-0.40152200	-6.39634600	-2.49114200
H	0.29018200	-4.88221700	-1.85654500
C	-2.41255400	-4.81606700	-1.22439400
H	-2.85986500	-5.27816400	-2.12420100
H	-3.22412400	-4.64874100	-0.49758000
H	-2.01124200	-3.83307100	-1.52055000
C	-1.85409300	-7.03864200	-0.12381800
H	-1.05791200	-7.62793500	0.35995400
H	-2.66327700	-6.88962700	0.60966700
H	-2.26260400	-7.64800700	-0.95155300
H	-0.91115000	-5.12004400	0.34065500
C	-0.40944900	-4.39769200	1.59793900
C	-0.09322600	-3.04791900	1.51310700
C	-0.29669600	-5.12910100	2.77318600
C	0.36202000	-2.39719300	2.67184400
H	-0.19342200	-2.49804600	0.57204800
C	0.15955400	-4.46946500	3.92654200
H	-0.55527800	-6.19197700	2.80758700
C	0.48683500	-3.10845500	3.87230300
H	0.61887800	-1.33435500	2.63568700
H	0.25853600	-5.01968900	4.86691500
H	0.84136300	-2.59837600	4.77177200

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -390.1859701
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -389.8284779

***t*Bu–H**
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.130747 (Hartree/Particle)
Thermal correction to Energy= 0.136352
Thermal correction to Enthalpy= 0.137297
Thermal correction to Gibbs Free Energy= 0.103241
Sum of electronic and zero-point Energies= -158.220710
Sum of electronic and thermal Energies= -158.215105
Sum of electronic and thermal Enthalpies= -158.214161
Sum of electronic and thermal Free Energies= -158.248216

C	-1.35880900	-5.74058300	-0.69920900
C	-0.82369700	-4.98911000	-1.92428400
H	0.27857000	-4.96727300	-1.93406700
H	-1.15671900	-5.47685400	-2.85723600
H	-1.18260900	-3.94683300	-1.94599900
C	-2.89193400	-5.72268600	-0.66606700
H	-3.30687200	-6.23708900	-1.55062800
H	-3.28129200	-6.23329100	0.23015200
H	-3.28288100	-4.69183400	-0.66506000
C	-0.82205700	-7.17657400	-0.65350800
H	0.28028500	-7.19472100	-0.64411100
H	-1.17672700	-7.71082400	0.24334200
H	-1.15825600	-7.74716700	-1.53709700
H	-0.99537000	-5.21550400	0.20414900

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -158.5324782
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -158.3793557

Figure A1.19
Non-ligated Ni(III) (Tetrahedral)
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.211223 (Hartree/Particle)
Thermal correction to Energy= 0.225662
Thermal correction to Enthalpy= 0.226607
Thermal correction to Gibbs Free Energy= 0.167821
Sum of electronic and zero-point Energies= -4471.112669
Sum of electronic and thermal Energies= -4471.098230
Sum of electronic and thermal Enthalpies= -4471.097286
Sum of electronic and thermal Free Energies= -4471.156071

C	2.85880600	0.74317800	0.23337800
C	3.89346800	-0.36358800	0.23547100
C	2.89142500	1.59192300	-1.03876300
H	3.79736600	-1.00840200	-0.65008500
H	3.80865900	-0.98854000	1.13475300
H	2.83855000	0.98998300	-1.95855600
H	2.09760800	2.35745600	-1.06205300
Br	1.03762700	-1.52014500	-2.04620800
Ni	1.11076700	-0.01515500	-0.20188300
C	0.91749900	-0.80812000	1.49745800
C	0.23763100	-0.12580100	2.51524500
C	1.28575200	-2.14699300	1.68565300
C	-0.07912200	-0.78179600	3.71312800
H	-0.04145600	0.92453500	2.38833100
C	0.97451500	-2.79953400	2.88509200
H	1.80903300	-2.68372300	0.89031400
H	-0.61299000	-0.24450900	4.50216000
H	1.26392600	-3.84500600	3.02485900
C	0.29169800	-2.11808000	3.90012700
H	0.05055000	-2.62804200	4.83649700
H	4.90621400	0.08337100	0.22516700
H	3.85381700	2.13871200	-1.06186100
C	2.86935900	1.59626600	1.48856300
H	2.00503800	2.27775800	1.52880400
H	2.86822500	0.98299600	2.39880000
H	3.78220400	2.22164500	1.49347700

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4472.2797924
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4471.7023257

Non-ligated Ni(III) (Square Planar)

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.211070 (Hartree/Particle)
Thermal correction to Energy= 0.225625
Thermal correction to Enthalpy= 0.226569
Thermal correction to Gibbs Free Energy= 0.166740
Sum of electronic and zero-point Energies= -4471.112594
Sum of electronic and thermal Energies= -4471.098040
Sum of electronic and thermal Enthalpies= -4471.097096
Sum of electronic and thermal Free Energies= -4471.156924

Ni	-0.69015100	-0.10048000	0.06690000
C	-1.96369900	1.24956000	-0.26283500
C	-3.75785000	3.24547600	-1.08695500
C	-3.28369100	0.91615600	-0.59356900
C	-1.54374900	2.58408400	-0.34634400
C	-2.43860100	3.58003200	-0.76273900
C	-4.17889400	1.91239800	-1.00231600
H	-3.61298600	-0.12420000	-0.53461900
H	-0.52004100	2.86087800	-0.07631200
H	-2.10321300	4.61904300	-0.82766500
H	-5.20867000	1.64572900	-1.25680800
Br	-1.01456200	-2.11044000	-1.14130800
C	-1.03216700	-0.11144300	1.98866700
H	-4.45861200	4.02270400	-1.40299600
C	0.07143200	-1.13149100	2.27540100
H	0.11860800	-1.28593800	3.37058600
H	-0.12193100	-2.10897700	1.81056400
H	1.07300700	-0.78180000	1.97154100
C	-2.41490100	-0.64855700	2.29100800
H	-3.19423400	0.09351200	2.07311600
H	-2.62479500	-1.55971000	1.71081700
H	-2.47953600	-0.90882600	3.36492000
C	-0.73489600	1.24114900	2.61122300
H	0.21051300	1.66488300	2.23478800
H	-1.53801100	1.96418300	2.41945300
H	-0.62753400	1.12405900	3.70638000

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4472.279756
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -4471.7027401

4,4'-dimethylbipyridine Ligand
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.212040 (Hartree/Particle)
Thermal correction to Energy= 0.224472
Thermal correction to Enthalpy= 0.225417
Thermal correction to Gibbs Free Energy= 0.170903
Sum of electronic and zero-point Energies= -573.414733
Sum of electronic and thermal Energies= -573.402300
Sum of electronic and thermal Enthalpies= -573.401356
Sum of electronic and thermal Free Energies= -573.455869

C	-2.31575100	-1.15742200	-0.05825600
C	-0.91697700	-1.27194600	0.02278700
C	-0.22447200	-0.70695500	1.10164900
C	-0.99218900	-0.04466300	2.07014800
C	-2.37809600	0.02559400	1.90563400
C	-3.07072300	-1.75985500	-1.20231200
C	-2.63843200	-2.95842800	-1.79813600
C	-3.35500200	-3.51359600	-2.86541400
C	-4.49796800	-2.81983100	-3.28994600
C	-4.85559900	-1.63801000	-2.63699400
H	-0.36149000	-1.78401300	-0.76571600
H	-0.51932900	0.41415800	2.94221800
H	-2.98834200	0.54166500	2.65702300
H	-1.75618600	-3.47459000	-1.41410900
H	-5.10737900	-3.19713900	-4.11514400
H	-5.74810300	-1.08816000	-2.96001800
N	-3.03302700	-0.50956800	0.87394100
N	-4.17073800	-1.11301100	-1.61872400
C	-2.91853600	-4.78894400	-3.53673600
H	-2.16322000	-5.32437400	-2.94346500
H	-3.77370400	-5.46175800	-3.70579800
H	-2.47910300	-4.57147800	-4.52509600
C	1.27668300	-0.77649400	1.19822700
H	1.60731200	-0.85611700	2.24488300
H	1.68075800	-1.63018200	0.63440200
H	1.72933200	0.14008200	0.78228300

UB3LYP-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -574.2558479
UM06/def2-TZVPP-CPCM(THF)//UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -573.7901558

^{1}F-DMA-O
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.435353 (Hartree/Particle)
Thermal correction to Energy= 0.465364
Thermal correction to Enthalpy= 0.466308
Thermal correction to Gibbs Free Energy= 0.371774
Sum of electronic and zero-point Energies= -5174.442026
Sum of electronic and thermal Energies= -5174.412014
Sum of electronic and thermal Enthalpies= -5174.411070
Sum of electronic and thermal Free Energies= -5174.505604

C	-1.99573800	1.70563600	1.27592200
O	-1.57857800	0.71672600	0.64048900
N	-2.89472400	2.56501500	0.75010400
C	-1.47410900	1.95364900	2.67628200
H	-1.11216300	2.98325600	2.81198000
H	-2.26334600	1.76787100	3.42184500
H	-0.65298600	1.24992700	2.85587800
C	-3.33995100	2.40820300	-0.63035700
H	-4.25568400	1.79961900	-0.69048700
H	-3.54156900	3.40275500	-1.05441600
H	-2.55717000	1.92011100	-1.22281600
C	-3.58663900	3.59887300	1.50728500
H	-4.67135200	3.39904700	1.50070200
H	-3.25493700	3.63050100	2.54901400

H	-3.41506200	4.58905900	1.05431700
Ni	-2.83422400	-0.70330200	-0.47307400
C	-2.12470800	-3.48520000	-0.24809200
C	-1.46424900	-2.23640700	-0.06587200
C	-0.92329800	-1.56582200	-1.20744300
C	-1.06246300	-2.17899900	-2.47563400
C	-1.73841200	-3.37384900	-2.65124100
C	-2.27633700	-4.02521900	-1.51351100
H	-2.51370100	-4.01365500	0.62537200
H	-1.14288900	-1.93603900	0.93594900
H	-1.85101900	-3.80954600	-3.64483900
H	-2.80536800	-4.97206300	-1.64706800
H	-0.24789300	-0.71828200	-1.08343100
Br	-0.30699000	-1.28484100	-3.99442100
C	-5.58488100	-0.71657100	-1.26670300
C	-6.73781400	-0.77640800	-2.10429200
C	-6.62620500	-0.92475200	-3.47360800
C	-5.31084700	-1.01892300	-4.02328900
C	-4.22414500	-0.96917600	-3.16702200
C	-5.62452000	-0.53277000	0.15671400
C	-6.81183900	-0.35572400	0.92827500
C	-6.75854700	-0.17742000	2.29830500
C	-5.47215700	-0.17843900	2.92135100
C	-4.35230300	-0.35121800	2.12428400
H	-7.72971900	-0.70607800	-1.65381300
H	-5.15633400	-1.12736700	-5.09888200
H	-3.20818600	-1.04370200	-3.56061600
H	-7.78206500	-0.35573300	0.42787800
H	-5.36804800	-0.05364900	4.00110500
H	-3.34962000	-0.36151400	2.56330400
N	-4.32004800	-0.82323300	-1.83343800
N	-4.39581800	-0.51921400	0.79480000
C	-7.99766800	0.01327800	3.13136200
H	-8.91250800	-0.01112300	2.52081600
H	-8.07819400	-0.77190300	3.90309800
H	-7.96779700	0.97738100	3.66821900
C	-7.82822500	-0.98815700	-4.37703000
H	-7.85017400	-1.93823500	-4.93878200
H	-8.77061600	-0.89980000	-3.81620200
H	-7.79867700	-0.18096600	-5.12951400

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5176.5999679
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5175.5019016

[1]F-DMA'
UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.434398 (Hartree/Particle)
Thermal correction to Energy= 0.465055
Thermal correction to Enthalpy= 0.465999
Thermal correction to Gibbs Free Energy= 0.367305
Sum of electronic and zero-point Energies= -5174.382824
Sum of electronic and thermal Energies= -5174.352168
Sum of electronic and thermal Enthalpies= -5174.351223
Sum of electronic and thermal Free Energies= -5174.449917

C	-1.97016600	-0.98194000	-1.08653400
O	-2.20401200	0.23211900	-0.94905100
N	-0.60758500	-1.45789200	-1.14294800
C	-3.05520500	-1.90925000	-1.62444700
H	-3.12003200	-1.79774700	-2.72214000
H	-2.91213600	-2.96911300	-1.38454000
H	-4.00633000	-1.56981000	-1.19390600
C	-0.25349500	-2.60168900	-1.99171600
H	-0.17849100	-2.30293900	-3.05367600
H	0.71643900	-3.00280500	-1.66692700
H	-0.99124600	-3.40058900	-1.88880200
C	0.42535300	-0.41680500	-1.13844900
H	0.58143400	-0.01349500	-2.15619400
H	0.11223800	0.39839900	-0.47949900
H	1.36587800	-0.85076800	-0.77147100
Ni	-1.23286100	-1.97005100	0.65837000
C	-1.08992900	-3.90407700	1.69927000
C	-2.39999500	-3.36935600	1.70329300
C	-2.63609200	-2.04654400	2.16848500
C	-1.53656200	-1.26833800	2.61729100
C	-0.22206000	-1.78959600	2.61961200
C	-0.01065000	-3.10841500	2.14799900
H	-0.90472400	-4.88789900	1.26762300
H	-3.23163500	-3.96770100	1.32849900
H	0.61175300	-1.18009900	2.96852300
H	1.00757500	-3.49857800	2.10094800
H	-3.64243600	-1.62574500	2.16820100
Br	-1.85461700	0.49234200	3.32735600
C	-0.09040200	-5.98907000	-1.79741600
C	0.72717800	-5.82898000	-2.92735000
C	2.08116800	-5.50137600	-2.77491200
C	2.55601200	-5.36665300	-1.46251900
C	1.67347400	-5.56036500	-0.39654700
C	-1.55072400	-6.27313800	-1.95183000
C	-2.01040200	-7.17779800	-2.92166800
C	-3.38412000	-7.41845300	-3.06355400
C	-4.24220200	-6.71770300	-2.20384900
C	-3.69645700	-5.83388600	-1.26960100
H	0.29925600	-5.92628100	-3.92752400
H	3.60125500	-5.11375200	-1.26868300
H	2.03505800	-5.46701800	0.63429100
H	-1.29511900	-7.71102700	-3.55197400
H	-5.32455600	-6.85832800	-2.25656300
H	-4.35677400	-5.27266200	-0.59793000
N	0.38261000	-5.86107300	-0.54841000
N	-2.38753300	-5.61150600	-1.13621600
C	-3.91142400	-8.36728900	-4.10664000
H	-3.18760700	-9.16524600	-4.32932600
H	-4.85947500	-8.82725000	-3.79075500
H	-4.10602100	-7.82680900	-5.04905000
C	2.96833300	-5.25888600	-3.96637600
H	4.01884800	-5.49575400	-3.74191900
H	2.64880300	-5.85264100	-4.83564100
H	2.92585600	-4.19588000	-4.26012500

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5176.5457794
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5175.463106

[1]G-DMA-O

UB3LYP-D3/def2-SVP-CPCM(THF)
Zero-point correction= 0.437417
(Hartree/Particle)
Thermal correction to Energy= 0.467940
Thermal correction to Enthalpy= 0.468884
Thermal correction to Gibbs Free Energy= 0.371580
Sum of electronic and zero-point Energies= -
5174.486401
Sum of electronic and thermal Energies= -
5174.455878
Sum of electronic and thermal Enthalpies= -
5174.454934
Sum of electronic and thermal Free Energies= -
5174.552238

C	-2.51811700	0.31763100	0.07638600
O	-1.75704900	-0.42918400	-0.58355500
N	-2.03794100	0.99075400	1.13756200
C	-3.96681200	0.45866400	-0.30611300
H	-4.55773600	-0.27525200	0.26498400
H	-4.36819500	1.46308700	-0.12181600
H	-4.04949800	0.20330700	-1.37052500
C	-2.87060900	1.84720400	1.97767100
H	-2.39333500	1.94038300	2.96236100
H	-2.97962400	2.85839700	1.55033500
H	-3.86665800	1.41301600	2.13146500
C	-0.62541000	0.90751900	1.49514000
H	-0.19668200	1.92010700	1.56276800
H	-0.50684800	0.41033900	2.47185100
H	-0.08655700	0.33533700	0.73370900
Ni	-2.17675500	-1.82835800	-1.86714500
C	-3.43413900	-3.49580300	1.78010300
C	-2.67291600	-2.89108000	0.76966300
C	-3.15204600	-2.77163900	-0.54921900
C	-4.43301900	-3.29451900	-0.81448900
C	-5.20936200	-3.88521500	0.19066900
C	-4.71214100	-3.99090300	1.49636400
H	-3.02949300	-3.57586900	2.79444400
H	-1.68660800	-2.48703600	1.01852400
H	-4.82632300	-3.24467200	-1.83340900
H	-6.20606200	-4.27154400	-0.04668700
H	-5.31338900	-4.45711600	2.28225500
Br	-2.08778200	-3.71370700	-3.31942000
C	-3.16586000	-0.65969400	-4.64107200
C	-3.62524100	-0.99946500	-5.91967800
C	-4.96027400	-1.38708400	-6.10195100
C	-5.77973200	-1.40094300	-4.96412000
C	-5.23882800	-1.03497200	-3.72942700
C	-1.74267500	-0.29293700	-4.39998500
C	-0.99936100	0.43769100	-5.33616700
C	0.33428100	0.77675600	-5.07833500
C	0.86918600	0.36373200	-3.84796800
C	0.07257000	-0.35560600	-2.96397400
H	-2.93801600	-0.99718100	-6.76814700
H	-6.82987100	-1.69394000	-5.03522200
H	-5.86283400	-1.03861300	-2.82874600
H	-1.47541400	0.76390200	-6.26241400
H	1.90000700	0.60148200	-3.57663900
H	0.45598600	-0.68479900	-1.99576300
N	-3.96721800	-0.67229400	-3.56429500
N	-1.19861900	-0.68518600	-3.23111300
C	1.16437100	1.54228400	-6.07178600
H	0.54561600	1.98976200	-6.86246500
H	1.73798500	2.34099500	-5.57658600
H	1.89556400	0.87062000	-6.55264800
C	-5.47169300	-1.81243900	-7.45188100
H	-6.55881200	-1.66825800	-7.53590100
H	-4.97664600	-1.25818600	-8.26334200
H	-5.26605300	-2.88448100	-7.61430200

UB3LYP-D3/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5176.6518013
UM06/def2-TZVPP-CPCM(THF)// UB3LYP-D3/def2-SVP-CPCM(THF)
HF= -5175.5492669

Appendix 2: Computational Methods, Results, Coordinates and Energies from Chapter 3 (Mechanistic Study of Nickel-Catalyzed Olefin Dicarbofunctionalization Enabled by Photochemical C–H Activation)

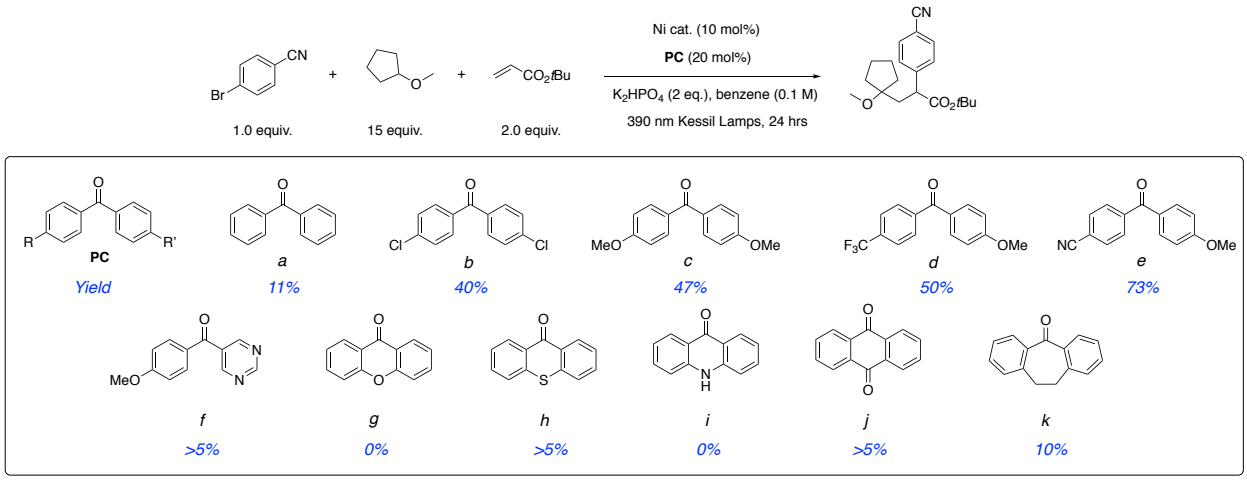
A2.1 Methods

All structural optimizations were performed at the (U)B3LYP[340-341]-D3[100]/def2-SVP[342-343] level of theory in benzene solvent using the CPCM implicit solvent model[352] with "opt=noeigen" keyword as implemented in Gaussian16.[353] Vibrational frequencies were computed at the same level to get thermal corrections (at 298 K; enthalpy and free energy) and to characterize the obtained stationary points as transition states (one and only one imaginary frequency) or minima (zero imaginary frequencies). Extensive conformational search was performed for all intermediates and transition states, and only the lowest-energy species were shown and discussed. Intrinsic reaction coordinate (IRC) calculations were performed for all transition states to ensure they are connected to the corresponding intermediates. To compare energetics, we also carried out single-point energy calculations using (U)B3LYP-D3/def2-TZVPP-CPCM(THF) and domain based local pair natural orbital coupled cluster method with single-, double-, and perturbative triple excitations and def2-TZVPP basis set along with def2-TZVPP/C as auxiliary basis set [noted as DLPNO-CCSD(T)/def2-TZVPP//(U)B3LYP-D3/def2-SVP-CPCM(benzene)] with ORCA (version 4.1.1). All structural figures were generated using CYLview.

Noncovalent interaction (NCI) analysis, also known as reduce density gradient (RDG) method,[354] was performed on Multiwfn to study the presence of noncovalent interactions (H-bonding) in the Giese addition. 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.[15]

A2.2 Supplementary Figures

Table A2.1 Calculation of HAT Catalyst[a]



Ketones	*a*	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	*k*
3P	65.4	64.7	66.2	62.5	60.4	60.2	70.1	62.1	61.2	58.7	62.9
Yield	11%	40%	47%	50%	73%	>5%	0%	>5%	0%	>5%	10%

[a]Electronic energy values given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of theory.

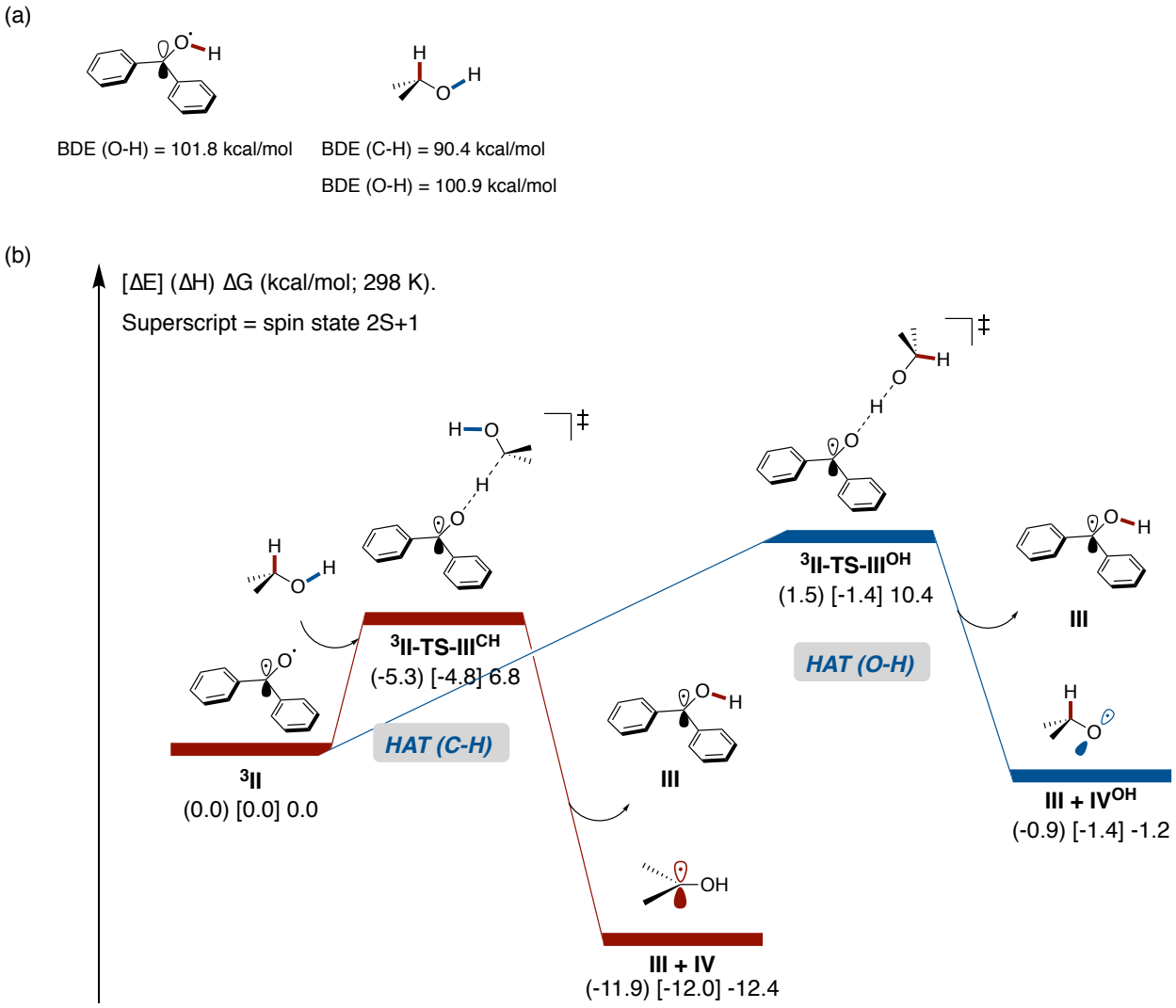


Figure A2.1 (a) Calculation of BDE of ketyl radical and active bonds in *i*-PrOH. BDE was calculated at the (U)B3LYP-D3/def2-TZVPP//(U)B3LYP-D3/def2-SVP level of theory. (b) Divergent HAT pathways from *i*-PrOH. Electronic (in parenthesis), enthalpy (in bracket) and free energy values given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of theory.

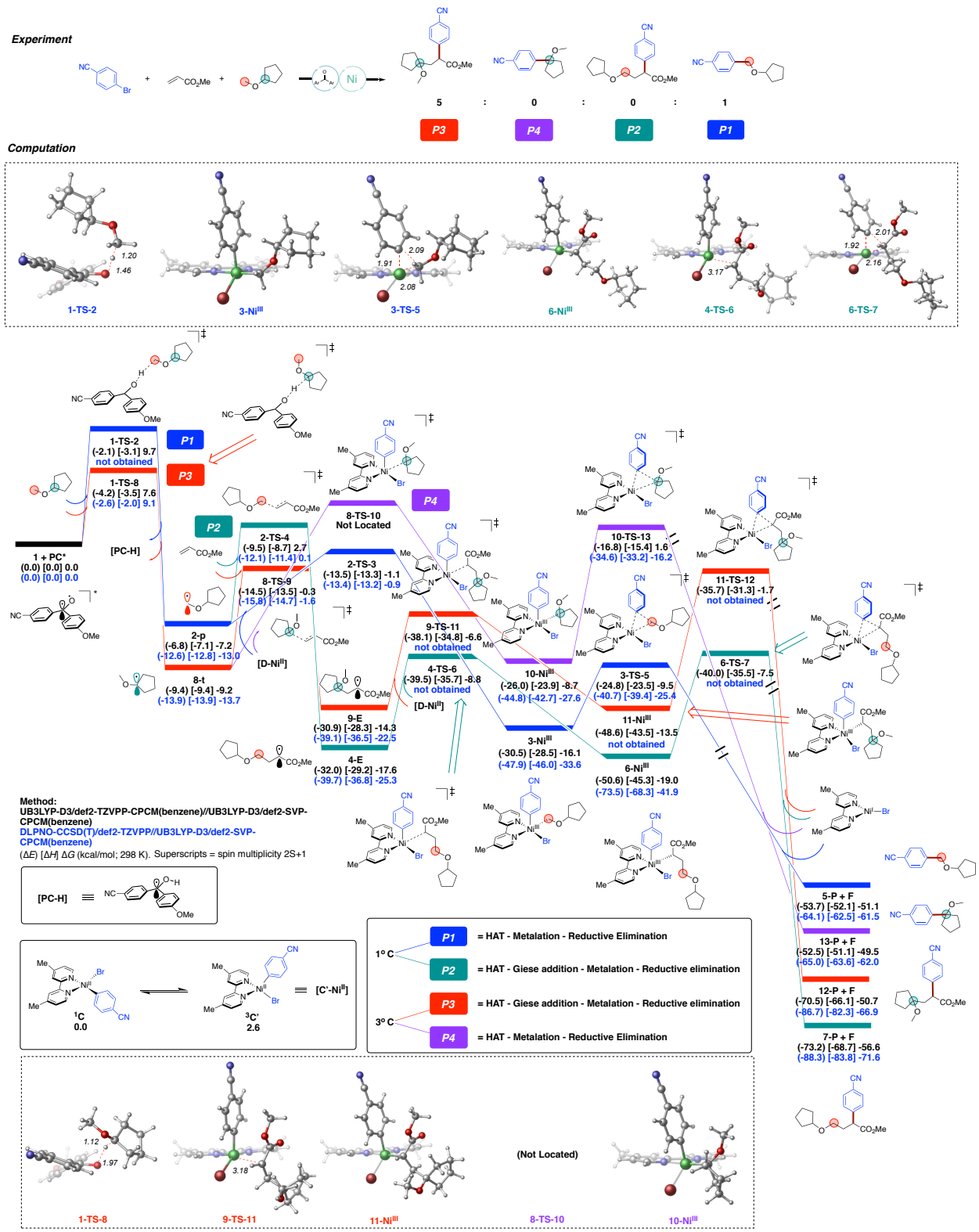


Figure A2.2 Calculation of divergent pathways forming DCF and CC products in the cyclopentyl methyl ether (CPME) system. Electronic (in parenthesis), enthalpy (in bracket) and free energy values given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-

D3/def2-SVP-CPCM(benzene) (black) and DLPNO-CCSD(T)/def2-TZVPP//(U)B3LYP-D3/def2-SVP-CPCM(benzene) (blue) levels of theory.

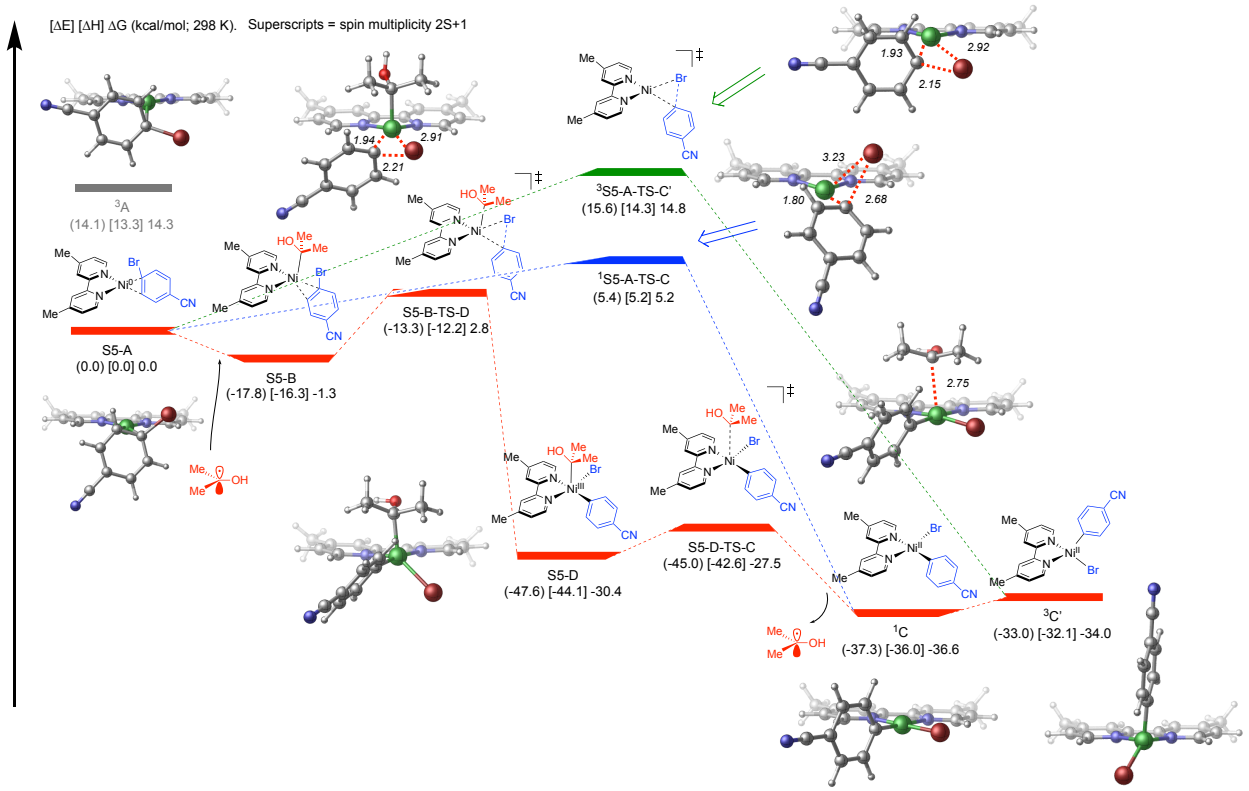


Figure A2.3 Calculation of Ni^0/Ni^{II} and $Ni^0/Ni^I/Ni^{III}/Ni^{II}$ pathways in the isopropyl alcohol system. Electronic (in parenthesis), enthalpy (in bracket) and free energy values given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of theory.

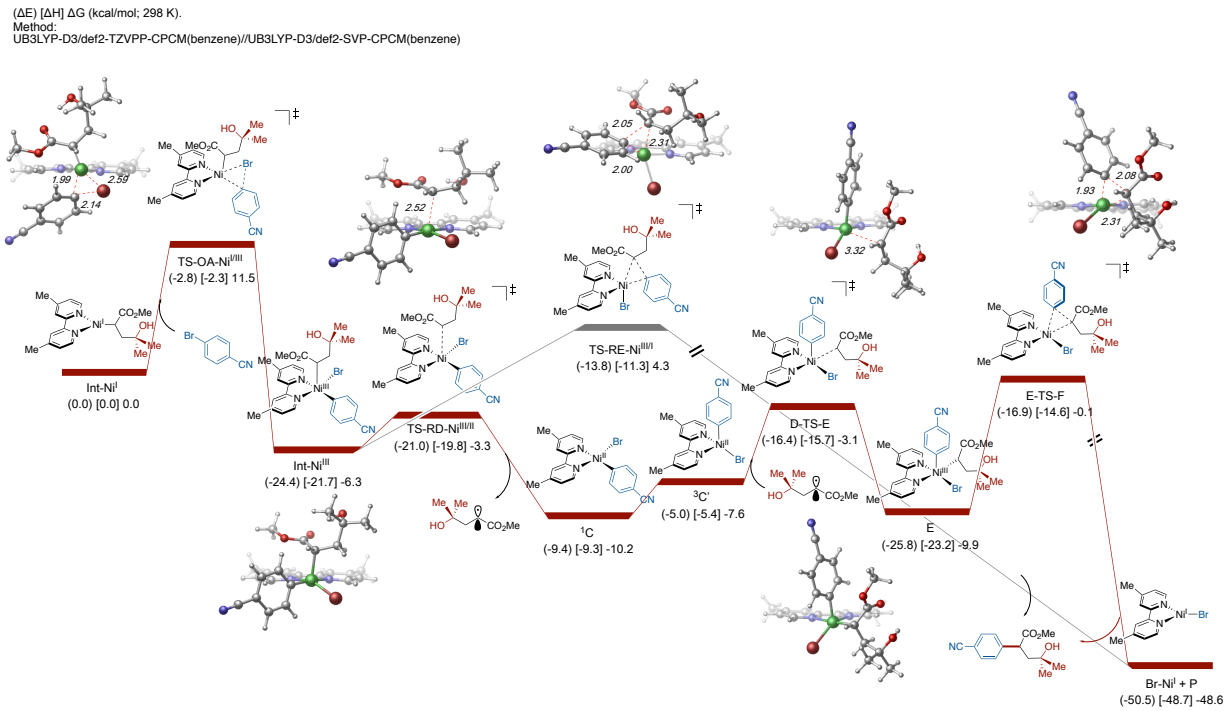


Figure A2.4 Calculation of Ni^0/Ni^{II} and $Ni^0/Ni^I/Ni^{III}/Ni^{II}$ pathways in the isopropyl alcohol system with α-ester radical. Electronic (in parenthesis), enthalpy (in bracket) and free energy values given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of theory.

To examine the different behavior of varied alkyl radicals in our proposed mechanism, we also explored the fate of Ni(III) intermediate (**Int-Ni^{III}**) with α-ester radical (presumably generated from radical addition to acrylate). Based on the energetics, oxidative addition of alkyl Ni(I) (via **TS-OA-Ni$^{I/III}$**) will lead to the desired Ni(III) intermediate. In turn, consistent with prior mechanistic model, the favored pathway is *radical dissociation* (via **TS-RD-Ni$^{III/II}$**) to afford the *singlet square planar* Ni(II) intermediate and the corresponding α-ester radical. Note that the barrier for direct C-C bond formation via **TS-RE-Ni$^{III/I}$** from the Ni(III) is much higher in energy. Finally, the square planar Ni(II) will need to undergo an isomerization to the tetrahedral Ni(II) to undergo productive (and energetically favored) C–C bond formation (after radical addition). Overall, the results presented here involving secondary α radical are consistent with our previous report that radical dissociation from the Ni(III) intermediate with "wrong" spatial arrangement is

more favorable than direct reductive elimination, and the alkyl radical needs to reassociate to the *tetrahedral* Ni(II) complex prior to reductive elimination.

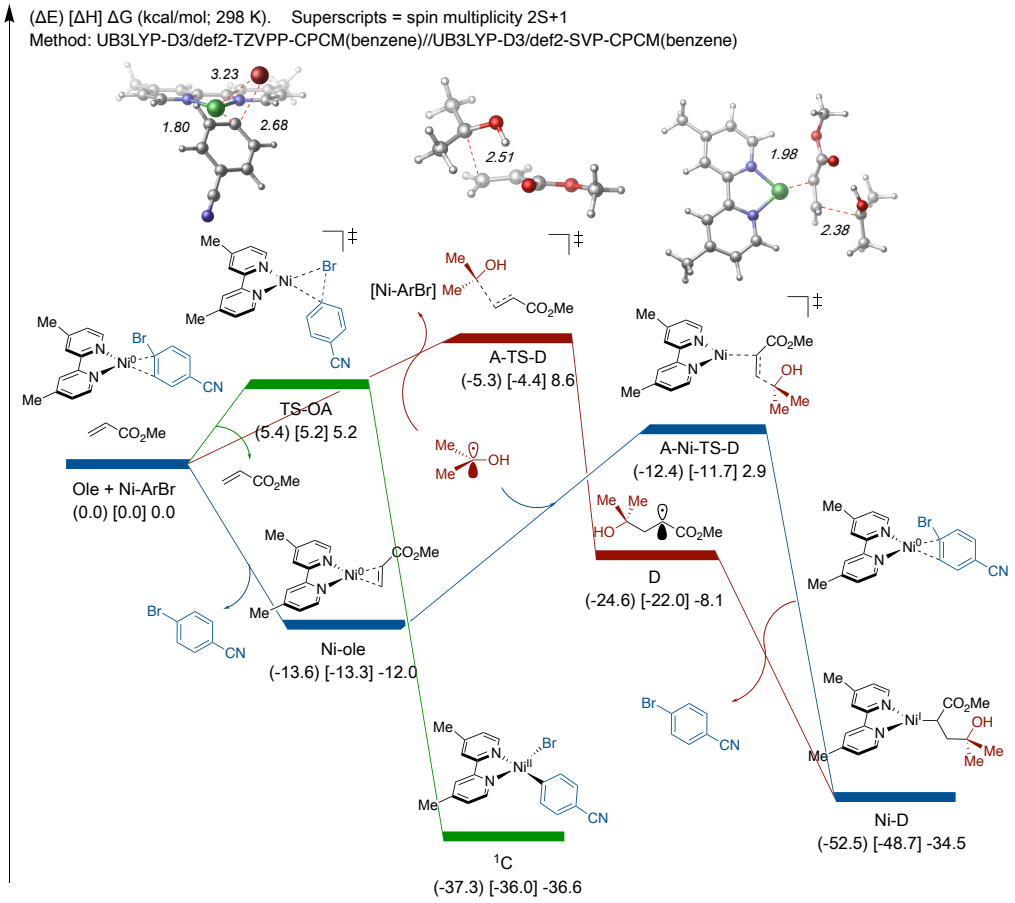


Figure A2.5 Comparison of divergent pathways forming α-ester radical and oxidative addition pathway from Ni(0) and aryl bromide. Electronic (in parenthesis), enthalpy (in bracket) and free energy values given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of theory.

We also considered the possibility of Ni species binding to alkene to facilitate the addition of alkyl radical to acrylate, and the energetics were shown above. Notably, in both cases (highly dependent on relative concentration of each species and solvation) both pathways will lead to rapid formation of the Ni(I)-alkyl intermediate, which, as we have shown above, will also converge to the square planar Ni(0) and lead to the same C–C bond formation [after isomerization to tetrahedral Ni(II) followed by radical addition/reductive elimination]. Overall, although the binding of Ni

center to olefin is thermodynamically favorable (barrier for decomplexation/association not calculated), the barrier for radical adding to the Ni(0)-bound alkene (blue, via **A-Ni-TS-D**) was found to be 14.9 kcal/mol with respect to **Ni-ole**. On the other hand, the barrier for direct radical addition to alkene (red, via **A-TS-D**) was 8.6 kcal/mol. These results show that the un-complexed *barriers* for Giese addition to alkene is lower than with the complex. Further, the barrier for oxidative addition from Ni(0)-ArBr is only 5.2 kcal/mol (see before), meaning that at low concentration of alkyl radical and/or alkene, computations showed that Ni(0) will quickly undergo oxidative addition to form the Ni(II) complex **^{1}C**. In parallel, radical addition to (un-complexed) olefin is also favorable. Finally, even if radical addition to complex-olefin proceeds, it will lead to alkyl Ni(I) **Ni-D** which, as shown above, will undergo facile oxidative addition followed by *radical dissociation* to form a square planar Ni(II) thus all pathways converging to the same intermediate. After that, the square planar Ni(II) will undergo isomerization to the tetrahedral Ni(II) followed by productive radical addition and reductive elimination.

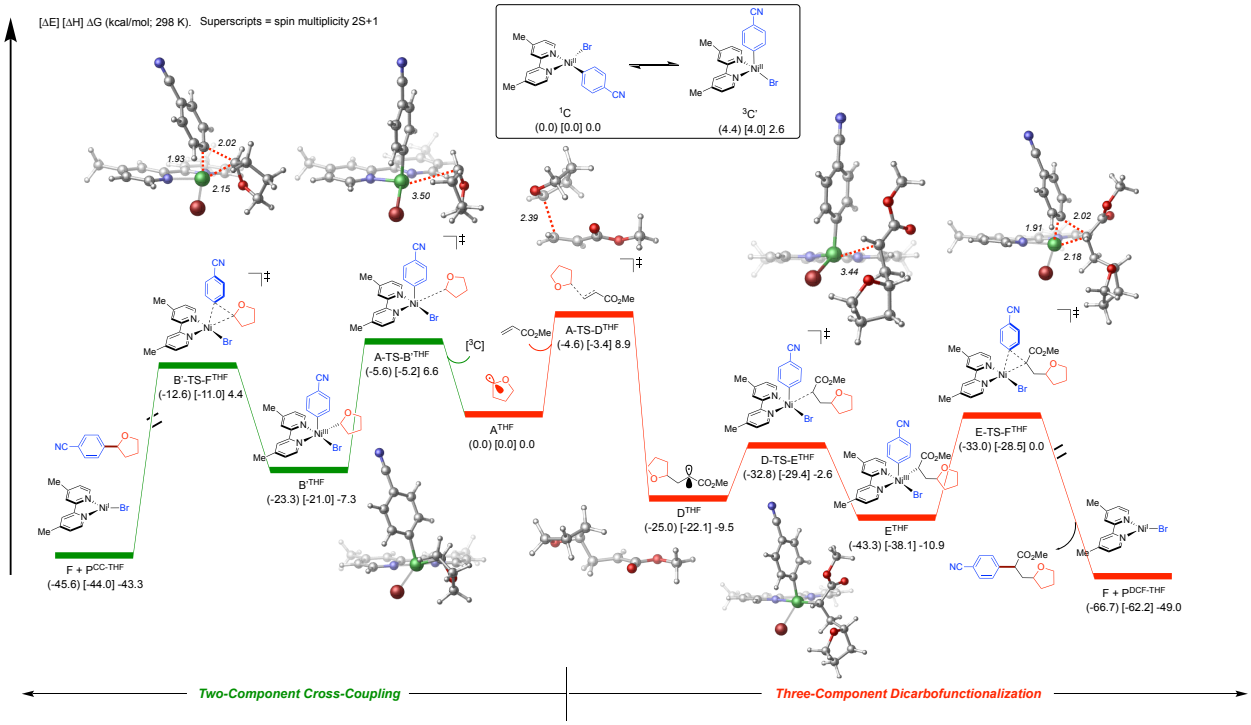
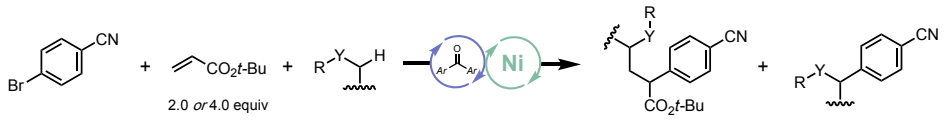


Figure A2.6 Calculation of divergent pathways towards DCF and CC products from Ni(II) complex, alkyl radical and olefin in the THF system. Electronic (in parenthesis), enthalpy (in bracket) and free energy values given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene)//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of theory.

Table A2.2 Computed Barrier for Giese Addition and Metalation of Different Substrates[a]



Entry	1	2	3	4	5	6	7	8	9	10	11
2 equiv. of acrylate (DCF:CC)	1:0	2.3:1	1:7.6†	2.7:1	1.3:1	1:1	1:1.3	1.1:1	1:1.3	1:6.1	4.4:1
Barrier for Giese Addition [a]	11.1	11.7	11.6	13.6	12.3	10.3	12.4	13.8	9.0	16.3	12.5
Barrier for Metalation [a]	11.5	/	/	/	12.2	12.4	/	/	14.8	10.1	/
Barrier for Giese Addition [b]	8.6	8.8	8.7	10.0	8.9	9.1	9.6	11.0	7.6	14.0	10.9
Barrier for Metalation [b]	6.6	/	/	/	6.6	6.6	/	/	8.1	7.1	/

†: using acrylonitrile in place of *t*Bu acrylate

[a] Free energy values given were calculated at the DLPNO-CCSD(T)/def2-TZVPP//(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of theory.
[b] Free energy values given were calculated at the (U)B3LYP-D3/def2-TZVPP-CPCM(benzene) //(U)B3LYP-D3/def2-SVP-CPCM(benzene) level of theory.

A2.3 Coordinates and Energies

Figure 3.2

A

C	-0.34885400	-0.30409300	2.42103500
C	-1.34898600	-1.41058500	2.31775600
H	-2.27071900	-1.06497100	1.82498400
H	-0.95670200	-2.26334300	1.73426700
H	-1.63716000	-1.80807100	3.31705900
C	-0.75302600	1.05727200	2.87559700
H	0.05601000	1.78447000	2.69826900
H	-1.65625900	1.39868600	2.34685200
H	-0.97683100	1.08175600	3.96540600
O	0.92231100	-0.64068800	2.82990300
H	1.10713700	-1.55542100	2.57559900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.093480 (Hartree/Particle)
Thermal correction to Energy= 0.099157
Thermal correction to Enthalpy= 0.100102
Thermal correction to Gibbs Free Energy= 0.065120
Sum of electronic and zero-point Energies= -193.474990
Sum of electronic and thermal Energies= -193.469313
Sum of electronic and thermal Enthalpies= -193.468368
Sum of electronic and thermal Free Energies= -193.503350
HF=-193.5684701
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-193.7976445
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-193.384634117296

^{1}C

C	-2.95592600	0.10967300	-0.42632600
C	-2.13688800	0.26429100	0.70876400
C	-2.64887800	1.00666700	1.79045300
C	-3.91052300	1.59817000	1.73824700
C	-4.70800300	1.45025500	0.58518800
C	-4.22028600	0.69303800	-0.49938200
Br	-1.26704800	-2.38717900	1.63783800
H	-2.04708200	1.12812900	2.69549800
H	-2.59734700	-0.47942500	-1.27502500
H	-4.83906400	0.56692200	-1.39115500
H	-4.28835500	2.17561000	2.58552800
C	2.40952500	-0.08261200	0.24464200
C	2.04715200	-2.18790600	1.14231800
C	3.40339900	-2.49329100	1.08749300
C	4.31231700	-1.54885400	0.58607000
C	3.78530600	-0.32351200	0.16105400
C	1.76004900	1.17579100	-0.17759300
C	-0.24589900	2.32209600	-0.37401500
C	0.38986000	3.43531000	-0.90981200
C	1.78068200	3.42775500	-1.09254600
C	2.45723600	2.26413400	-0.71163600
H	1.30550700	-2.89370100	1.52423800
H	3.74711300	-3.46932200	1.43687100
H	4.45419300	0.44062600	-0.23493000
H	-1.32442100	2.31129700	-0.22594000
H	-0.20758400	4.30740000	-1.18365100
H	3.53878500	2.20772500	-0.83396300
N	1.55612500	-1.01042400	0.73112600
N	0.41176500	1.20570300	-0.00972200
Ni	-0.38343500	-0.41490900	0.74500600
C	2.49815700	4.61637600	-1.66834700
H	2.09710800	4.86550200	-2.66413900
H	2.34795200	5.50347000	-1.03156100
H	3.57836700	4.43826000	-1.76389900
C	5.78357900	-1.85043100	0.51018000
H	6.17727300	-2.11258900	1.50547500
H	5.96598200	-2.71778000	-0.14516300
H	6.35922300	-0.99809200	0.12281700
C	-6.00142600	2.06433500	0.51590700
N	-7.04832700	2.56701900	0.45779000

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.304972 (Hartree/Particle)
Thermal correction to Energy= 0.328052
Thermal correction to Enthalpy= 0.328996
Thermal correction to Gibbs Free Energy= 0.246282
Sum of electronic and zero-point Energies= -4979.154063
Sum of electronic and thermal Energies= -4979.130983
Sum of electronic and thermal Enthalpies= -4979.130039
Sum of electronic and thermal Free Energies= -4979.212753
HF=-4979.4590352
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4980.9686485
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4976.621685424276

^{3}C'

C	-2.37859000	1.50062200	0.11727800
C	-3.34140300	2.42253700	0.54511800
C	-2.94837200	3.63106000	1.13313900
C	-1.56906300	3.86075300	1.27343100
C	-0.66728200	2.89904400	0.83144200
C	-2.69901200	0.18879400	-0.50271600
C	-3.99534400	-0.26526800	-0.77198200
C	-4.19074700	-1.52273800	-1.35783500
C	-3.04685300	-2.28178000	-1.65893000
C	-1.78742800	-1.76989300	-1.36538400
H	-4.40262000	2.20231700	0.42724100
H	-1.19870100	4.78167400	1.72861600
H	0.41182900	3.03641000	0.93822400

H	-4.85842500	0.35553800	-0.53037300
H	-3.13627700	-3.26692200	-2.12146000
H	-0.86585600	-2.31387400	-1.58809900
N	-1.06018500	1.75380500	0.26205700
N	-1.62493600	-0.56959000	-0.79896700
Br	1.75545500	-0.46949900	-1.90342200
Ni	0.17420800	0.18558200	-0.24385900
C	0.45600200	-0.56122000	1.56987100
C	-0.50130000	-0.47594700	2.60020000
C	1.65135900	-1.24850600	1.86585700
C	-0.29186900	-1.03516400	3.86122000
H	-1.44828100	0.04469600	2.41973100
C	1.89149800	-1.81414100	3.11930500
H	2.41405200	-1.34598200	1.08690500
H	-1.05178000	-0.95574600	4.64292400
H	2.82759600	-2.33969700	3.32450500
C	0.91555300	-1.71044600	4.13059500
C	-3.95197100	4.64715600	1.60382000
H	-4.98529000	4.31184300	1.43819100
H	-3.82089500	4.85130000	2.67880600
H	-3.80891400	5.60398200	1.07575300
C	-5.56709800	-2.05198200	-1.65366600
H	-5.76526800	-2.95912500	-1.05930900
H	-6.34916300	-1.31421200	-1.42597800
H	-5.65459000	-2.33770400	-2.71408800
C	1.14549900	-2.28764600	5.42333800
N	1.32860600	-2.75409600	6.47247300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.303703 (Hartree/Particle)
Thermal correction to Energy= 0.327376
Thermal correction to Enthalpy= 0.328320
Thermal correction to Gibbs Free Energy= 0.243434
Sum of electronic and zero-point Energies= -4979.151831
Sum of electronic and thermal Energies= -4979.128158
Sum of electronic and thermal Enthalpies= -4979.127214
Sum of electronic and thermal Free Energies= -4979.212100
HF=-4979.4555336
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4980.9616702
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4976.625103352761

A-TS-B (S5-D-TS-C)

Ni	-0.55576900	0.11134400	-0.66804200
C	-1.79112000	1.54927900	-0.84453500
C	-3.52560400	3.76110200	-1.27822900
C	-2.99045400	1.69566900	-0.12086800
C	-1.51037800	2.52690800	-1.82208000
C	-2.35286500	3.61635500	-2.04460500
C	-3.84086700	2.78283100	-0.31296900
H	-3.28244200	0.92662600	0.59745700
H	-0.60206800	2.43993200	-2.42634900
H	-2.10984000	4.35936000	-2.80811400
H	-4.75921700	2.87730700	0.27150600
N	1.01689900	1.25421100	-0.14580100
C	3.28716400	2.56651800	0.90345200
C	0.97639900	2.55524100	0.19447600
C	2.17991300	0.57911200	0.04042900
C	3.31766100	1.21214700	0.55899700
C	2.06852400	3.23927400	0.71176100
N	0.90778400	-1.31314400	-0.64185200
C	3.10874000	-3.06363100	-0.54881400
C	0.76128200	-2.61748500	-0.91474100
C	2.13245400	-0.85521200	-0.30215500
C	3.24667700	-1.70214900	-0.26183800
C	1.82027400	-3.51748100	-0.87300000
H	0.02137500	3.05676600	0.04400100
H	4.23486400	0.64222300	0.70697900
H	1.96483000	4.29646100	0.96496700
H	-0.25223900	-2.92584200	-1.18144000
H	4.22889300	-1.30509300	-0.00533400
H	1.63812700	-4.57002700	-1.10038800
Br	-2.22459600	-1.29424400	-1.63265200
C	-0.51666100	-0.31058600	2.04890400
C	4.28075300	-4.00568300	-0.52100200
H	4.47693100	-4.40628400	-1.52937000
H	5.19621300	-3.51318000	-0.16375700
H	4.07139000	-4.86851800	0.13137700
C	4.49340700	3.27879300	1.44896800
H	5.32115100	2.58582300	1.65574600
H	4.85052200	4.03371300	0.72861400
H	4.24535800	3.81576500	2.37834000
C	-1.45737900	-1.46582200	1.96668600
H	-2.39961400	-1.17517300	1.48449500
H	-1.01963600	-2.28233700	1.37581100
H	-1.68292300	-1.85912700	2.98068800
C	-0.95185900	0.97436100	2.67726700
H	-0.22652200	1.78438500	2.49073200
H	-1.92269600	1.30206800	2.28742000
H	-1.04339200	0.85803100	3.77780500
O	0.76546600	-0.70676400	2.33649400
H	1.30527100	0.06723800	2.54983900
C	-4.39012700	4.88616000	-1.48128400
N	-5.08836100	5.80186100	-1.64271700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.400782 (Hartree/Particle)
Thermal correction to Energy= 0.429793
Thermal correction to Enthalpy= 0.430737
Thermal correction to Gibbs Free Energy= 0.338090
Sum of electronic and zero-point Energies= -5172.649518
Sum of electronic and thermal Energies= -5172.620507
Sum of electronic and thermal Enthalpies= -5172.619563
Sum of electronic and thermal Free Energies= -5172.712210
HF=-5173.0503001
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.778422
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5170.012657626478

B (S5-D)

Ni	-0.53973700	0.14320000	-0.29890300
C	-1.88953000	1.51549100	-0.49177400
C	-3.72379400	3.56357400	-1.21866100
C	-3.23328600	1.47720500	-0.07958100
C	-1.50714400	2.58517800	-1.32464100
C	-2.39460300	3.60149300	-1.67968300
C	-4.13998600	2.47819400	-0.42200500
H	-3.60001100	0.64030700	0.51844200
H	-0.49747400	2.61978100	-1.74199600
H	-2.06658800	4.42103100	-2.32353200
H	-5.17646400	2.42353800	-0.08102600
N	1.23336900	1.32746300	0.03058300
C	3.64254200	2.53790400	0.82940500
C	1.27594400	2.62340200	0.36403600
C	2.36594600	0.59850100	0.10621900
C	3.58003700	1.17951100	0.49800600
C	2.44427300	3.26569400	0.76206800
N	0.96019200	-1.28214300	-0.37802400
C	3.10903300	-3.08229200	-0.54207700
C	0.74838900	-2.58130100	-0.61483100
C	2.22259400	-0.84542300	-0.20695100
C	3.31336200	-1.71858400	-0.30203800
C	1.78159100	-3.51052100	-0.68719000
H	0.32881600	3.16324900	0.31315400
H	4.48221200	0.57182100	0.56619100
H	2.41539700	4.32576400	1.02266600
H	-0.29128600	-2.87052400	-0.77584500
H	4.33028700	-1.34186100	-0.19302400
H	1.54770500	-4.56160700	-0.86883100
Br	-1.60698700	-0.93187400	-2.28097900
C	-0.80781100	-0.07217200	1.71047000
C	4.25747600	-4.04570900	-0.66409700
H	4.40182700	-4.33421500	-1.71900500
H	5.19912700	-3.60995800	-0.30085800
H	4.05735300	-4.97070000	-0.10149900
C	4.93346500	3.19583700	1.23141400
H	5.70424100	2.45820000	1.49640200
H	5.32212200	3.80652800	0.39880200
H	4.78392800	3.87340700	2.08595300
C	-1.75297300	-1.25720500	1.73277800
H	-2.67537800	-1.05685700	1.17327200
H	-1.27247500	-2.14368400	1.29682800
H	-2.02210900	-1.50306600	2.77740900
C	-1.28723200	1.14074000	2.48787900
H	-0.60778700	1.99613100	2.34685000
H	-2.29041500	1.46398400	2.19593900
H	-1.29851400	0.88561500	3.56399100
O	0.42271700	-0.50118300	2.23389400
H	0.94246900	0.27743500	2.47349600
C	-4.64275000	4.60764300	-1.56433300
N	-5.38598300	5.45773900	-1.84148800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.402420 (Hartree/Particle)
Thermal correction to Energy= 0.431649
Thermal correction to Enthalpy= 0.432593
Thermal correction to Gibbs Free Energy= 0.337558
Sum of electronic and zero-point Energies= -5172.655461
Sum of electronic and thermal Energies= -5172.626233
Sum of electronic and thermal Enthalpies= -5172.625288
Sum of electronic and thermal Free Energies= -5172.720323
HF=-5173.0578813
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.7825675
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5170.035403514842

B-TS-F

Ni	-0.49974800	0.42929400	-0.78654600
C	-1.80620800	1.74627300	-0.20118900
C	-3.29336800	4.17242400	-0.36401100
C	-3.04530900	1.80968200	-0.88407100
C	-1.37578700	2.93113500	0.44214000
C	-2.08310900	4.12504600	0.35731000
C	-3.76953300	2.99270200	-0.97723800
H	-3.42304900	0.91280200	-1.37759500
H	-0.46354100	2.91184100	1.04346100
H	-1.71092900	5.02419600	0.85394500
H	-4.71050900	3.01554200	-1.53175400
N	1.32645000	1.53200400	-0.48416000
C	3.78033600	2.80366300	0.02375600
C	1.48809100	2.83779800	-0.72667600
C	2.38361300	0.81458100	-0.05068100
C	3.60983700	1.42919500	0.23308800
C	2.68560800	3.50942100	-0.49736600
N	1.06257900	-1.09597100	-0.60199700
C	2.94188000	-2.93402200	0.37917300
C	0.87766100	-2.41006300	-0.75914600
C	2.19034900	-0.65986100	-0.01393100
C	3.13901400	-1.55256100	0.50121100
C	1.78540500	-3.35843200	-0.29322100
H	0.61293200	3.36426800	-1.11248800
H	4.45135000	0.83428600	0.58864500
H	2.75931000	4.57563700	-0.72174600
H	-0.03530500	-2.69124100	-1.29234900
H	4.03697800	-1.18119500	0.99619400
H	1.58782800	-4.42104100	-0.45101000
Br	-1.56672500	-0.72246400	-2.71803800
C	-1.61237600	0.16568700	1.23375900
C	3.92053700	-3.92486400	0.94850200
H	4.10426400	-4.75006200	0.24335400
H	4.88257000	-3.45434800	1.19734600
H	3.51514400	-4.37274900	1.87173500
C	5.07765300	3.49556800	0.34023700
H	5.91047000	2.78337100	0.42922500
H	5.32984000	4.23963800	-0.43050700
H	4.99428900	4.03677500	1.29827600
C	-2.01385800	-1.24620700	0.84232400
H	-2.75503300	-1.22886600	0.03388400
H	-1.16042200	-1.84257700	0.51146500
H	-2.45455800	-1.75224600	1.72054800
C	-2.70702900	0.78499300	2.09856600
H	-2.47454200	1.81292400	2.40895400
H	-3.67347500	0.79792600	1.57902400
H	-2.80100000	0.15935000	3.00372200
O	-0.39201500	0.16435700	1.91072000
H	-0.28097600	1.01594600	2.35579700

C	-4.03160100	5.39505300	-0.45883700
N	-4.62915000	6.39029400	-0.53203700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.402216 (Hartree/Particle)
Thermal correction to Energy= 0.430969
Thermal correction to Enthalpy= 0.431913
Thermal correction to Gibbs Free Energy= 0.338221
Sum of electronic and zero-point Energies= -5172.635878
Sum of electronic and thermal Energies= -5172.607125
Sum of electronic and thermal Enthalpies= -5172.606181
Sum of electronic and thermal Free Energies= -5172.699873
HF=-5173.038094
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.764352
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5170.017704334534

A-TS-B'

C	2.98893100	1.34924900	1.15585900
C	3.89562200	0.16500700	1.10395800
H	3.78175600	-0.37815200	0.15132600
H	3.67156700	-0.53393600	1.92151300
C	-2.13315900	1.34589100	-0.24784600
C	-2.89578500	2.49224600	0.00414600
C	-2.25813600	3.70787200	0.29031300
C	-0.85178300	3.71954200	0.31713000
C	-0.15537900	2.54462500	0.05885800
C	-2.68298900	0.00058000	-0.55559000
C	-4.04525900	-0.30660600	-0.57434500
C	-4.47204000	-1.61236700	-0.86130100
C	-3.48009600	-2.57234500	-1.10889300
C	-2.13833300	-2.19775800	-1.06975300
H	-3.98513600	2.44788900	-0.02194000
H	-0.30342700	4.63700900	0.54033900
H	0.92945000	2.43186400	0.06932800
H	-4.78396800	0.46627100	-0.35777800
H	-3.74511100	-3.60884400	-1.32591000
H	-1.33919600	-2.92301900	-1.24393300
N	-0.78899500	1.39736900	-0.21395300
N	-1.75014400	-0.94738200	-0.80895300
Br	1.94465100	0.01515200	-2.22812700
Ni	0.20017100	-0.32488800	-0.57645800
C	0.52471300	-1.11495900	1.19842900
C	0.05513600	-0.55320900	2.40191500
C	1.22812500	-2.33331500	1.29526000
C	0.28507600	-1.15041400	3.64069700
H	-0.49706200	0.39189100	2.37488600
C	1.46479900	-2.96044800	2.51925100
H	1.62410700	-2.80097400	0.38688500
H	-0.07859100	-0.68695300	4.56138900
H	2.01705200	-3.90239000	2.56722600
C	0.99594500	-2.36705500	3.70834000
C	-3.04179000	4.96685300	0.54290500
H	-2.65305700	5.50236600	1.42294800
H	-2.94771900	5.65149400	-0.31699400
H	-4.11034100	4.76211500	0.69899700
C	-5.93734600	-1.94407200	-0.92874800
H	-6.11510900	-3.02702100	-0.87200000
H	-6.49861800	-1.45069200	-0.12001100
H	-6.35850300	-1.58162300	-1.88224200
H	4.96155400	0.46885800	1.19113000
C	2.64081500	2.00083400	2.44848600
H	3.47886400	2.61616400	2.84337700
H	1.77546300	2.67472600	2.33582500
H	2.39572800	1.24243300	3.20665700
C	1.23591300	-2.99424700	4.97494600
N	1.42811700	-3.50222900	6.00314200
O	3.01361000	2.21523000	0.08944400
H	3.01575200	1.68454200	-0.73601800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.398693 (Hartree/Particle)
Thermal correction to Energy= 0.428802
Thermal correction to Enthalpy= 0.429746
Thermal correction to Gibbs Free Energy= 0.331039
Sum of electronic and zero-point Energies= -5172.648928
Sum of electronic and thermal Energies= -5172.618819
Sum of electronic and thermal Enthalpies= -5172.617875
Sum of electronic and thermal Free Energies= -5172.716582
HF=-5173.0476208
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.7754139
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5170.007622406840

B'

C	2.38674300	0.70319400	0.21121900
C	3.35545300	-0.42764700	-0.11548000
H	3.20845300	-0.80570000	-1.13638900
H	3.23919800	-1.25898700	0.59294500
C	-1.99146500	1.46062900	0.04714600
C	-2.90524200	2.48686700	0.31567100
C	-2.45592600	3.79392600	0.53932000
C	-1.07286100	4.01612800	0.45816100
C	-0.21877000	2.94952400	0.19237900
C	-2.39651700	0.06499500	-0.25955000
C	-3.72553800	-0.37917900	-0.29414300
C	-4.01434300	-1.70610700	-0.63304500
C	-2.92872400	-2.54534000	-0.93561900
C	-1.63596100	-2.03672400	-0.87505900
H	-3.97429100	2.27592200	0.34317400
H	-0.65707100	5.01646300	0.59607400
H	0.86053300	3.07916000	0.09458400
H	-4.54228200	0.30378000	-0.05995400
H	-3.08917300	-3.58888400	-1.21457300
H	-0.76438800	-2.65488700	-1.10359000
N	-0.66256500	1.69914300	0.01425400
N	-1.38203800	-0.76961800	-0.54100500
Br	0.92337300	-0.08088200	-2.71017700
Ni	0.53512800	0.00117200	-0.22717700
C	0.45905700	-0.80188300	1.52849300

C	-0.14547600	-0.18165400	2.63438700
C	0.84289500	-2.14830000	1.65834700
C	-0.35644900	-0.86736300	3.82982800
H	-0.45580200	0.86438500	2.56876200
C	0.64252000	-2.85514400	2.84513300
H	1.30717500	-2.66859400	0.81446600
H	-0.82635500	-0.36792500	4.68048500
H	0.94871100	-3.90068200	2.92723600
C	0.03849500	-2.21562100	3.94494800
C	-3.40760200	4.91475200	0.85544500
H	-3.18254200	5.80547900	0.24853800
H	-4.45383800	4.62620500	0.68124900
H	-3.30817000	5.21165900	1.91314600
C	-5.42632100	-2.22253100	-0.68340200
H	-5.68140400	-2.54834900	-1.70518000
H	-5.54241300	-3.10053900	-0.02785600
H	-6.15431000	-1.45966100	-0.37361400
H	4.38924400	-0.04403700	-0.03232800
C	2.59197600	1.25423400	1.60942500
H	1.77703000	1.92713700	1.91108000
H	2.66194100	0.45075000	2.35193000
H	3.53233800	1.83384900	1.61855600
C	-0.17757000	-2.93020200	5.16936700
N	-0.35608100	-3.50890500	6.16155900
O	2.50144500	1.78331100	-0.67087800
H	2.32528000	1.45009900	-1.57491700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.402717 (Hartree/Particle)
Thermal correction to Energy= 0.431707
Thermal correction to Enthalpy= 0.432652
Thermal correction to Gibbs Free Energy= 0.338878
Sum of electronic and zero-point Energies= -5172.675440
Sum of electronic and thermal Energies= -5172.646450
Sum of electronic and thermal Enthalpies= -5172.645506
Sum of electronic and thermal Free Energies= -5172.739279
HF=-5173.078157
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.8017283
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5170.066193230873

B'-TS-F

C	2.38670900	0.62068800	0.61004300
C	3.54727900	-0.35327200	0.59961900
H	3.46910500	-1.05652300	-0.24087400
H	3.60548100	-0.91929500	1.53784600
C	-2.03298500	1.56226300	0.00323700
C	-2.93779900	2.60456000	0.24000300
C	-2.48072800	3.92171700	0.36640200
C	-1.09952400	4.13626700	0.22738400
C	-0.25628100	3.05362800	-0.00066700
C	-2.43950400	0.15026700	-0.20824000
C	-3.73766600	-0.33518600	-0.00723600
C	-4.02925400	-1.68184500	-0.25641800
C	-2.97779300	-2.49403400	-0.71402400
C	-1.71022100	-1.94652900	-0.88242900
H	-4.00619800	2.39755400	0.30757100
H	-0.68034400	5.14271300	0.29194800
H	0.82071600	3.17646600	-0.12819000
H	-4.52480000	0.32800500	0.35307500
H	-3.14376100	-3.55116900	-0.93255400
H	-0.85913700	-2.53832600	-1.22891600
N	-0.70505200	1.79390600	-0.08862800
N	-1.44939200	-0.65879000	-0.63325400
Br	1.53185100	-1.12280800	-2.33537800
Ni	0.43989300	0.09191700	-0.41321200
C	0.80828000	-0.70564100	1.29300300
C	0.07899900	-0.24575600	2.40997800
C	1.13670700	-2.07760500	1.24253400
C	-0.34338700	-1.11456900	3.41079200
H	-0.19099000	0.80942600	2.48279000
C	0.72196700	-2.95928700	2.23623500
H	1.69409000	-2.46019900	0.38567200
H	-0.92714000	-0.74011200	4.25493200
H	0.96818600	-4.02130000	2.16566500
C	-0.02788200	-2.48757500	3.33399800
C	-3.42045600	5.06580700	0.63160000
H	-3.27870200	5.86859100	-0.10939700
H	-4.47226400	4.74807100	0.60446900
H	-3.22017800	5.50496000	1.62309100
C	-5.40430500	-2.24957800	-0.03281800
H	-5.75549900	-2.78858800	-0.92706800
H	-5.38898500	-2.97715000	0.79570600
H	-6.13659700	-1.46754600	0.21297000
H	4.47761700	0.22910600	0.47775800
C	2.41085200	1.55853900	1.79662600
H	1.51104900	2.18513100	1.84770100
H	2.50265700	1.00550200	2.73924400
H	3.28247900	2.22666700	1.68705700
C	-0.46879800	-3.38911200	4.35521000
N	-0.83239400	-4.12012200	5.18355100
O	2.39423500	1.43004100	-0.55286500
H	2.55336300	0.85634100	-1.33297200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.402217 (Hartree/Particle)
Thermal correction to Energy= 0.430521
Thermal correction to Enthalpy= 0.431465
Thermal correction to Gibbs Free Energy= 0.340026
Sum of electronic and zero-point Energies= -5172.658902
Sum of electronic and thermal Energies= -5172.630598
Sum of electronic and thermal Enthalpies= -5172.629654
Sum of electronic and thermal Free Energies= -5172.721092
HF=-5173.0611185
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.7834431
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5170.043291122486

F

Ni	0.03233200	0.43854100	2.37428500

N	-1.22126000	1.78636300	1.65716700
C	-3.08993200	3.51217600	0.47448000
C	-1.33869800	3.05450100	2.07732800
C	-2.01496700	1.34333100	0.65331600
C	-2.95563600	2.18666900	0.04718600
C	-2.25041200	3.94265100	1.51982100
N	-0.80929600	-0.67550200	1.02859700
C	-2.18037800	-2.10025600	-0.98309100
C	-0.52169200	-1.96671700	0.77263900
C	-1.78065500	-0.06979900	0.29130000
C	-2.47261900	-0.75995300	-0.71144700
C	-1.17123500	-2.70378900	-0.20696300
H	-0.66675100	3.34215500	2.89064500
H	-3.58725100	1.81351900	-0.76020500
H	-2.30912000	4.96637900	1.89621600
H	0.26453700	-2.40752300	1.39043500
H	-3.24687500	-0.25040300	-1.28692400
H	-0.89392800	-3.74807000	-0.36793400
Br	1.49136000	0.93260300	4.10225800
C	-2.90219000	-2.87460900	-2.05208300
H	-3.40461600	-3.75765400	-1.62370700
H	-3.65984200	-2.26160000	-2.56082000
H	-2.19413500	-3.24668000	-2.81103300
C	-4.08696300	4.45090600	-0.14941500
H	-4.78921700	4.83376100	0.60920100
H	-3.57776800	5.32645800	-0.58479300
H	-4.66998300	3.96224700	-0.94298400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.214556 (Hartree/Particle)
Thermal correction to Energy= 0.230691
Thermal correction to Enthalpy= 0.231635
Thermal correction to Gibbs Free Energy= 0.166314
Sum of electronic and zero-point Energies= -4655.572211
Sum of electronic and thermal Energies= -4655.556076
Sum of electronic and thermal Enthalpies= -4655.555132
Sum of electronic and thermal Free Energies= -4655.620454
HF=-4655.7867678
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4656.9522739
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4653.326579669174

P^CC

C	2.70923800	0.39927000	0.99986900
C	3.93420400	0.05349200	1.86226900
H	4.06477600	-1.03876500	1.93328200
H	3.85321900	0.45149500	2.88392100
C	1.43025200	-0.25891200	1.54269000
C	1.10037700	-0.19972500	2.90825600
C	0.53801300	-0.89784100	0.66794300
C	-0.07537700	-0.76882300	3.39083100
H	1.76625700	0.30142300	3.61321700
C	-0.64220800	-1.47412700	1.13544100
H	0.77643600	-0.93458700	-0.39540200
H	-0.31620800	-0.71615400	4.45432500
H	-1.32494200	-1.96888900	0.44184900
C	-0.95785800	-1.41586000	2.50467400
H	4.83185100	0.48483400	1.39487300
C	2.50148000	1.91783200	0.92721600
H	1.65675700	2.14866400	0.26145800
H	2.28862300	2.33404700	1.92251400
H	3.40720800	2.39554100	0.52342700
C	-2.16986800	-2.00841000	2.99530400
N	-3.15035900	-2.48775900	3.39302700
O	2.95621600	-0.00865700	-0.34387300
H	3.20609800	-0.94372600	-0.33704900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.187559 (Hartree/Particle)
Thermal correction to Energy= 0.198839
Thermal correction to Enthalpy= 0.199783
Thermal correction to Gibbs Free Energy= 0.150394
Sum of electronic and zero-point Energies= -517.113576
Sum of electronic and thermal Energies= -517.102296
Sum of electronic and thermal Enthalpies= -517.101352
Sum of electronic and thermal Free Energies= -517.150741
HF=-517.3011351
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-517.8827394
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-516.759587569435

A-TS-D

C	-5.29864800	4.47809000	-2.64546400
H	-4.37043400	4.51790100	-3.23613700
H	-6.07303400	3.95061100	-3.22141700
H	-5.64149600	5.52312100	-2.49662400
C	-5.05294000	3.81090100	-1.33374600
C	-4.15335400	1.54636200	-1.93582000
H	-4.78375400	1.28849100	-1.08513500
H	-4.59097800	1.45335500	-2.93203300
C	-2.80977200	1.68071300	-1.76741500
C	-6.20629200	3.36278900	-0.48879600
H	-5.86124100	2.75290300	0.36173800
H	-6.74359500	4.23903900	-0.07110900
H	-6.92872200	2.77487900	-1.07484400
H	-2.12015700	1.76093200	-2.61051100
O	-3.95767200	4.27882400	-0.69469300
H	-3.74230100	3.68159800	0.05129100
C	-2.24554600	1.81650100	-0.42738700
O	-2.88928500	2.05960800	0.59315300
O	-0.90763400	1.68088700	-0.40680700
C	-0.26575200	1.85981600	0.85607800
H	-0.61984300	1.11616700	1.58663700
H	0.80865800	1.73143400	0.67535900
H	-0.46638300	2.86480300	1.25938900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.190823 (Hartree/Particle)
Thermal correction to Energy= 0.203080
Thermal correction to Enthalpy= 0.204024

Thermal correction to Gibbs Free Energy= 0.151878
Sum of electronic and zero-point Energies= -499.644195
Sum of electronic and thermal Energies= -499.631938
Sum of electronic and thermal Enthalpies= -499.630994
Sum of electronic and thermal Free Energies= -499.683140
HF=-499.8350179
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-500.4155434
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-499.377669396735

D

C	-4.85466700	4.27729600	-2.51015400
H	-3.78425300	4.34185400	-2.75760900
H	-5.39640200	3.85583700	-3.37070800
H	-5.22314700	5.29858800	-2.32880300
C	-5.06056500	3.43035300	-1.25283400
C	-4.48262500	1.98324000	-1.45586100
H	-4.79380100	1.38835300	-0.57980500
H	-4.95524300	1.54803800	-2.34946100
C	-3.00479700	1.92521200	-1.56641200
C	-6.55103500	3.32184800	-0.90480500
H	-6.68461400	2.75744300	0.03183800
H	-6.96916300	4.32955600	-0.75846600
H	-7.12136900	2.81600900	-1.70032000
H	-2.49319800	1.91162500	-2.53103500
O	-4.37016900	4.10035100	-0.20741800
H	-4.10723900	3.45198800	0.46675800
C	-2.19420300	1.95338000	-0.36259300
O	-2.64721900	2.05350600	0.77373600
O	-0.87528300	1.85907600	-0.61376900
C	-0.00887400	1.89935900	0.52119100
H	-0.22233700	1.06481000	1.20722600
H	1.01292600	1.81849500	0.13080000
H	-0.13289900	2.84350800	1.07421400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.194060 (Hartree/Particle)
Thermal correction to Energy= 0.205834
Thermal correction to Enthalpy= 0.206778
Thermal correction to Gibbs Free Energy= 0.156072
Sum of electronic and zero-point Energies= -499.673876
Sum of electronic and thermal Energies= -499.662102
Sum of electronic and thermal Enthalpies= -499.661158
Sum of electronic and thermal Free Energies= -499.711864
HF=-499.8679363
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-500.4463221
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-499.419444581568

D-TS-E

Ni	-5.17269000	-0.00342200	0.57017900
C	-6.29694000	0.43277300	-1.00340000
C	-5.79314000	0.51345400	-2.31689000
C	-7.68804100	0.59782400	-0.84330800
C	-6.61748100	0.75177800	-3.41838600
H	-4.72038900	0.39073700	-2.49540500
C	-8.53579800	0.83979700	-1.92419900
H	-8.11570300	0.54213300	0.16181000
C	-8.00279300	0.91946400	-3.22646600
H	-6.20019800	0.81300500	-4.42665300
H	-9.60992000	0.97166400	-1.77182200
Br	-6.41506400	-0.24019600	2.63053800
C	-2.66309400	-0.86777200	-0.61580500
C	-1.41726300	-0.84000400	-1.25282400
C	-0.79422200	0.38259800	-1.53378300
C	-1.48162900	1.55026400	-1.16745500
C	-2.71987700	1.45377400	-0.53964900
C	-3.40746100	-2.11870100	-0.31786400
C	-2.93202000	-3.40495600	-0.59975200
C	-3.71831400	-4.52550500	-0.30314200
C	-4.97636500	-4.29628700	0.27876900
C	-5.38421700	-2.99247900	0.53924900
H	-0.92812500	-1.77015000	-1.54241300
H	-1.06217300	2.53658500	-1.37657700
H	-3.29523800	2.34597300	-0.28006200
H	-1.94896400	-3.54300300	-1.05011800
H	-5.63501400	-5.12951900	0.53233100
H	-6.34357600	-2.76186200	1.00846300
N	-3.28854600	0.27411700	-0.25432800
N	-4.61747000	-1.93655200	0.24586600
C	-3.24206300	-5.92354500	-0.58663400
C	0.55344000	0.45145700	-2.19696400
H	1.30880500	0.82472900	-1.48514900
H	0.88407700	-0.53146700	-2.56073800
H	0.53764500	1.15388200	-3.04492900
H	-2.26415900	-5.93076600	-1.08815700
H	-3.96443400	-6.45788800	-1.22440100
H	-3.15448500	-6.49759900	0.35028400
C	-8.86068600	1.17663500	-4.34656300
N	-9.55429900	1.38864200	-5.25517900
C	-5.07716500	4.81609700	4.21480500
H	-6.08036000	4.94111500	3.77998100
H	-5.14121700	4.11770600	5.06307800
H	-4.74391800	5.79641200	4.58877400
C	-4.09690700	4.31323800	3.15315600
C	-4.57961800	2.94966600	2.55670700
H	-3.76462500	2.57020700	1.91725900
H	-4.71369700	2.22680800	3.37319700
C	-5.82855700	3.03017300	1.75755000
C	-2.69653000	4.12017400	3.75015900
H	-1.98826900	3.80854800	2.96553700
H	-2.33998900	5.07188500	4.17322600
H	-2.69325800	3.35731500	4.54505900
H	-6.79624000	2.77946500	2.19099900
O	-4.04956000	5.31850100	2.14618900
H	-3.86652700	4.90274500	1.28800300
C	-5.80210300	3.53948900	0.40160400
O	-4.77350800	3.86197500	-0.19926600
O	-7.01676900	3.62768400	-0.15211000
C	-7.07256400	4.02434700	-1.52413300

H	-6.53316600	3.29896900	-2.15053700
H	-8.13428600	4.03510100	-1.79516500
H	-6.62741200	5.02174400	-1.65965800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.499525 (Hartree/Particle)
Thermal correction to Energy= 0.535878
Thermal correction to Enthalpy= 0.536822
Thermal correction to Gibbs Free Energy= 0.424795
Sum of electronic and zero-point Energies= -5478.849419
Sum of electronic and thermal Energies= -5478.813066
Sum of electronic and thermal Enthalpies= -5478.812122
Sum of electronic and thermal Free Energies= -5478.924148
HF=-5479.3489435
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5481.4261926

E

Ni	0.93891600	0.64738100	0.74815900
C	1.47948700	1.61152400	-0.82384500
C	2.08877500	3.23118300	-3.02694200
C	2.20213600	2.79773200	-0.64176900
C	1.06910500	1.23092700	-2.10664200
C	1.36679700	2.03517300	-3.20748900
C	2.50491700	3.60955000	-1.73483200
H	2.53174700	3.08190100	0.36073000
H	0.52821300	0.29450900	-2.25361800
H	1.04729700	1.74031000	-4.20958600
H	3.06926500	4.53436600	-1.59582300
N	-1.01959400	1.61297800	0.73911400
C	-3.51130200	2.88463200	0.65466100
C	-1.14303400	2.89171900	1.11171900
C	-2.09916100	0.93308600	0.31068100
C	-3.35857100	1.54887700	0.26539900
C	-2.36012500	3.56349000	1.08270300
N	-0.59003300	-0.88974300	-0.16892400
C	-2.65255200	-2.61684700	-0.97311300
C	-0.31566200	-2.11694700	-0.62734400
C	-1.87110400	-0.47269600	-0.13065400
C	-2.91921200	-1.31910100	-0.51908600
C	-1.30719900	-3.00629700	-1.03641000
H	-0.22656800	3.37351500	1.45819900
H	-4.22951700	0.99593400	-0.08497300
H	-2.40764400	4.60918600	1.39368000
H	0.74400000	-2.37174100	-0.70146100
H	-3.95246600	-0.97627700	-0.47120100
H	-1.02555300	-3.99492100	-1.40522900
Br	1.54088600	1.71351800	2.95517200
C	-3.75791700	-3.55805400	-1.36604300
H	-3.91346500	-4.31117500	-0.57494700
H	-4.71012000	-3.03086200	-1.52075900
H	-3.50345700	-4.10506800	-2.28676600
C	-4.84935000	3.57066100	0.62436500
H	-5.62424700	2.94159000	0.16416600
H	-5.17361300	3.82180300	1.64789900
H	-4.78968200	4.51782700	0.06517600
C	2.40347500	4.05678900	-4.15716500
N	2.65735500	4.72369300	-5.07439500
C	4.73156100	-1.34884900	2.81419200
H	5.06343000	-0.48854200	2.21584900
H	4.23018300	-0.97379000	3.71841600
H	5.62550800	-1.91900400	3.10986600
C	3.79618600	-2.24208600	1.99961200
C	2.49508800	-1.48733400	1.59303700
H	1.81370000	-2.21464000	1.12648300
H	2.01120300	-1.13773700	2.51693800
C	2.72256900	-0.31879100	0.64511100
C	3.41112600	-3.49404600	2.79945000
H	2.76929500	-4.15640800	2.19516300
H	4.31742300	-4.05398100	3.07648400
H	2.86343100	-3.23173200	3.71831300
H	3.41559700	0.43140000	1.03839400
O	4.54171700	-2.62247200	0.84121700
H	3.93891800	-3.04587500	0.21283400
C	3.12884100	-0.73440000	-0.72478100
O	2.70905400	-1.71676700	-1.32067000
O	4.02122800	0.10069800	-1.27173100
C	4.40792700	-0.16483900	-2.61996000
H	3.53329000	-0.11987100	-3.28675500
H	5.12753400	0.61719400	-2.89079500
H	4.87120000	-1.15950300	-2.70567400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.502514 (Hartree/Particle)
Thermal correction to Energy= 0.538833
Thermal correction to Enthalpy= 0.539778
Thermal correction to Gibbs Free Energy= 0.428923
Sum of electronic and zero-point Energies= -5478.866556
Sum of electronic and thermal Energies= -5478.830236
Sum of electronic and thermal Enthalpies= -5478.829292
Sum of electronic and thermal Free Energies= -5478.940147
HF=-5479.3690699
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5481.4411026
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5476.087074516803

E-TS-F

Ni	0.71969800	0.61065600	0.87543900
C	1.73951700	1.24597200	-0.62907300
C	1.94568900	3.10151600	-2.74781900
C	2.36850800	2.49522400	-0.43417800
C	1.26690800	0.92206200	-1.91984800
C	1.35396400	1.83895300	-2.96100000
C	2.45650200	3.41694900	-1.47101800
H	2.75798100	2.74458200	0.55444300
H	0.83683300	-0.06048000	-2.10821500
H	0.96527200	1.58226700	-3.94889100
H	2.92440200	4.38874600	-1.29927800
N	-1.12511600	1.62228000	0.82829100
C	-3.59418800	2.93351800	0.67491100
C	-1.24563300	2.89298300	1.23028700
C	-2.19872700	0.97156600	0.34247200

C	-3.44678100	1.60434200	0.26047700
C	-2.45136100	3.58338900	1.16695100
N	-0.67742000	-0.84821900	-0.08944900
C	-2.69556000	-2.53453300	-1.07957700
C	-0.38248300	-2.06017000	-0.57705800
C	-1.95830000	-0.42435500	-0.12058900
C	-2.98331300	-1.25052300	-0.60058400
C	-1.34970800	-2.92891300	-1.07574700
H	-0.33608200	3.34725700	1.63011000
H	-4.31118500	1.07184700	-0.13555600
H	-2.49825000	4.62134400	1.50327600
H	0.67717900	-2.32313500	-0.60889600
H	-4.01492300	-0.89909100	-0.60837000
H	-1.04879600	-3.90399800	-1.46454100
Br	1.52483800	1.67421000	3.01653700
C	-3.77981700	-3.45503100	-1.56808400
H	-4.02889300	-4.19375800	-0.78714900
H	-4.70024700	-2.90752900	-1.81677100
H	-3.45307500	-4.01895100	-2.45486300
C	-4.91753600	3.64475700	0.60137100
H	-5.69989200	3.01389900	0.15648800
H	-5.24858500	3.94741600	1.60833100
H	-4.83045600	4.56546700	0.00228000
C	2.03693800	4.04560100	-3.82032300
N	2.10817900	4.81104800	-4.69285500
C	4.74689200	-1.08749200	2.63762000
H	5.14073900	-0.32265400	1.95313400
H	4.21230500	-0.58189300	3.45483900
H	5.60475200	-1.63951700	3.05061900
C	3.82124600	-2.04931500	1.89247800
C	2.52586700	-1.33620800	1.39947200
H	1.86606300	-2.09801000	0.96372100
H	2.02907400	-0.94244000	2.29679800
C	2.80747700	-0.22925500	0.37067100
C	3.41405900	-3.21846600	2.79959500
H	2.76529500	-3.92526900	2.25573500
H	4.31136400	-3.76192000	3.13238700
H	2.86588300	-2.86546500	3.68699800
H	3.52037300	0.49737900	0.76263800
O	4.58619200	-2.53963900	0.78839500
H	4.00786400	-3.07834400	0.22928000
C	3.27604300	-0.81520200	-0.92132700
O	2.78404200	-1.79812000	-1.45160200
O	4.27624000	-0.11964600	-1.46951800
C	4.74244000	-0.56749200	-2.74353100
H	3.92805400	-0.54009300	-3.48381000
H	5.54389800	0.12168100	-3.03541500
H	5.12778700	-1.59623200	-2.67610900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.502906 (Hartree/Particle)
Thermal correction to Energy= 0.538491
Thermal correction to Enthalpy= 0.539435
Thermal correction to Gibbs Free Energy= 0.430304
Sum of electronic and zero-point Energies= -5478.851012
Sum of electronic and thermal Energies= -5478.815426
Sum of electronic and thermal Enthalpies= -5478.814482
Sum of electronic and thermal Free Energies= -5478.923613
HF=-5479.3539175
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5481.4269675
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5476.071812475649

p^DCF

C	2.05188800	0.54394800	-1.09543900
C	-0.10936800	1.90701400	-2.27980000
C	1.77546500	1.87781900	-0.75740300
C	1.23050700	-0.09987100	-2.03715400
C	0.16129300	0.56956200	-2.62719600
C	0.70766800	2.55949800	-1.33815500
H	2.40589400	2.39156500	-0.02744700
H	1.44325600	-1.13332700	-2.31647600
H	-0.46867700	0.06160200	-3.35987200
H	0.50339200	3.59708600	-1.06744100
C	-1.21078500	2.60183800	-2.88432200
N	-2.10214400	3.16376300	-3.37305700
C	4.35302300	-0.85016600	2.46664300
H	4.85900200	-0.04663700	1.91161900
H	3.58847800	-0.40367200	3.11987100
H	5.10806700	-1.34606000	3.09486800
C	3.72954400	-1.86902200	1.51092800
C	2.65596400	-1.22501700	0.60169500
H	2.13976900	-2.01829700	0.03589000
H	1.89542400	-0.74000000	1.23328600
C	3.19405600	-0.19537300	-0.41170100
C	3.09767500	-3.02393400	2.29976100
H	2.69097800	-3.78487200	1.61340600
H	3.85662200	-3.50415400	2.93572000
H	2.27447400	-2.66982500	2.94001900
H	3.81854700	0.54684300	0.10147600
O	4.82013300	-2.36124300	0.72459600
H	4.46957200	-2.97869300	0.06590000
C	4.06544800	-0.87688700	-1.45997500
O	3.79114200	-1.92575600	-2.00420900
O	5.14832300	-0.15364500	-1.75129300
C	6.04263300	-0.70632300	-2.72465300
H	5.52225200	-0.87958600	-3.67838400
H	6.84615900	0.02842700	-2.85358500
H	6.45264200	-1.66215800	-2.36468900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.287863 (Hartree/Particle)
Thermal correction to Energy= 0.306029
Thermal correction to Enthalpy= 0.306973
Thermal correction to Gibbs Free Energy= 0.240327
Sum of electronic and zero-point Energies= -823.310603
Sum of electronic and thermal Energies= -823.292437
Sum of electronic and thermal Enthalpies= -823.291493
Sum of electronic and thermal Free Energies= -823.358139
HF=-823.5984659
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-824.5282222

DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-822.791861407660

Figure 3.3
TS-17

C	-6.46057100	3.02123900	-0.76422500
H	-6.92347500	2.37005500	-1.52701000
H	-6.27959000	2.41538700	0.13520800
H	-7.20412000	3.80251900	-0.50159500
C	-5.18962200	3.63290300	-1.26064400
C	-3.93267700	1.52560100	-1.82284000
H	-4.51481600	1.07218700	-1.01840200
H	-4.39208200	1.60383100	-2.80948600
C	-2.60637100	1.74747500	-1.64607100
C	-4.20743100	4.23056300	-0.31435700
H	-3.25197700	4.42150700	-0.82775000
H	-4.57513400	5.19764100	0.08466700
H	-4.01705700	3.55055200	0.52730200
H	-1.96399000	2.10888000	-2.45213300
O	-5.24072600	4.28922600	-2.45659700
H	-5.96954900	3.94127100	-2.99006900
C	-1.99566300	1.58148100	-0.32170200
O	-2.58212200	1.28119900	0.70371500
O	-0.66315200	1.81873900	-0.35207500
C	0.02586800	1.69975600	0.89024800
H	-0.06877800	0.68146500	1.29949000
H	1.07935200	1.92699200	0.68331700
H	-0.37544500	2.40683500	1.63372200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.190348 (Hartree/Particle)
Thermal correction to Energy= 0.203037
Thermal correction to Enthalpy= 0.203981
Thermal correction to Gibbs Free Energy= 0.149969
Sum of electronic and zero-point Energies= -499.639122
Sum of electronic and thermal Energies= -499.626433
Sum of electronic and thermal Enthalpies= -499.625489
Sum of electronic and thermal Free Energies= -499.679500
HF=-499.8294698
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-500.4124648
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-499.373944293896

TS-18

C	-4.41977400	1.03922300	-1.92214300
H	-5.19891000	1.17846700	-1.17137400
H	-4.68321200	0.49299100	-2.82987000
C	-3.11872700	1.26127800	-1.59065200
H	-2.29743400	1.01577300	-2.26749300
C	-2.77168100	1.95687800	-0.35020600
O	-3.55647600	2.36944900	0.48710200
O	-1.43123700	2.11825300	-0.22563000
C	-0.98811000	2.80803000	0.93973900
H	-1.29405200	2.27740700	1.85542300
H	0.10680900	2.85132100	0.87729600
H	-1.40584200	3.82680900	0.97890200
C	-5.17943700	3.21875900	-2.78816800
O	-4.00306200	3.89341900	-2.85746100
C	-5.87611700	2.80747400	-4.05003700
H	-5.22507800	2.25211000	-4.74115700
H	-6.73615000	2.16683900	-3.80710100
H	-6.26468700	3.69183800	-4.59795500
C	-5.98764200	3.67582100	-1.61561300
H	-5.36551300	3.68778400	-0.70890300
H	-6.37558200	4.70046500	-1.78685600
H	-6.84916700	3.01294000	-1.44807200
C	-3.13660400	3.68281900	-3.95690800
H	-2.20410100	4.21681700	-3.72983500
H	-2.90873800	2.61233800	-4.09318000
H	-3.55930100	4.08262100	-4.89520000

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.218766 (Hartree/Particle)
Thermal correction to Energy= 0.232620
Thermal correction to Enthalpy= 0.233565
Thermal correction to Gibbs Free Energy= 0.177051
Sum of electronic and zero-point Energies= -538.885574
Sum of electronic and thermal Energies= -538.871719
Sum of electronic and thermal Enthalpies= -538.870775
Sum of electronic and thermal Free Energies= -538.927289
HF=-539.1043395
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-539.7275358
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-538.595815110508

TS-19

C	-5.01673100	3.83797500	-1.39894700
C	-4.18450000	1.51998100	-1.87956300
H	-4.80744600	1.33556900	-1.00353000
H	-4.64325300	1.38543500	-2.86133000
C	-2.83568400	1.62606300	-1.73795500
H	-2.15752200	1.64361500	-2.59382500
O	-3.95760100	4.28557000	-0.70302000
H	-3.75325800	3.65697000	0.02263700
C	-2.24722500	1.80877600	-0.41319800
O	-2.87011500	2.11888200	0.60210400
O	-0.91553800	1.63188400	-0.40259500
C	-0.25047600	1.84892100	0.84287700
H	-0.61222900	1.14620200	1.60923300
H	0.81747000	1.68549800	0.65284600
H	-0.42091600	2.87501300	1.20437200
H	-5.84958900	3.40206400	-0.83052100
C	-5.29148600	4.55027700	-2.67428000
H	-6.08933400	4.04849600	-3.24139900
H	-5.60985000	5.59736700	-2.49286200
H	-4.38042500	4.59338200	-3.29431300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.163039 (Hartree/Particle)

Thermal correction to Energy= 0.173909
Thermal correction to Enthalpy= 0.174854
Thermal correction to Gibbs Free Energy= 0.125648
Sum of electronic and zero-point Energies= -460.374268
Sum of electronic and thermal Energies= -460.363398
Sum of electronic and thermal Enthalpies= -460.362454
Sum of electronic and thermal Free Energies= -460.411660
HF=-460.5373076
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-461.0753566
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-460.129152905038

int-19

C	-5.02845100	3.33652200	-1.52134400
C	-4.48859000	1.87337500	-1.59963800
H	-4.86558700	1.34320600	-0.70754100
H	-4.92587000	1.39517200	-2.48967400
C	-3.00744500	1.76900800	-1.62474900
H	-2.44720100	1.65636000	-2.55530500
O	-4.46341400	4.05345400	-0.44435600
H	-4.18906300	3.43056900	0.24955700
C	-2.26009500	1.87822800	-0.38534500
O	-2.76953400	2.09618300	0.71046800
O	-0.93526200	1.71565200	-0.55123300
C	-0.12961500	1.82655900	0.62356600
H	-0.41026300	1.06180100	1.36450300
H	0.90774000	1.67907000	0.29945200
H	-0.24825800	2.81862000	1.08638400
H	-6.12688500	3.24007800	-1.38655900
C	-4.76726100	4.12822800	-2.79666700
H	-5.25492600	3.65935900	-3.66557500
H	-5.16015100	5.15022200	-2.68407900
H	-3.68487100	4.20037700	-2.98909500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.166671 (Hartree/Particle)
Thermal correction to Energy= 0.177107
Thermal correction to Enthalpy= 0.178051
Thermal correction to Gibbs Free Energy= 0.130080
Sum of electronic and zero-point Energies= -460.407719
Sum of electronic and thermal Energies= -460.397283
Sum of electronic and thermal Enthalpies= -460.396338
Sum of electronic and thermal Free Energies= -460.444309
HF=-460.5743894
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-461.1098148
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-460.173329643468

19

Ni	0.93579600	0.64878600	0.75148400
C	1.47364200	1.61194300	-0.82214900
C	2.08036800	3.23042700	-3.02662900
C	2.19414600	2.79955900	-0.64101400
C	1.06407000	1.22926400	-2.10454000
C	1.36053100	2.03298600	-3.20611500
C	2.49562700	3.61083000	-1.73484500
H	2.52320300	3.08527400	0.36122800
H	0.52480200	0.29180300	-2.25075500
H	1.04168300	1.73657000	-4.20795600
H	3.05831800	4.53677000	-1.59664400
N	-1.02266400	1.61444600	0.74032500
C	-3.51398300	2.88650100	0.65085300
C	-1.14674300	2.89304400	1.11322400
C	-2.10137900	0.93486900	0.30920600
C	-3.36058000	1.55088100	0.26140800
C	-2.36366900	3.56498300	1.08180900
N	-0.59166300	-0.88888000	-0.16487500
C	-2.65198900	-2.61406900	-0.97858700
C	-0.31628300	-2.11627200	-0.62205300
C	-1.87257700	-0.47081900	-0.13192200
C	-2.91959300	-1.31623200	-0.52531400
C	-1.30672700	-3.00473900	-1.03571900
H	-0.23098200	3.37460100	1.46188800
H	-4.23086900	0.99816400	-0.09093100
H	-2.41172700	4.61053600	1.39317600
H	0.74340600	-2.37205700	-0.69165100
H	-3.95275700	-0.97252000	-0.48214200
H	-1.02428400	-3.99354800	-1.40341200
Br	1.53584100	1.71342400	2.95756100
C	-3.75643500	-3.55407300	-1.37690900
H	-3.91860100	-4.30521400	-0.58525100
H	-4.70663500	-3.02544600	-1.53891400
H	-3.49696300	-4.10346000	-2.29479800
C	-4.85180400	3.57281900	0.61769300
H	-5.62611400	2.94349000	0.15686800
H	-5.17764900	3.82518500	1.64041400
H	-4.79093000	4.51936200	0.05756700
C	2.39382400	4.05545600	-4.15763300
N	2.64670900	4.72186200	-5.07548800
C	4.76554000	-1.36407000	2.81228100
H	5.11973800	-0.50203500	2.22698800
H	4.27074400	-0.99011600	3.72100800
H	5.64490700	-1.95889700	3.10256500
C	3.81424900	-2.21772500	1.98576700
C	2.50628400	-1.48369100	1.59849500
H	1.82345600	-2.21589700	1.14119400
H	2.03166200	-1.13687500	2.52870500
C	2.72063000	-0.31306200	0.64665400
H	3.41367200	0.43921000	1.03698300
O	4.53782300	-2.65850300	0.84485200
H	3.91677900	-3.04935500	0.21383100
C	3.12690200	-0.73090000	-0.72270800
O	2.71066200	-1.71764300	-1.31420600
O	4.01625700	0.10472900	-1.27329900
C	4.40312800	-0.16445000	-2.62093800
H	3.52809800	-0.12327900	-3.28743900
H	5.12103100	0.61819800	-2.89442700
H	4.86827600	-1.15848100	-2.70346500
H	3.50547700	-3.08968400	2.60034200

UB3LYP-D3/def2-SVP-CPCM(benzene)

Zero-point correction= 0.475108 (Hartree/Particle)
Thermal correction to Energy= 0.510067
Thermal correction to Enthalpy= 0.511011
Thermal correction to Gibbs Free Energy= 0.402761
Sum of electronic and zero-point Energies= -5439.600097
Sum of electronic and thermal Energies= -5439.565138
Sum of electronic and thermal Enthalpies= -5439.564194
Sum of electronic and thermal Free Energies= -5439.672444
HF=-5440.0752046
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5442.1042535
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5436.840624039104

TS-20

C	-4.96009400	3.88440000	-1.36011300
C	-4.15591100	1.53580100	-1.92534800
H	-4.85255800	1.20798400	-1.15199200
H	-4.52833500	1.57780500	-2.95058000
C	-2.82548000	1.66230500	-1.67198000
H	-2.11654900	1.91564300	-2.46561300
O	-3.82802000	4.39264400	-0.82447200
H	-3.65082300	3.99256900	0.03986600
H	-5.72827700	3.52143000	-0.66572700
C	-5.34450400	4.45758300	-2.67514600
H	-6.17732000	3.89217500	-3.11879400
H	-5.66294900	5.51607700	-2.58256300
H	-4.48819000	4.43769900	-3.36990800
C	-2.30982200	1.63035000	-0.34683400
N	-1.91148900	1.64066600	0.74887700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.118086 (Hartree/Particle)
Thermal correction to Energy= 0.126919
Thermal correction to Enthalpy= 0.127863
Thermal correction to Gibbs Free Energy= 0.083183
Sum of electronic and zero-point Energies= -324.872392
Sum of electronic and thermal Energies= -324.863559
Sum of electronic and thermal Enthalpies= -324.862615
Sum of electronic and thermal Free Energies= -324.907295
HF=-324.9904775
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-325.371597
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-324.672953593238

int-20

C	-5.00892800	3.46880700	-1.40901100
C	-4.52195200	1.99718900	-1.55654100
H	-4.76133600	1.47202600	-0.61468500
H	-5.10210700	1.51351000	-2.35789300
C	-3.05924900	1.87413900	-1.84616700
H	-2.70419700	1.73321500	-2.87127200
O	-4.31169100	4.13826700	-0.37634400
H	-4.46266100	3.67713300	0.46008600
H	-6.09282400	3.41356100	-1.17847100
C	-4.82000700	4.28663400	-2.67813200
H	-5.35223000	3.82921900	-3.52605100
H	-5.20684200	5.30516000	-2.52626400
H	-3.75043400	4.36274400	-2.92941000
C	-2.09232000	2.02811200	-0.85447900
N	-1.28354600	2.13041500	-0.01069200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.121851 (Hartree/Particle)
Thermal correction to Energy= 0.129989
Thermal correction to Enthalpy= 0.130933
Thermal correction to Gibbs Free Energy= 0.088525
Sum of electronic and zero-point Energies= -324.910041
Sum of electronic and thermal Energies= -324.901903
Sum of electronic and thermal Enthalpies= -324.900959
Sum of electronic and thermal Free Energies= -324.943367
HF=-325.0318921
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-325.4094553
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-324.719263036445

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Ni	-4.80731500	1.26436800	0.38636200
C	-6.03042800	1.19105200	-1.08686800
C	-5.59377500	1.00605700	-2.40135600
C	-7.39650800	1.16016400	-0.78638600
C	-6.51674900	0.76378200	-3.41886100
H	-4.53028800	1.06407600	-2.64244700
C	-8.33001000	0.92201500	-1.79719200
H	-7.73200700	1.31828500	0.24179100
C	-7.89303300	0.71608800	-3.12009500
H	-6.17892100	0.61463800	-4.44672100
H	-9.39740000	0.89658300	-1.56709000
Br	-5.89130600	1.21298500	2.66725000
C	-2.54309700	-0.32791900	-0.60766100
C	-1.30458500	-0.70305600	-1.14056300
C	-0.37101000	0.26919700	-1.51936200
C	-0.74068300	1.61019500	-1.33942500
C	-1.98918800	1.91176500	-0.80573000
C	-3.57968600	-1.30631700	-0.19590800
C	-3.44758900	-2.69148200	-0.35323500
C	-4.48366000	-3.54885900	0.03538400
C	-5.63557900	-2.95706100	0.57744200
C	-5.69986200	-1.57529300	0.71149100
H	-1.05674900	-1.75714600	-1.26253700
H	-0.06477400	2.42212300	-1.61495600
H	-2.29665600	2.94833900	-0.67884500
H	-2.54043700	-3.11135000	-0.78703900

H	-6.48391100	-3.56761300	0.89309800
H	-6.57307200	-1.07721900	1.13527700
N	-2.87333900	0.97278200	-0.44348000
N	-4.69514000	-0.77259600	0.33926700
C	-4.37438800	-5.04105600	-0.11074600
C	0.96278400	-0.09772200	-2.10700700
H	1.14895900	-1.17976400	-2.06089000
H	1.01214000	0.21497200	-3.16329700
H	1.77801600	0.42230000	-1.57982500
H	-4.32434800	-5.51853400	0.88204700
H	-3.47959700	-5.33472600	-0.67722900
H	-5.26184100	-5.44944600	-0.61923300
C	-8.84594800	0.46046100	-4.16211300
N	-9.61617800	0.24772700	-5.00573400
C	-3.92726300	5.38753600	3.32350800
H	-3.78484800	4.54142200	4.01665500
H	-2.93435200	5.74689000	3.00704700
H	-4.43613400	6.19595700	3.86970000
C	-4.77379500	4.95036300	2.12832500
C	-4.06713900	3.83006400	1.33257000
H	-3.13107500	4.22817700	0.91197300
H	-3.77553300	3.04626200	2.05043400
C	-4.97332800	3.24691500	0.22814900
H	-6.02766500	3.44557500	0.46216300
O	-6.07873700	4.57868900	2.53054200
H	-6.05263500	3.66515200	2.87220400
C	-4.65897900	3.75783800	-1.08173500
N	-4.34244200	4.14184700	-2.13375200
H	-4.91154800	5.81300400	1.45118800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.430716 (Hartree/Particle)
Thermal correction to Energy= 0.462750
Thermal correction to Enthalpy= 0.463694
Thermal correction to Gibbs Free Energy= 0.362477
Sum of electronic and zero-point Energies= -5304.105355
Sum of electronic and thermal Energies= -5304.073321
Sum of electronic and thermal Enthalpies= -5304.072377
Sum of electronic and thermal Free Energies= -5304.173594
HF=-5304.5360709
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5306.4092282
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5301.397993088009

Figure 3.4
TS-22

C	-6.39911300	3.59024400	-1.75341300
H	-6.25527400	3.14500300	-2.74987200
H	-7.07874300	2.95375100	-1.16813200
H	-6.89540400	4.57205900	-1.89779600
C	-5.08873500	3.75476900	-1.06032800
C	-4.27580800	1.38781300	-0.96658200
H	-4.20059900	1.53203400	0.11225400
H	-5.20678400	0.96704500	-1.35068200
C	-3.17473700	1.45635600	-1.76765300
C	-5.03298100	4.09521500	0.39559800
H	-4.01409400	3.97155300	0.80039800
H	-5.32997000	5.15073100	0.56515200
H	-5.71486400	3.45792100	0.97783100
H	-3.23164100	1.21592900	-2.83319700
O	-4.13516100	4.28782500	-1.86542300
H	-3.30381600	4.39603900	-1.37862900
C	-1.94780300	2.00508400	-1.30629700
N	-0.96215000	2.49585600	-0.92111300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.146050 (Hartree/Particle)
Thermal correction to Energy= 0.156161
Thermal correction to Enthalpy= 0.157106
Thermal correction to Gibbs Free Energy= 0.109390
Sum of electronic and zero-point Energies= -364.142477
Sum of electronic and thermal Energies= -364.132365
Sum of electronic and thermal Enthalpies= -364.131421
Sum of electronic and thermal Free Energies= -364.179137
HF=-364.2885268
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-364.7123084
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-363.921552742328

Radical (from *i*Pr$_2$O)

C	-5.45954100	3.55773900	-2.92762700
O	-4.49130500	4.52611700	-3.02439500
C	-5.70484100	2.90497900	-4.24901900
H	-4.75207600	2.66754500	-4.74852800
H	-6.28559200	1.97685600	-4.13104800
H	-6.27653500	3.56643200	-4.93677000
C	-3.96711600	5.15969500	-1.84929000
H	-4.13539100	4.50137200	-0.97782300
C	-6.60305200	3.73504100	-1.97469400
H	-6.28153100	3.98958300	-0.95288000
H	-7.29540100	4.54090700	-2.30680100
H	-7.19121400	2.80643700	-1.91698800
C	-2.46607000	5.30820400	-2.06738300
H	-1.99097700	5.79444800	-1.20111300
H	-2.00014400	4.32273600	-2.21808500
H	-2.27289400	5.92187500	-2.96190400
C	-4.66073200	6.50103800	-1.62397000
H	-4.51974300	7.14786700	-2.50470700
H	-5.74077200	6.37170400	-1.46335000
H	-4.23966300	7.01363300	-0.74447200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.177749 (Hartree/Particle)
Thermal correction to Energy= 0.187254
Thermal correction to Enthalpy= 0.188198
Thermal correction to Gibbs Free Energy= 0.143440
Sum of electronic and zero-point Energies= -311.250032
Sum of electronic and thermal Energies= -311.240527

Sum of electronic and thermal Enthalpies= -311.239583
Sum of electronic and thermal Free Energies= -311.284340
HF=-311.4277804
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-311.7837789
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-311.094799922802

TS-23

C	-4.84130600	1.50111200	-1.61002600
H	-5.35918100	1.88270900	-0.72807800
H	-5.42066400	0.91355800	-2.32306900
C	-3.47909400	1.45329900	-1.60710200
H	-2.91324700	0.97850400	-2.41155700
C	-2.71462000	2.09424200	-0.53951600
O	-3.17628100	2.70944700	0.40872200
O	-1.37655900	1.95283700	-0.72259100
C	-0.54045600	2.56171300	0.25775100
H	-0.75748900	2.16916000	1.26348600
H	0.49283300	2.32531800	-0.02641100
H	-0.68684500	3.65357500	0.27456200
C	-5.54227500	3.48130200	-2.84498200
O	-4.43732700	4.25362100	-2.93834800
C	-5.85234500	2.85099400	-4.16757900
H	-4.94741400	2.39481500	-4.59720200
H	-6.63480100	2.08407100	-4.07366000
H	-6.21154900	3.61685000	-4.88374400
C	-3.93845800	5.04082400	-1.83537100
H	-4.15472200	4.51094700	-0.89375000
C	-6.68580900	3.87611600	-1.95758200
H	-6.36252100	4.16613100	-0.94802200
H	-7.24746600	4.72827100	-2.39184800
H	-7.38813200	3.03523300	-1.86137800
C	-2.42910800	5.11630600	-2.02493900
H	-1.96970500	5.67733300	-1.19695100
H	-1.98561600	4.11222400	-2.05577000
H	-2.18917300	5.62891300	-2.97020400
C	-4.58072400	6.42593300	-1.83713200
H	-4.39502500	6.92644900	-2.80086900
H	-5.66632300	6.38033600	-1.67573800
H	-4.14487500	7.04344000	-1.03618500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.275442 (Hartree/Particle)
Thermal correction to Energy= 0.291632
Thermal correction to Enthalpy= 0.292577
Thermal correction to Gibbs Free Energy= 0.231745
Sum of electronic and zero-point Energies= -617.418252
Sum of electronic and thermal Energies= -617.402062
Sum of electronic and thermal Enthalpies= -617.401117
Sum of electronic and thermal Free Energies= -617.461949
HF=-617.6936939
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-618.4021595
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-617.086919544197

TS-24

C	-4.73982000	1.42483000	-1.74173700
H	-5.48651300	1.56994500	-0.95942900
H	-5.05208800	0.88531500	-2.63627600
C	-3.40770900	1.57509000	-1.47443700
H	-2.65123400	1.31932200	-2.22228100
C	-5.55985300	3.48193000	-2.83690300
O	-4.45071400	4.24306300	-2.97043000
C	-5.97042200	2.90585000	-4.15657400
H	-5.09570400	2.50850800	-4.69346300
H	-6.71315900	2.10441500	-4.02988100
H	-6.42508200	3.68942500	-4.79564100
C	-3.90524600	5.03272800	-1.89153500
H	-4.10881000	4.52522600	-0.93455100
C	-6.63539700	3.84936600	-1.85777900
H	-6.24482900	4.08539800	-0.85775700
H	-7.20909800	4.72987500	-2.21223000
H	-7.34730800	3.01697400	-1.75787500
C	-2.40116200	5.07661000	-2.11894100
H	-1.91027400	5.64385900	-1.31413800
H	-1.98178100	4.06141300	-2.13324700
H	-2.17621800	5.56220100	-3.08182700
C	-4.52909900	6.42584600	-1.89169900
H	-4.36222500	6.91261900	-2.86568000
H	-5.61088400	6.39281700	-1.70236800
H	-4.06576900	7.04630400	-1.10888000
C	-2.93046700	2.14301300	-0.26366400
N	-2.54581500	2.63384700	0.72187300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.230620 (Hartree/Particle)
Thermal correction to Energy= 0.244512
Thermal correction to Enthalpy= 0.245456
Thermal correction to Gibbs Free Energy= 0.189480
Sum of electronic and zero-point Energies= -481.917932
Sum of electronic and thermal Energies= -481.904039
Sum of electronic and thermal Enthalpies= -481.903095
Sum of electronic and thermal Free Energies= -481.959071
HF=-482.1485515
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-482.7001059
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-481.632858900733

Figure 3.5
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C	0.29689400	1.96215900	-2.78830600
C	1.02936400	2.57413200	-3.91210600
C	0.89668000	2.03552200	-5.31905800
C	0.28780900	3.37065400	-4.99307000
H	2.01166700	2.96613200	-3.62929100

H	0.21630100	1.19108900	-5.45838800
H	1.79583100	2.00875900	-5.94183600
H	-0.80058800	3.41959900	-4.89873100
H	0.76185600	4.27742000	-5.38106000
C	0.37426500	2.53802000	-1.41152700
H	-0.27929700	3.43069400	-1.29207400
H	0.06203700	1.80548700	-0.64489500
H	1.40248500	2.85059600	-1.17369200
O	-0.89220200	1.37500500	-3.16222700
H	-1.35635500	1.06082100	-2.37500400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.128188 (Hartree/Particle)
Thermal correction to Energy= 0.135296
Thermal correction to Enthalpy= 0.136240
Thermal correction to Gibbs Free Energy= 0.096901
Sum of electronic and zero-point Energies= -270.775382
Sum of electronic and thermal Energies= -270.768274
Sum of electronic and thermal Enthalpies= -270.767330
Sum of electronic and thermal Free Energies= -270.806669
HF=-270.9035695
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-271.2139238
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-270.625455129203

TS-32

C	-4.23590100	1.32771300	-2.02494800
H	-4.90496400	1.31391600	-1.16574300
H	-4.67361400	1.08302800	-2.99532400
C	-2.88109000	1.32769700	-1.85359700
H	-2.19227800	1.13041100	-2.67817100
C	-2.28941500	1.67900700	-0.57013300
O	-2.86939600	2.26119900	0.35086600
O	-0.99408400	1.33533700	-0.47103300
C	-0.32202600	1.70037800	0.73512400
H	-0.78241500	1.20867100	1.60593300
H	0.71727900	1.36900900	0.61906100
H	-0.35990900	2.78977500	0.89181200
C	-5.00552300	3.67165700	-1.69612600
C	-6.28836400	3.71661200	-2.42314500
C	-7.48797400	2.94547700	-1.91413400
C	-7.48767400	4.44037500	-1.80386800
H	-6.18107700	3.80775900	-3.50781000
H	-7.34266700	2.37539400	-0.99270000
H	-8.13667300	2.47206200	-2.65655900
H	-7.33173200	4.87458400	-0.81293700
H	-8.12633100	5.02251200	-2.47440600
C	-3.82181900	4.41261600	-2.23321300
H	-3.91619300	5.49332800	-2.00736700
H	-2.88566300	4.06150700	-1.77331300
H	-3.73915500	4.29497900	-3.32333400
O	-5.12695500	3.55945700	-0.35555400
H	-4.27913000	3.21284300	0.02361200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.225654 (Hartree/Particle)
Thermal correction to Energy= 0.239167
Thermal correction to Enthalpy= 0.240111
Thermal correction to Gibbs Free Energy= 0.184895
Sum of electronic and zero-point Energies= -576.948629
Sum of electronic and thermal Energies= -576.935117
Sum of electronic and thermal Enthalpies= -576.934172
Sum of electronic and thermal Free Energies= -576.989388
HF=-577.1742834
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-577.835512
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-576.621558226388

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C	-4.34114700	1.90320200	-2.04030700
H	-4.95304800	1.24269000	-1.39861300
H	-4.56064800	1.63812700	-3.08454800
C	-2.89567800	1.65945100	-1.78919500
H	-2.23750300	1.33885000	-2.60007000
C	-2.28002900	1.81646100	-0.48605500
O	-2.83025500	2.29298800	0.50559500
O	-1.00511800	1.39239500	-0.45896900
C	-0.31277900	1.52900300	0.78413600
H	-0.81333800	0.95038000	1.57589800
H	0.70004600	1.14447400	0.61398900
H	-0.27461300	2.58434000	1.09572400
C	-4.88993700	3.35493300	-1.77089700
C	-6.25948100	3.45829600	-2.44038200
C	-7.48155100	2.88851800	-1.77106100
C	-7.30856800	4.38486600	-1.88496500
H	-6.21096100	3.37520700	-3.53157500
H	-7.33728700	2.45381100	-0.77847100
H	-8.23411900	2.39464500	-2.39272100
H	-7.05450500	4.92440300	-0.96959600
H	-7.93704300	4.93431000	-2.59190900
C	-3.94495600	4.41693300	-2.35222400
H	-4.38944700	5.41402700	-2.21642000
H	-2.97635400	4.39886900	-1.82845300
H	-3.76230200	4.25407500	-3.42666500
O	-5.07418500	3.56973200	-0.38784800
H	-4.29833900	3.20911500	0.08639600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.228512 (Hartree/Particle)
Thermal correction to Energy= 0.241757
Thermal correction to Enthalpy= 0.242701
Thermal correction to Gibbs Free Energy= 0.187790
Sum of electronic and zero-point Energies= -576.974674
Sum of electronic and thermal Energies= -576.961428
Sum of electronic and thermal Enthalpies= -576.960484

Sum of electronic and thermal Free Energies= -577.015395
HF=-577.2031851
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-577.8611919
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-576.659393983904

TS-33

C	0.24729100	2.04013100	-2.77286300
C	1.06885100	2.46300200	-3.81464600
C	0.85850700	2.11238100	-5.25040800
C	0.27691000	3.47998700	-5.24504400
H	1.98947300	2.98311700	-3.54426700
H	0.14859700	1.29285300	-5.41633400
H	1.77423800	1.97430000	-5.84059100
H	-0.79048500	3.61560400	-5.06555400
H	0.87893500	4.34953600	-5.51480100
C	0.35917400	2.50502000	-1.35773900
H	-0.46646700	3.19526200	-1.08814200
H	0.31300800	1.65832500	-0.64714300
H	1.30660500	3.03600400	-1.18835900
O	-0.86305900	1.30264000	-3.10739900
H	-1.38502900	1.12442500	-2.31477500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.125566 (Hartree/Particle)
Thermal correction to Energy= 0.132815
Thermal correction to Enthalpy= 0.133759
Thermal correction to Gibbs Free Energy= 0.094330
Sum of electronic and zero-point Energies= -270.761884
Sum of electronic and thermal Energies= -270.754635
Sum of electronic and thermal Enthalpies= -270.753691
Sum of electronic and thermal Free Energies= -270.793120
HF=-270.8874499
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-271.2006897
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-270.608807117228

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C	0.19421500	2.09126800	-2.65316600
C	0.99145200	2.56349300	-3.62814900
C	0.76673000	2.33789100	-5.10968200
C	0.30300200	3.58853900	-5.79300800
H	1.83206800	3.19754000	-3.33493700
H	0.01777800	1.53661600	-5.23156500
H	1.70300400	1.98073300	-5.57377200
H	-0.69865900	3.97603100	-5.58336200
H	1.00338700	4.24556300	-6.31693100
C	0.39901700	2.34227400	-1.18716700
H	-0.47988900	2.85142900	-0.75221900
H	0.52758300	1.39003300	-0.64115300
H	1.28477200	2.96512600	-1.00406200
O	-0.89450300	1.32292500	-2.97584700
H	-1.32360900	1.00962500	-2.16984700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.125566 (Hartree/Particle)
Thermal correction to Energy= 0.132815
Thermal correction to Enthalpy= 0.133759
Thermal correction to Gibbs Free Energy= 0.094330
Sum of electronic and zero-point Energies= -270.761884
Sum of electronic and thermal Energies= -270.754635
Sum of electronic and thermal Enthalpies= -270.753691
Sum of electronic and thermal Free Energies= -270.793120
HF=-270.8874499
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-271.217969
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-270.627498300399

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C	-4.22627600	2.16338900	-1.20934500
H	-3.94003800	3.00584700	-0.57953400
H	-5.28531400	2.01021600	-1.42109000
C	-3.33313300	1.17809300	-1.49999900
H	-3.64003500	0.29179400	-2.06508200
C	-1.95406600	1.23447000	-1.14659500
N	-0.82477500	1.23885200	-0.86243600
C	-2.57597700	5.51658600	-0.59007600
C	-3.06029800	5.64186400	-1.83749100
C	-2.98062800	4.56780700	-2.89100700
C	-4.24002000	3.77869400	-3.07992900
H	-3.56257000	6.57806400	-2.09468200
H	-2.14762800	3.87650800	-2.66890600
H	-2.71315700	5.03470300	-3.86374800
H	-5.20265200	4.22353300	-2.80885200
H	-4.26269800	3.00130700	-3.84942800
C	-2.63739600	6.57604600	0.47056300
H	-3.19846800	6.21451500	1.35029300
H	-1.62161600	6.83875600	0.81746100
H	-3.11965400	7.49040800	0.09983700
O	-1.99779300	4.33172800	-0.21682800
H	-1.55503100	4.41813100	0.63722300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.178577 (Hartree/Particle)
Thermal correction to Energy= 0.190946
Thermal correction to Enthalpy= 0.191890
Thermal correction to Gibbs Free Energy= 0.138346
Sum of electronic and zero-point Energies= -441.442181
Sum of electronic and thermal Energies= -441.429812
Sum of electronic and thermal Enthalpies= -441.428868
Sum of electronic and thermal Free Energies= -441.482412
HF=-441.6207579

UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-442.1294273
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-441.162609989374

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C	-4.44948600	2.56708600	-1.75548800
H	-4.71776000	3.19125300	-0.89023800
H	-5.28478600	1.86480000	-1.93123900
C	-3.22294800	1.76845700	-1.43848600
H	-2.89024800	0.98877500	-2.13213200
C	-2.43080200	2.00786400	-0.32076300
N	-1.77072100	2.24206500	0.62213600
C	-2.27474100	5.37782400	-0.73467400
C	-3.21861800	5.34350300	-1.69248700
C	-3.15172200	4.48565200	-2.92432000
C	-4.30128100	3.46159300	-3.00954800
H	-4.11832800	5.94845800	-1.54084300
H	-2.18524900	3.95884300	-2.94111100
H	-3.18695100	5.10969200	-3.83609800
H	-5.26259500	3.98505200	-3.15434300
H	-4.15548500	2.82579300	-3.90003400
C	-2.38825500	6.13145900	0.55855200
H	-2.32673000	5.42871600	1.40962800
H	-1.55329700	6.84426900	0.66759900
H	-3.33918900	6.67687200	0.63259300
O	-1.09050100	4.71222400	-0.92025800
H	-0.83153100	4.27666000	-0.09249600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.183672 (Hartree/Particle)
Thermal correction to Energy= 0.195078
Thermal correction to Enthalpy= 0.196023
Thermal correction to Gibbs Free Energy= 0.145728
Sum of electronic and zero-point Energies= -441.494736
Sum of electronic and thermal Energies= -441.483330
Sum of electronic and thermal Enthalpies= -441.482386
Sum of electronic and thermal Free Energies= -441.532680
HF=-441.6784082
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-442.1810323
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-441.221614305262

TS-35

C	-4.14460700	1.23404800	-2.16346300
H	-4.96948200	1.17870300	-1.45386100
H	-4.38119500	1.11072500	-3.22246900
C	-2.85282400	1.29339800	-1.75149200
H	-2.02274700	1.28648800	-2.46410900
C	-4.98326100	3.72312800	-1.75760600
C	-6.30928600	3.70984700	-2.39479200
C	-7.45673300	2.92927600	-1.78836500
C	-7.49470900	4.42840300	-1.73968800
H	-6.26810900	3.75812400	-3.48687800
H	-7.25123600	2.40154200	-0.85314100
H	-8.13173200	2.40856100	-2.47349000
H	-7.29983700	4.90885300	-0.77717800
H	-8.18793900	4.96299100	-2.39553600
C	-3.83565700	4.47257700	-2.34237900
H	-3.84573400	5.53646500	-2.02858000
H	-2.87178200	4.04349300	-2.01428700
H	-3.86416000	4.44248000	-3.44125700
O	-5.01796100	3.56792500	-0.40398800
H	-4.12293400	3.58556600	-0.03250000
C	-2.51460800	1.50672400	-0.38417000
N	-2.25775500	1.73284600	0.73021800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.180508 (Hartree/Particle)
Thermal correction to Energy= 0.192155
Thermal correction to Enthalpy= 0.193099
Thermal correction to Gibbs Free Energy= 0.141926
Sum of electronic and zero-point Energies= -441.444513
Sum of electronic and thermal Energies= -441.432866
Sum of electronic and thermal Enthalpies= -441.431922
Sum of electronic and thermal Free Energies= -441.483095
HF=-441.6250213
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-442.1304755
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-441.166010613767

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C	-4.30087700	1.87956300	-2.16188800
H	-5.01109200	1.17572000	-1.69793700
H	-4.32993000	1.72812700	-3.25101600
C	-2.91627400	1.61828900	-1.66611200
H	-2.06851100	1.61549600	-2.35777700
C	-4.84682600	3.31451600	-1.83572400
C	-6.25679400	3.42145900	-2.40834300
C	-7.44408000	2.91203000	-1.63550300
C	-7.24529200	4.39727900	-1.82734900
H	-6.28101100	3.28569800	-3.49471200
H	-7.25038100	2.51248700	-0.63679600
H	-8.24474500	2.41193800	-2.18787700
H	-6.91940500	4.96891900	-0.95481800
H	-7.90624200	4.93309600	-2.51459400
C	-3.95085000	4.40376500	-2.43382000
H	-4.37153700	5.39404200	-2.20529500
H	-2.93117400	4.35175800	-2.01708500
H	-3.87559600	4.29899300	-3.52722600
O	-4.94901300	3.46843800	-0.42777400
H	-4.07461700	3.64752800	-0.05800200
C	-2.62002500	1.45580000	-0.31331800
N	-2.37161500	1.32302100	0.82605300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.183580 (Hartree/Particle)
Thermal correction to Energy= 0.194597

Thermal correction to Enthalpy= 0.195542
Thermal correction to Gibbs Free Energy= 0.146166
Sum of electronic and zero-point Energies= -441.476039
Sum of electronic and thermal Energies= -441.465022
Sum of electronic and thermal Enthalpies= -441.464078
Sum of electronic and thermal Free Energies= -441.513454
HF=-441.6596195
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-442.160472
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-441.206058893034

TS-36

C	-4.13285900	1.49839100	-2.19707200
H	-4.99186800	1.49802400	-1.52276600
H	-4.22121000	0.95131900	-3.13628500
C	-2.91525100	1.89237600	-1.73980200
H	-2.02551100	1.84708500	-2.36845800
C	-2.27648800	5.27234500	-2.27836400
C	-3.49474600	5.22675300	-2.84243300
C	-3.95076700	4.21722500	-3.85815800
C	-5.10137700	3.37016900	-3.40288300
H	-4.22088600	5.98753900	-2.53934500
H	-3.10248300	3.58082800	-4.16274400
H	-4.26104000	4.74535300	-4.78643600
H	-5.71654100	3.70915000	-2.56422200
H	-5.59810800	2.72615000	-4.13534900
C	-1.85385900	6.28870600	-1.25542700
H	-1.51062100	5.79242800	-0.33215000
H	-1.00159500	6.87815600	-1.63449100
H	-2.67305700	6.97213300	-0.99265900
O	-1.29324800	4.39266700	-2.66384300
H	-0.91224400	3.99763700	-1.86042000
C	-2.76834400	2.48345600	-0.40475800
O	-3.62925000	2.57655900	0.44423100
O	-1.49320800	2.93134400	-0.19194400
C	-1.21274100	3.41473300	1.12481200
H	-1.31264700	2.60357700	1.86234800
H	-0.17949000	3.78248800	1.10444000
H	-1.90319000	4.22435900	1.40390200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.223812 (Hartree/Particle)
Thermal correction to Energy= 0.238100
Thermal correction to Enthalpy= 0.239044
Thermal correction to Gibbs Free Energy= 0.182274
Sum of electronic and zero-point Energies= -576.942781
Sum of electronic and thermal Energies= -576.928493
Sum of electronic and thermal Enthalpies= -576.927549
Sum of electronic and thermal Free Energies= -576.984318
HF=-577.1665925
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-577.8312694
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-576.617229776715

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C	-3.89899200	1.86065900	-2.59106100
H	-4.46394900	1.05772600	-2.08200000
H	-3.49885100	1.44153500	-3.52807600
C	-2.76666100	2.28574800	-1.72207300
H	-1.75950800	2.38850700	-2.12788300
C	-2.07849100	5.13664000	-2.65237200
C	-3.41903500	5.00992200	-2.61808700
C	-4.25695600	4.22234300	-3.58416300
C	-4.90699500	2.98807900	-2.93052500
H	-3.93804800	5.47853300	-1.77722700
H	-3.64933900	3.91256900	-4.44971800
H	-5.06447200	4.86689400	-3.97678100
H	-5.41881300	3.28849000	-2.00143700
H	-5.67738700	2.57130800	-3.60155600
C	-1.26622100	5.84305100	-1.60896400
H	-0.64132500	5.11201200	-1.06710500
H	-0.59872900	6.59549500	-2.06551600
H	-1.90866300	6.34747200	-0.87511100
O	-1.36553900	4.53336500	-3.65313600
H	-0.42509900	4.72446200	-3.54518300
C	-2.98485200	2.67551900	-0.34728000
O	-4.05468300	2.63713800	0.24261400
O	-1.84424100	3.12710300	0.24560600
C	-1.97843900	3.58132800	1.58866400
H	-2.34865900	2.77801400	2.24518500
H	-0.97876600	3.90080400	1.90991000
H	-2.68291700	4.42653500	1.65119600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.228144 (Hartree/Particle)
Thermal correction to Energy= 0.242309
Thermal correction to Enthalpy= 0.243254
Thermal correction to Gibbs Free Energy= 0.186069
Sum of electronic and zero-point Energies= -576.989435
Sum of electronic and thermal Energies= -576.975269
Sum of electronic and thermal Enthalpies= -576.974325
Sum of electronic and thermal Free Energies= -577.031509
HF=-577.2175786
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-577.8789909
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-576.669748077964

Table A2.1

Ground state (singlet spin state) ***a***

C	-6.41504500	0.74026100	-0.39513100
C	-6.76753900	1.93998400	-1.02693500
C	-5.94140400	3.05711500	-0.91162600

C	-4.73837100	2.98392700	-0.18616500
C	-4.39544800	1.77801800	0.45042800
C	-5.23430700	0.66438200	0.35036300
H	-7.06528400	-0.13423300	-0.47979900
H	-7.69247200	2.00266700	-1.60561100
H	-6.21063100	4.00571600	-1.38040600
H	-3.48347200	1.71486700	1.04668300
H	-4.96564300	-0.26475000	0.85895200
C	-3.92045100	4.23690400	-0.05462600
O	-4.46676800	5.32883900	-0.10526900
C	-2.43335600	4.15238200	0.13924000
C	-1.65201300	3.11137900	-0.39260700
C	-1.79683400	5.21111500	0.81216700
C	-0.26253800	3.12422200	-0.24071000
H	-2.12674500	2.30086400	-0.94841500
C	-0.41278200	5.21283600	0.98000900
H	-2.41067800	6.02728800	1.19838800
C	0.35768900	4.16810900	0.45304900
H	0.33755700	2.31724200	-0.66826400
H	0.07069600	6.03217900	1.51780200
H	1.44346200	4.17180400	0.57874300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.191845 (Hartree/Particle)
Thermal correction to Energy= 0.202489
Thermal correction to Enthalpy= 0.203433
Thermal correction to Gibbs Free Energy= 0.154325
Sum of electronic and zero-point Energies= -576.049627
Sum of electronic and thermal Energies= -576.038983
Sum of electronic and thermal Enthalpies= -576.038039
Sum of electronic and thermal Free Energies= -576.087147
HF=-576.2414719
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-576.8727891

Triplet spin state ***a***

C	-6.68733300	1.08108100	-0.63480500
C	-5.80015500	1.76945000	-1.48029600
C	-4.77717600	2.54963300	-0.95331000
C	-4.58877300	2.63449700	0.45235900
C	-5.50596600	1.94866800	1.29779300
C	-6.53526600	1.18521200	0.75434500
H	-7.49246500	0.47632200	-1.05837700
H	-5.92202600	1.70603700	-2.56475800
H	-4.12503900	3.11367300	-1.62184100
H	-5.37512600	2.00676600	2.37977300
H	-7.22158500	0.65545100	1.42005800
C	-3.54530400	3.45156200	1.04081200
O	-3.78471900	3.88884200	2.26502500
C	-2.27477000	3.85335100	0.46979700
C	-1.61706100	3.08099400	-0.52534300
C	-1.61792300	5.01608500	0.96367000
C	-0.39022500	3.48930000	-1.03601300
H	-2.07049000	2.15345300	-0.87810200
C	-0.38161500	5.40168000	0.45348200
H	-2.10992300	5.61803700	1.72966700
C	0.23880700	4.65022400	-0.55362200
H	0.09482300	2.88921600	-1.81034100
H	0.10063300	6.30476800	0.83654700
H	1.20629900	4.95881100	-0.95626300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.188417 (Hartree/Particle)
Thermal correction to Energy= 0.199452
Thermal correction to Enthalpy= 0.200396
Thermal correction to Gibbs Free Energy= 0.149624
Sum of electronic and zero-point Energies= -575.949841
Sum of electronic and thermal Energies= -575.938806
Sum of electronic and thermal Enthalpies= -575.937862
Sum of electronic and thermal Free Energies= -575.988634
HF=-576.1382581
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-576.7686266

Ground state (singlet spin state) ***b***

C	-6.40993400	0.75049400	-0.39711900
C	-6.77635800	1.94871400	-1.02360300
C	-5.94439600	3.05827800	-0.90258100
C	-4.73608700	2.98240100	-0.18662600
C	-4.39378500	1.77195700	0.44065100
C	-5.22784700	0.65690600	0.34394900
H	-7.70604500	2.00243800	-1.59211100
H	-6.22027600	4.00758900	-1.36560500
H	-3.48133900	1.69897200	1.03470900
H	-4.96936900	-0.27934600	0.84072000
C	-3.91913200	4.23429900	-0.05462800
O	-4.46535000	5.32604500	-0.10553300
C	-2.43352500	4.14966400	0.13988700
C	-1.64850800	3.10716500	-0.38235600
C	-1.79564300	5.21345700	0.80305500
C	-0.26065600	3.11509300	-0.23353300
H	-2.11571100	2.29057400	-0.93526200
C	-0.41435700	5.22476500	0.97584100
H	-2.40583500	6.03492400	1.18326700
C	0.34639300	4.17028400	0.45447400
H	0.35076700	2.31291700	-0.64924500
H	0.07945800	6.04177500	1.50410100
Cl	-7.45034600	-0.64590600	-0.53705900
Cl	2.08126800	4.17829800	0.65990000

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.172552 (Hartree/Particle)
Thermal correction to Energy= 0.185634
Thermal correction to Enthalpy= 0.186578
Thermal correction to Gibbs Free Energy= 0.130700
Sum of electronic and zero-point Energies= -1495.005168
Sum of electronic and thermal Energies= -1494.992085
Sum of electronic and thermal Enthalpies= -1494.991141
Sum of electronic and thermal Free Energies= -1495.047020
HF=-1495.1777197

UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-1496.1274472

Triplet spin state ***b***

C	-6.49351100	0.76503700	-0.42066000
C	-6.85045200	2.01184200	-0.95281200
C	-5.97634100	3.08487800	-0.83449400
C	-4.71760500	2.93832700	-0.18463900
C	-4.40114400	1.67248400	0.37992500
C	-5.26770900	0.59699500	0.24752100
H	-7.80569800	2.12764600	-1.46761300
H	-6.24152400	4.05047400	-1.26777900
H	-3.47432100	1.54323800	0.94073700
H	-5.01385500	-0.37508300	0.67366200
C	-3.84426400	4.08456200	-0.04771100
O	-4.43438500	5.26400100	-0.10273900
C	-2.40935400	4.10849800	0.14178000
C	-1.56688300	3.05830400	-0.31487700
C	-1.79519200	5.24981400	0.73202500
C	-0.19246800	3.11842400	-0.13454100
H	-1.99899800	2.19914500	-0.82997100
C	-0.41768800	5.31637600	0.89789000
H	-2.42360800	6.07022400	1.08194600
C	0.38404500	4.24752200	0.47377600
H	0.44769200	2.30376000	-0.47731100
H	0.04393800	6.18677100	1.36717000
Cl	-7.58192100	-0.59075800	-0.57701100
Cl	2.11463400	4.31927300	0.69102000

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.169215 (Hartree/Particle)
Thermal correction to Energy= 0.182706
Thermal correction to Enthalpy= 0.183650
Thermal correction to Gibbs Free Energy= 0.126100
Sum of electronic and zero-point Energies= -1494.906267
Sum of electronic and thermal Energies= -1494.892777
Sum of electronic and thermal Enthalpies= -1494.891832
Sum of electronic and thermal Free Energies= -1494.949382
HF=-1495.0754822
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-1496.0243305

Ground state (singlet spin state) ***c***

C	-6.47226800	0.82135200	-0.44610000
C	-6.82461200	2.04477700	-1.04642700
C	-5.98444800	3.14754500	-0.90325900
C	-4.77429800	3.06519900	-0.19505000
C	-4.44031200	1.83572100	0.40927300
C	-5.27672100	0.73244200	0.29189400
H	-7.74681400	2.14565800	-1.61825600
H	-6.26004000	4.10568000	-1.34863400
H	-3.52941900	1.74802300	1.00387100
H	-5.03211300	-0.21871900	0.76873300
C	-3.95858900	4.31145700	-0.04667500
O	-4.50433600	5.40793500	-0.09771700
C	-2.47920300	4.22416900	0.16377400
C	-1.67942200	3.17461500	-0.33338700
C	-1.84038700	5.29061800	0.81755100
C	-0.30028400	3.18710300	-0.16495400
H	-2.13748900	2.35181100	-0.88486700
C	-0.46032900	5.30838800	1.01146800
H	-2.45349400	6.11885800	1.17874700
C	0.32335800	4.24808700	0.51861700
H	0.32711900	2.38539400	-0.55933600
H	-0.00499500	6.14638900	1.53880000
C	-8.43608500	-0.29676600	-1.22947200
H	-8.85207300	-1.30936900	-1.14691600
H	-9.15351400	0.42337100	-0.79812100
H	-8.28453200	-0.05592400	-2.29648100
C	2.37051200	5.19956900	1.30841500
H	3.43100900	4.91655100	1.28638600
H	2.24642500	6.17041200	0.79708800
H	2.04799800	5.30455600	2.35936000
O	-7.21221000	-0.30651700	-0.51651100
O	1.66568100	4.16550400	0.64565200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.256811 (Hartree/Particle)
Thermal correction to Energy= 0.272536
Thermal correction to Enthalpy= 0.273480
Thermal correction to Gibbs Free Energy= 0.212710
Sum of electronic and zero-point Energies= -804.874852
Sum of electronic and thermal Energies= -804.859127
Sum of electronic and thermal Enthalpies= -804.858183
Sum of electronic and thermal Free Energies= -804.918953
HF=-805.131663
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-806.0286281

Triplet spin state ***c***

C	-6.53261800	0.79871900	-0.49176200
C	-6.86455900	2.06127400	-1.01688000
C	-5.98319100	3.12844900	-0.87208100
C	-4.73460000	2.98057600	-0.20497600
C	-4.43944300	1.70348800	0.35551900
C	-5.30708200	0.63933200	0.19832800
H	-7.80161100	2.21712100	-1.55177600
H	-6.23778200	4.10059800	-1.29687900
H	-3.52192400	1.56471100	0.92989300
H	-5.07718200	-0.34283400	0.61701300
C	-3.86618700	4.12575500	-0.03775000
O	-4.45406900	5.30685000	-0.09240800
C	-2.43614200	4.14235400	0.18183000
C	-1.57658400	3.09912600	-0.27101900
C	-1.82475200	5.27497100	0.78948800
C	-0.21114800	3.16293900	-0.06735100
H	-1.99874200	2.24252400	-0.79923100
C	-0.44818700	5.34700800	0.98050700
H	-2.46086800	6.09284500	1.13119800
C	0.37628100	4.28584700	0.56316500
H	0.44767300	2.35921300	-0.40318500
H	-0.02632500	6.22654900	1.46722600
C	-8.56333300	-0.22420000	-1.23004000

H	-9.01018100	-1.22547900	-1.17397200
H	-9.23224800	0.49800700	-0.72903400
H	-8.45799400	0.06387800	-2.29118000
C	2.38966600	5.34442400	1.29872200
H	3.45895500	5.09542900	1.30005400
H	2.23612900	6.27309100	0.72077300
H	2.05811800	5.51263900	2.33887700
O	-7.30683300	-0.30703700	-0.58448500
O	1.72088100	4.24571800	0.70888400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.253160 (Hartree/Particle)
Thermal correction to Energy= 0.269371
Thermal correction to Enthalpy= 0.270315
Thermal correction to Gibbs Free Energy= 0.207609
Sum of electronic and zero-point Energies= -804.774067
Sum of electronic and thermal Energies= -804.757856
Sum of electronic and thermal Enthalpies= -804.756912
Sum of electronic and thermal Free Energies= -804.819619
HF=-805.0272277
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-805.9231245

Ground state (singlet spin state) ***d***

C	-6.36973300	0.71620600	-0.44952600
C	-6.70318400	1.90811700	-1.10698200
C	-5.90328500	3.03529600	-0.93978200
C	-4.74804700	2.98087900	-0.14111800
C	-4.42713500	1.78259600	0.51687000
C	-5.23770500	0.65540600	0.36883500
H	-7.58676500	1.94791800	-1.74670500
H	-6.16028000	3.97729600	-1.42749400
H	-3.55177200	1.73168300	1.16627600
H	-4.98839100	-0.27257200	0.88598800
C	-3.96008800	4.25259800	0.04651600
O	-4.55574000	5.32088400	0.05390000
C	-2.48052200	4.19888500	0.22250300
C	-1.67438200	3.14273700	-0.25268100
C	-1.84661300	5.29816300	0.82730300
C	-0.29364000	3.18227000	-0.11189000
H	-2.12831700	2.29239200	-0.76418300
C	-0.46458800	5.34380500	0.99143200
H	-2.46638100	6.12734500	1.17447400
C	0.32626500	4.27778600	0.52018100
H	0.33877400	2.37603500	-0.48826400
H	-0.01198000	6.20643500	1.47973400
C	2.37378800	5.28808300	1.23364000
H	3.43717200	5.01823900	1.19841100
H	2.22441100	6.23742600	0.69028200
H	2.07124900	5.42469700	2.28659600
O	1.66949900	4.22056800	0.62241400
C	-7.27266100	-0.48442300	-0.58215800
F	-8.28731800	-0.43858000	0.30513400
F	-7.82882500	-0.55874900	-1.80534600
F	-6.61515700	-1.63778100	-0.36545200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.229078 (Hartree/Particle)
Thermal correction to Energy= 0.245918
Thermal correction to Enthalpy= 0.246862
Thermal correction to Gibbs Free Energy= 0.181595
Sum of electronic and zero-point Energies= -1027.249523
Sum of electronic and thermal Energies= -1027.232683
Sum of electronic and thermal Enthalpies= -1027.231739
Sum of electronic and thermal Free Energies= -1027.297006
HF=-1027.478601
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-1028.6485529

Triplet spin state ***d***

C	-6.46329800	0.72174200	-0.40521700
C	-6.84735600	1.96660700	-0.93335000
C	-5.98723100	3.05237500	-0.87016500
C	-4.69793800	2.93147800	-0.27332500
C	-4.33558700	1.66833500	0.27631600
C	-5.20115100	0.58769000	0.20256600
H	-7.82498000	2.07265000	-1.40797800
H	-6.28391400	4.01228400	-1.29698300
H	-3.37508700	1.54933200	0.78039600
H	-4.90447900	-0.37522600	0.62343500
C	-3.84106500	4.07782000	-0.19999300
O	-4.27166800	5.27651900	-0.50809200
C	-2.40541000	4.11703600	0.07986100
C	-1.50661000	3.12832300	-0.41262100
C	-1.85539500	5.23667000	0.76493500
C	-0.15490600	3.21423000	-0.15057100
H	-1.89295500	2.29330600	-0.99897500
C	-0.49296500	5.33598500	1.01410700
H	-2.53016300	6.01705200	1.11842900
C	0.37436400	4.31880200	0.56727800
H	0.54085300	2.44821300	-0.49869800
H	-0.11268200	6.19625600	1.56428500
C	2.33315100	5.37802600	1.44279500
H	3.40439800	5.14224400	1.46568900
H	2.18153400	6.33386500	0.91305500
H	1.95922100	5.47181300	2.47664300
O	1.70242800	4.30344200	0.76108000
C	-7.41461000	-0.43667600	-0.42244700
F	-8.16549500	-0.49945900	0.70273000
F	-8.28062600	-0.36968600	-1.45338900
F	-6.77173000	-1.61940400	-0.51288900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.225979 (Hartree/Particle)
Thermal correction to Energy= 0.243161
Thermal correction to Enthalpy= 0.244105
Thermal correction to Gibbs Free Energy= 0.177183
Sum of electronic and zero-point Energies= -1027.153230
Sum of electronic and thermal Energies= -1027.136049
Sum of electronic and thermal Enthalpies= -1027.135104

Sum of electronic and thermal Free Energies= -1027.202026
HF=-1027.3792093
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-1028.5490008

Ground state (singlet spin state) ***e***

C	-6.37817800	0.70790500	-0.45755100
C	-6.70535700	1.90809700	-1.11977100
C	-5.90320900	3.03087700	-0.94621600
C	-4.75282900	2.97468100	-0.14052600
C	-4.43808400	1.77757400	0.52399100
C	-5.24534400	0.65087000	0.37474000
H	-7.58875500	1.95159400	-1.75934400
H	-6.15697300	3.97403800	-1.43325000
H	-3.56879300	1.72900300	1.18162400
H	-5.00402400	-0.27401000	0.90160400
C	-3.96480600	4.24694500	0.05182600
O	-4.56439900	5.31278200	0.06339500
C	-2.48633100	4.19298000	0.22617600
C	-1.68167900	3.13321700	-0.24412500
C	-1.85085300	5.29518500	0.82451500
C	-0.30096900	3.17228500	-0.10506700
H	-2.13625900	2.28037000	-0.75093800
C	-0.46881200	5.34054300	0.98643000
H	-2.46946600	6.12662100	1.16828500
C	0.32063900	4.27112500	0.51996500
H	0.33038500	2.36348900	-0.47760800
H	-0.01477700	6.20543400	1.46930300
C	2.37034500	5.28401300	1.22418900
H	3.43306400	5.01185900	1.18925100
H	2.22172400	6.22982900	0.67469900
H	2.06919900	5.42754100	2.27651800
O	1.66337000	4.21350000	0.62048900
C	-7.20399100	-0.45514800	-0.62647100
N	-7.87079500	-1.39587200	-0.76366200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.222942 (Hartree/Particle)
Thermal correction to Energy= 0.237961
Thermal correction to Enthalpy= 0.238906
Thermal correction to Gibbs Free Energy= 0.179384
Sum of electronic and zero-point Energies= -782.638276
Sum of electronic and thermal Energies= -782.623257
Sum of electronic and thermal Enthalpies= -782.622313
Sum of electronic and thermal Free Energies= -782.681834
HF=-782.8612185
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-783.7305667

Triplet spin state ***e***

C	-6.48944900	0.72644100	-0.32952700
C	-6.88372400	1.98041700	-0.85985000
C	-6.02109700	3.05959400	-0.82715600
C	-4.71205500	2.94032500	-0.26662100
C	-4.33565700	1.67880300	0.28454500
C	-5.19979400	0.60030800	0.24693700
H	-7.87627400	2.08748600	-1.30265500
H	-6.32892200	4.01878600	-1.24788200
H	-3.36162400	1.56395700	0.76318300
H	-4.89484300	-0.35706500	0.67455100
C	-3.85478600	4.07958100	-0.22800000
O	-4.26237800	5.27463400	-0.55898200
C	-2.41359000	4.11656000	0.05216900
C	-1.51666700	3.14551600	-0.47294900
C	-1.86888600	5.21704200	0.76831200
C	-0.16472600	3.22583900	-0.20973700
H	-1.90463900	2.32697100	-1.08124200
C	-0.50739500	5.31133100	1.02163200
H	-2.54604000	5.98618000	1.14151500
C	0.36147600	4.30931800	0.54227800
H	0.53277400	2.47214000	-0.58020500
H	-0.12799100	6.15503900	1.59724100
C	2.31909900	5.34396100	1.45104000
H	3.38989800	5.10626900	1.46554600
H	2.16735900	6.31561000	0.95151800
H	1.94477800	5.40328800	2.48702000
O	1.68724700	4.29132500	0.73449500
C	-7.37754100	-0.39002600	-0.36701300
N	-8.10051000	-1.30230600	-0.39769300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.220092 (Hartree/Particle)
Thermal correction to Energy= 0.235412
Thermal correction to Enthalpy= 0.236357
Thermal correction to Gibbs Free Energy= 0.175398
Sum of electronic and zero-point Energies= -782.544829
Sum of electronic and thermal Energies= -782.529509
Sum of electronic and thermal Enthalpies= -782.528564
Sum of electronic and thermal Free Energies= -782.589523
HF=-782.764921
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-783.6342397

Ground state (singlet spin state) ***f***

C	-3.93849200	4.29236600	-0.05712700
O	-4.54386100	5.35215500	0.02536700
C	-2.46573700	4.22105400	0.14073300
C	-1.65770000	3.17987400	-0.36428300
C	-1.83762400	5.28414700	0.81371600
C	-0.28105500	3.19831600	-0.18753800
H	-2.10294800	2.36012400	-0.93051900
C	-0.46022300	5.30822600	1.01223900
H	-2.45915600	6.10057400	1.18688100
C	0.33259700	4.25702900	0.51048500
H	0.35314900	2.40413000	-0.58560500
H	-0.01179300	6.14200800	1.55174200
C	2.37099100	5.21117700	1.32139100
H	3.43201300	4.93126000	1.29844900
H	2.24408500	6.18663900	0.82049900
H	2.04395500	5.30004700	2.37200100
O	1.67110900	4.18152600	0.64260800
C	-6.27628300	0.92250000	-0.87055700

N	-5.23259700	0.72107900	-0.06423700
C	-4.45799300	1.77999600	0.18605800
C	-4.71876200	3.04398400	-0.36207100
C	-5.86728100	3.13346200	-1.16606300
N	-6.63850700	2.08085400	-1.43265100
H	-3.61227100	1.62631300	0.86510000
H	-6.90537600	0.05114900	-1.08980200
H	-6.14833800	4.09938500	-1.59985600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.200738 (Hartree/Particle)
Thermal correction to Energy= 0.213754
Thermal correction to Enthalpy= 0.214698
Thermal correction to Gibbs Free Energy= 0.159912
Sum of electronic and zero-point Energies= -722.528850
Sum of electronic and thermal Energies= -722.515834
Sum of electronic and thermal Enthalpies= -722.514890
Sum of electronic and thermal Free Energies= -722.569676
HF=-722.7295878
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-723.5354141

Triplet spin state ***f***

C	-6.55336400	0.79577100	-0.47006000
C	-6.81553500	2.06487200	-1.02509500
C	-5.96614900	3.12650800	-0.74525900
C	-4.81802500	2.96083700	0.08024200
C	-4.60171700	1.68598600	0.67679700
C	-5.43284900	0.62441800	0.38558300
H	-7.66972300	2.22412000	-1.68260600
H	-6.15962600	4.10693500	-1.18171100
H	-3.76983600	1.54655300	1.36888700
H	-5.26105200	-0.36519900	0.81348100
C	-3.97590300	4.11854000	0.37986100
O	-4.70875500	5.19381900	0.52561900
C	-8.45753900	-0.22805100	-1.49553100
H	-8.89168700	-1.23551300	-1.50417100
H	-9.19330900	0.48288300	-1.08284700
H	-8.20418400	0.06797700	-2.52774500
O	-7.29642600	-0.30106500	-0.68011200
C	0.09573600	4.26359700	1.09064400
N	-0.37197800	3.14687100	0.51145100
C	-1.67485200	3.08582000	0.27426300
C	-2.56700000	4.13627900	0.62834000
C	-1.93824100	5.27626200	1.20816500
N	-0.63420200	5.33312700	1.43623700
H	-2.04776100	2.18717800	-0.23029800
H	1.17254500	4.30795500	1.28893100
H	-2.54616100	6.14437600	1.48885400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.197459 (Hartree/Particle)
Thermal correction to Energy= 0.210789
Thermal correction to Enthalpy= 0.211733
Thermal correction to Gibbs Free Energy= 0.155477
Sum of electronic and zero-point Energies= -722.432443
Sum of electronic and thermal Energies= -722.419113
Sum of electronic and thermal Enthalpies= -722.418169
Sum of electronic and thermal Free Energies= -722.474425
HF=-722.629902
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-723.4350388

Ground state (singlet spin state) ***g***

C	-6.14508100	0.70098300	-0.27630300
C	-6.84689500	1.91961000	-0.34611500
C	-6.15039300	3.11852400	-0.27671600
C	-4.74898600	3.12975700	-0.13723400
C	-4.06626700	1.90057000	-0.06945800
C	-4.76134500	0.68442100	-0.13861900
H	-6.68934900	-0.24503000	-0.33061400
H	-7.93361800	1.91852100	-0.45435000
H	-6.65835200	4.08370800	-0.32741300
H	-4.19756700	-0.24831800	-0.08273400
C	-4.00427100	4.40564300	-0.06321300
O	-4.55178800	5.50035500	-0.11688300
C	-2.54098400	4.24495400	0.08133300
C	-1.96662700	2.96104300	0.13814700
C	-1.69593200	5.36850100	0.16505200
C	-0.58064100	2.79606300	0.27505200
C	-0.32285400	5.21499600	0.30080200
H	-2.16385700	6.35394600	0.11900400
C	0.23171200	3.92194400	0.35541300
H	-0.17211600	1.78489800	0.31536300
H	0.32634500	6.09082400	0.36516400
H	1.31198600	3.79656500	0.46214500
O	-2.71401900	1.82608400	0.06450300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.175253 (Hartree/Particle)
Thermal correction to Energy= 0.185366
Thermal correction to Enthalpy= 0.186310
Thermal correction to Gibbs Free Energy= 0.139261
Sum of electronic and zero-point Energies= -650.045704
Sum of electronic and thermal Energies= -650.035591
Sum of electronic and thermal Enthalpies= -650.034647
Sum of electronic and thermal Free Energies= -650.081696
HF=-650.220957
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-650.9336767

Triplet spin state ***g***

C	-6.14896900	0.68282100	-0.26596200
C	-6.83761700	1.91032900	-0.34905500
C	-6.15983800	3.12589600	-0.28021300
C	-4.75376500	3.15658700	-0.14252700
C	-4.07872200	1.89616900	-0.06328700
C	-4.75839400	0.67974600	-0.12474200
H	-6.69522100	-0.26075100	-0.31595200

H	-7.92293600	1.90904100	-0.47822000
H	-6.68989000	4.07709300	-0.34249400
H	-4.18415200	-0.24557700	-0.05364600
C	-3.98830300	4.37336200	-0.06160500
O	-4.56931100	5.53446500	-0.11828300
C	-2.55988000	4.26527000	0.08427700
C	-1.95533500	2.96817100	0.13101100
C	-1.69669800	5.38088000	0.16835600
C	-0.57802400	2.79032300	0.26069200
C	-0.32144600	5.20272500	0.30557300
H	-2.14076500	6.37651300	0.13470700
C	0.24886000	3.91400700	0.34620600
H	-0.18087200	1.77409900	0.28501500
H	0.32602000	6.07907400	0.39151900
H	1.32856500	3.79141700	0.44833000
O	-2.72420900	1.84690400	0.06262600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.170183 (Hartree/Particle)
Thermal correction to Energy= 0.180807
Thermal correction to Enthalpy= 0.181751
Thermal correction to Gibbs Free Energy= 0.132896
Sum of electronic and zero-point Energies= -649.937724
Sum of electronic and thermal Energies= -649.927099
Sum of electronic and thermal Enthalpies= -649.926155
Sum of electronic and thermal Free Energies= -649.975010
HF=-650.1079061
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-650.8218954

Ground state (singlet spin state) ***h***

C	-6.40239700	0.72412600	-0.30295700
C	-6.95639800	2.01459000	-0.35600300
C	-6.12236900	3.11990200	-0.27320000
C	-4.72405300	2.98067000	-0.13628400
C	-4.18081500	1.67844900	-0.08387800
C	-5.02994900	0.55555400	-0.16830100
H	-7.04833100	-0.15497000	-0.36726200
H	-8.03554500	2.14575700	-0.46167700
H	-6.52046100	4.13513900	-0.31124200
H	-4.60301300	-0.44982000	-0.12721300
C	-3.91666900	4.22985600	-0.05679400
O	-4.46480500	5.32616000	-0.11219000
C	-2.43753000	4.13541700	0.09109800
C	-1.72165500	2.92037400	0.16090500
C	-1.71462400	5.34592300	0.16527400
C	-0.31836300	2.93507500	0.30102900
C	-0.33444000	5.35888900	0.30344700
H	-2.28791100	6.27266700	0.10937400
C	0.36567300	4.14225100	0.37138500
H	0.23003100	1.99105800	0.35422100
H	0.20449200	6.30725200	0.35904800
H	1.45303400	4.13853200	0.48009400
S	-2.46573100	1.32917100	0.08426400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.171959 (Hartree/Particle)
Thermal correction to Energy= 0.182738
Thermal correction to Enthalpy= 0.183682
Thermal correction to Gibbs Free Energy= 0.134723
Sum of electronic and zero-point Energies= -972.963681
Sum of electronic and thermal Energies= -972.952902
Sum of electronic and thermal Enthalpies= -972.951958
Sum of electronic and thermal Free Energies= -973.000917
HF=-973.1356404
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-973.900182

Triplet spin state ***h***

C	-6.40141200	0.69985000	-0.30380300
C	-6.94109800	2.00232800	-0.35538900
C	-6.12793100	3.12672800	-0.27372600
C	-4.72164400	3.01721500	-0.13527800
C	-4.19524000	1.68075900	-0.08459100
C	-5.02369600	0.54729300	-0.16779900
H	-7.04902000	-0.17603800	-0.36895600
H	-8.02151100	2.13186600	-0.46184600
H	-6.54575700	4.13285900	-0.31346000
H	-4.58027300	-0.45111800	-0.12515700
C	-3.91237300	4.22083200	-0.05439600
O	-4.48686100	5.36968600	-0.11061800
C	-2.46820600	4.15513500	0.08882500
C	-1.71498000	2.93324600	0.16239500
C	-1.71673200	5.35440100	0.16470600
C	-0.31544800	2.92507200	0.30151500
C	-0.33361500	5.33928700	0.30237100
H	-2.27102100	6.29157500	0.11053300
C	0.38459100	4.12705000	0.37253800
H	0.21764600	1.97195600	0.35336100
H	0.20747100	6.28777300	0.35729300
H	1.47047800	4.12670900	0.48060000
S	-2.48519600	1.36755700	0.08401900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.168039 (Hartree/Particle)
Thermal correction to Energy= 0.179202
Thermal correction to Enthalpy= 0.180146
Thermal correction to Gibbs Free Energy= 0.129454
Sum of electronic and zero-point Energies= -972.866280
Sum of electronic and thermal Energies= -972.855117
Sum of electronic and thermal Enthalpies= -972.854173
Sum of electronic and thermal Free Energies= -972.904865
HF=-973.0343192
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-973.8012367

Ground state (singlet spin state) ***i***

C	-6.20235900	0.70444900	-0.28324100
C	-6.87376200	1.94168500	-0.34980600

C	-6.14197200	3.11776400	-0.27595400
C	-4.74037000	3.09466900	-0.13547200
C	-4.07405700	1.84590700	-0.06915100
C	-4.82261400	0.65025400	-0.14498200
H	-6.77071300	-0.22738000	-0.34097800
H	-7.96005700	1.97025400	-0.45871900
H	-6.62247300	4.09706700	-0.32389900
H	-4.30689400	-0.31240900	-0.09455300
C	-3.98298900	4.36331400	-0.05945100
O	-4.53259300	5.46210900	-0.11272100
C	-2.51778500	4.21723200	0.08467100
C	-1.91783500	2.93490100	0.14430700
C	-1.70011700	5.36166700	0.16446000
C	-0.51603700	2.82576300	0.28150400
C	-0.32405200	5.25066500	0.29950200
H	-2.19591500	6.33325900	0.11543300
C	0.26374500	3.97118800	0.35746100
H	-0.05408900	1.83593500	0.32668200
H	0.30118200	6.14401400	0.36048500
H	1.34724900	3.87397400	0.46344400
N	-2.70441900	1.80721800	0.06793800
H	-2.25200100	0.90129100	0.11513600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.188299 (Hartree/Particle)
Thermal correction to Energy= 0.198560
Thermal correction to Enthalpy= 0.199504
Thermal correction to Gibbs Free Energy= 0.152298
Sum of electronic and zero-point Energies= -630.201710
Sum of electronic and thermal Energies= -630.191449
Sum of electronic and thermal Enthalpies= -630.190505
Sum of electronic and thermal Free Energies= -630.237711
HF=-630.3900092
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-631.075555

Triplet spin state ***i***

C	-6.20290300	0.67734000	-0.28209900
C	-6.85976100	1.91796900	-0.34701600
C	-6.15227400	3.12374400	-0.27585500
C	-4.75039600	3.12972800	-0.13578900
C	-4.09329600	1.85372200	-0.07051800
C	-4.80947000	0.64828300	-0.14288700
H	-6.76747400	-0.25472100	-0.33925700
H	-7.94747800	1.94314400	-0.45565500
H	-6.65979300	4.08758300	-0.32645100
H	-4.27186200	-0.30232600	-0.09066200
C	-3.98120100	4.36020400	-0.05865100
O	-4.55170000	5.50019100	-0.11377200
C	-2.53931200	4.24704700	0.08233300
C	-1.91148600	2.95620100	0.14411000
C	-1.69873200	5.37466800	0.16437500
C	-0.52102800	2.81551200	0.27883500
C	-0.31329600	5.22682100	0.29911800
H	-2.16658800	6.35862900	0.11901200
C	0.28655600	3.95728100	0.35714000
H	-0.08158100	1.81518500	0.32102900
H	0.31513200	6.11951100	0.36031600
H	1.36812100	3.85738800	0.46192900
N	-2.72202900	1.84440000	0.06645000
H	-2.26715500	0.93441200	0.11457200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.184337 (Hartree/Particle)
Thermal correction to Energy= 0.194877
Thermal correction to Enthalpy= 0.195822
Thermal correction to Gibbs Free Energy= 0.147198
Sum of electronic and zero-point Energies= -630.105784
Sum of electronic and thermal Energies= -630.095244
Sum of electronic and thermal Enthalpies= -630.094299
Sum of electronic and thermal Free Energies= -630.142923
HF=-630.2901209
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-630.9779687

Ground state (singlet spin state) ***j***

C	-6.27789000	0.70964500	-0.28931100
C	-6.90451800	1.96229400	-0.35118500
C	-6.14353700	3.12882700	-0.27560500
C	-4.75009100	3.05579600	-0.13756600
C	-4.11931400	1.79476800	-0.07501700
C	-4.89227300	0.62742800	-0.15183500
H	-6.87485900	-0.20358300	-0.34880100
H	-7.99001400	2.02564600	-0.45881300
H	-6.60885900	4.11504600	-0.32168300
H	-4.38223800	-0.33619700	-0.10143400
C	-3.96306300	4.32340900	-0.06019600
O	-4.50889500	5.41492500	-0.11481700
C	-2.48123100	4.20172500	0.08674900
C	-1.85043100	2.94070900	0.14930100
C	-1.70827400	5.36906000	0.16364100
C	-0.45699000	2.86767000	0.28741500
C	-0.32266900	5.28686900	0.30120300
H	-2.21832800	6.33267700	0.11323100
C	0.30396300	4.03422200	0.36307900
H	0.00835000	1.88146300	0.33349100
H	0.27429200	6.20009800	0.36075900
H	1.38945300	3.97087200	0.47077500
C	-2.63746200	1.67309500	0.07184200
O	-2.09161700	0.58158100	0.12633600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.181184 (Hartree/Particle)
Thermal correction to Energy= 0.192175
Thermal correction to Enthalpy= 0.193120
Thermal correction to Gibbs Free Energy= 0.143846
Sum of electronic and zero-point Energies= -688.125973
Sum of electronic and thermal Energies= -688.114981
Sum of electronic and thermal Enthalpies= -688.114037
Sum of electronic and thermal Free Energies= -688.163310

HF=-688.3071564
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-689.0601208

Triplet spin state ***j***

C	-6.26266100	0.70848600	-0.28579600
C	-6.89521300	1.96792100	-0.34771300
C	-6.13562300	3.12853500	-0.27292100
C	-4.73619000	3.07223300	-0.13546200
C	-4.10250600	1.80122100	-0.07333200
C	-4.88699500	0.62069700	-0.15058000
H	-6.85917400	-0.20520000	-0.34460700
H	-7.98066700	2.02916300	-0.45429100
H	-6.59573800	4.11779400	-0.31802600
H	-4.39491400	-0.35316900	-0.10237600
C	-3.96890000	4.33476400	-0.06034400
O	-4.52020000	5.43682400	-0.11470900
C	-2.50278900	4.20041600	0.08388100
C	-1.86549400	2.93125400	0.14670300
C	-1.71309700	5.36263000	0.16195900
C	-0.45462700	2.85980300	0.28598500
C	-0.33300100	5.28299800	0.29824600
H	-2.22887700	6.32375300	0.11117800
C	0.29573100	4.02165600	0.36023600
H	0.02974400	1.88206100	0.33385600
H	0.26548600	6.19493400	0.35742200
H	1.38132600	3.95776100	0.46751600
C	-2.66668100	1.73203400	0.06769800
O	-2.08542900	0.57035500	0.12436200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.177538 (Hartree/Particle)
Thermal correction to Energy= 0.188835
Thermal correction to Enthalpy= 0.189779
Thermal correction to Gibbs Free Energy= 0.139145
Sum of electronic and zero-point Energies= -688.035692
Sum of electronic and thermal Energies= -688.024395
Sum of electronic and thermal Enthalpies= -688.023451
Sum of electronic and thermal Free Energies= -688.074085
HF=-688.2132297
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-688.9665519

Ground state (singlet spin state) ***k***

C	-0.79208700	-0.86019300	-4.72006100
C	0.62785700	-0.36669800	-4.81880200
C	0.75551500	0.80712200	-5.79576500
C	-1.82310500	-0.02565800	-4.24212200
C	0.33981200	2.15994800	-5.25597700
C	-0.67932200	2.38286600	-4.29487700
H	1.00419000	-0.06023300	-3.82719300
H	0.17037500	0.58001400	-6.70609200
H	1.27310200	-1.19026400	-5.15870400
H	1.80256900	0.88618900	-6.12680500
C	-1.61901200	1.36082600	-3.68963500
O	-2.33321500	1.69950500	-2.75523700
C	-3.44776800	-1.81049900	-4.60149900
C	-2.42624200	-2.63947800	-5.07651600
C	-1.11411900	-2.16452300	-5.12562700
C	-3.13975000	-0.52109000	-4.17377000
H	-4.47833600	-2.17086900	-4.55773300
H	-2.64997000	-3.65707400	-5.40695800
H	-0.31565500	-2.81890000	-5.48603500
H	-3.91848600	0.13086700	-3.77452800
C	1.04910600	3.27400300	-5.74272600
C	0.78793600	4.57175700	-5.30911100
C	-0.20202300	4.78916400	-4.34528700
C	-0.91492500	3.70430400	-3.85053200
H	1.84022300	3.10765000	-6.47911900
H	1.36276200	5.40860300	-5.71415900
H	-0.41631900	5.79796300	-3.98448300
H	-1.69462400	3.85198300	-3.10280200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.227768 (Hartree/Particle)
Thermal correction to Energy= 0.239431
Thermal correction to Enthalpy= 0.240375
Thermal correction to Gibbs Free Energy= 0.189355
Sum of electronic and zero-point Energies= -653.388563
Sum of electronic and thermal Energies= -653.376900
Sum of electronic and thermal Enthalpies= -653.375955
Sum of electronic and thermal Free Energies= -653.426976
HF=-653.616331
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-654.3263673

Triplet spin state ***k***

C	-0.81160800	-0.83219800	-4.75934700
C	0.56520300	-0.28159200	-5.02455900
C	0.55918800	0.88508800	-6.03708400
C	-1.91176600	0.02030500	-4.43246800
C	0.31513500	2.22136500	-5.38621400
C	-0.77236700	2.42851800	-4.48153200
H	1.02836500	0.06640000	-4.08368900
H	-0.20897400	0.68517000	-6.80569700
H	1.20290500	-1.09516600	-5.40133600
H	1.52376300	0.92172800	-6.56505500
C	-1.80569400	1.44893100	-4.19793100
O	-2.87498500	1.96848200	-3.60036200
C	-3.38787500	-1.94590100	-4.36127300
C	-2.30658800	-2.77571200	-4.67630300
C	-1.04317600	-2.20348900	-4.88510800
C	-3.19771500	-0.57367900	-4.25260900
H	-4.38574500	-2.36746700	-4.21678500
H	-2.44234400	-3.85507100	-4.77621800
H	-0.20388300	-2.84901300	-5.15949100
H	-4.05176500	0.07323100	-4.04462600
C	1.19783400	3.27706100	-5.62277200
C	1.04035500	4.53750500	-5.02775500
C	-0.01905000	4.74458600	-4.13802700
C	-0.90188600	3.70790800	-3.86076700
H	2.04279500	3.10682100	-6.29616200
H	1.74927500	5.33919700	-5.24718500

H -0.14748800 5.71160200 -3.64536200
H -1.70341600 3.86267700 -3.13643800
UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.224311
(Hartree/Particle)
Thermal correction to Energy= 0.236348
Thermal correction to Enthalpy= 0.237293
Thermal correction to Gibbs Free Energy= 0.184438
Sum of electronic and zero-point Energies= -
653.292286
Sum of electronic and thermal Energies= -
653.280249
Sum of electronic and thermal Enthalpies= -
653.279305
Sum of electronic and thermal Free Energies= -
653.332159
HF=-653.5165974
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-654.2261988

Figure A2.1
Ketyl radical III

C	-6.65213500	1.07656500	-0.61916200
C	-5.77121700	1.75229200	-1.47594200
C	-4.75450000	2.55301000	-0.96465700
C	-4.57704300	2.70291800	0.43634900
C	-5.48476200	2.01533100	1.28706300
C	-6.50139900	1.21840600	0.76509600
H	-7.44855400	0.45001700	-1.02746900
H	-5.89123300	1.66536100	-2.55911900
H	-4.10992400	3.10621000	-1.64885700
H	-5.35664200	2.07518400	2.37123300
H	-7.17444400	0.69013500	1.44570100
C	-3.56680500	3.56973400	1.00989500
C	-2.28152500	3.91167100	0.45183200
C	-1.65075800	3.13222200	-0.55533600
C	-1.57232000	5.03787600	0.95160100
C	-0.40142100	3.48591600	-1.05628600
H	-2.13293100	2.22341300	-0.91737100
C	-0.32363200	5.38092100	0.44320800
H	-2.02941900	5.63907000	1.73812700
C	0.27087600	4.61509300	-0.56905200
H	0.06295200	2.86444500	-1.82666000
H	0.19493800	6.25876700	0.83820400
H	1.25154700	4.88832800	-0.96602700
O	-3.82269000	4.11925100	2.23339200
H	-4.77791300	4.11793200	2.38885400

UB3LYP-D3/def2-SVP
Zero-point correction= 0.202063
(Hartree/Particle)
Thermal correction to Energy= 0.213118
Thermal correction to Enthalpy= 0.214062
Thermal correction to Gibbs Free Energy= 0.164012
Sum of electronic and zero-point Energies= -
576.607153
Sum of electronic and thermal Energies= -
576.596099
Sum of electronic and thermal Enthalpies= -
576.595155
Sum of electronic and thermal Free Energies= -
576.645204
HF=-576.8092164
UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP
HF=-577.4419177

Triplet Ketone

C	-6.67425200	1.11124700	-0.62304800
C	-5.78099900	1.78175800	-1.47558800
C	-4.75680400	2.56546300	-0.95729700
C	-4.57348700	2.67258700	0.44731000
C	-5.49723300	2.00512200	1.29960600
C	-6.52728100	1.23772400	0.76439600
H	-7.48046600	0.50315800	-1.03990100
H	-5.89952200	1.70195300	-2.55946200
H	-4.09968900	3.11739000	-1.63116300
H	-5.36962200	2.08162600	2.38082000
H	-7.21890000	0.72200900	1.43577500
C	-3.52813600	3.49314200	1.02668300
C	-2.25354400	3.87758000	0.45290800
C	-1.59726900	3.08443900	-0.52600900
C	-1.59235100	5.04514600	0.92706400
C	-0.36729900	3.47693400	-1.04069300
H	-2.05479000	2.15221300	-0.86089100
C	-0.35330700	5.41518000	0.41306100
H	-2.08420400	5.66198300	1.68122500
C	0.26584200	4.64300900	-0.57841600
H	0.11738600	2.85976700	-1.80186900
H	0.13264400	6.32268500	0.78094100
H	1.23591300	4.93958100	-0.98403500
O	-3.76975600	3.95229400	2.24182700

UB3LYP-D3/def2-SVP
Zero-point correction= 0.188518
(Hartree/Particle)
Thermal correction to Energy= 0.199528
Thermal correction to Enthalpy= 0.200472
Thermal correction to Gibbs Free Energy= 0.149814
Sum of electronic and zero-point Energies= -
575.947506
Sum of electronic and thermal Energies= -
575.936496
Sum of electronic and thermal Enthalpies= -
575.935552
Sum of electronic and thermal Free Energies= -
575.986210
HF=-576.136024
UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP
HF=-576.7662586

H radical

H 1.82744000 0.40918200 0.01606800
UB3LYP-D3/def2-SVP
Zero-point correction= 0.000000
(Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.010654
Sum of electronic and zero-point Energies= -
0.501259
Sum of electronic and thermal Energies= -
0.499843
Sum of electronic and thermal Enthalpies= -
0.498898

Sum of electronic and thermal Free Energies= -0.511913
HF=-0.5012589
UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP
HF=-0.5021542

***i*-PrOH**

C	-0.30959400	-0.28470100	2.24521800
C	-1.37426700	-1.37894600	2.32997900
H	-2.29918700	-1.08237500	1.80931000
H	-1.01641000	-2.31485200	1.86730200
H	-1.61551100	-1.59003300	3.38442900
C	-0.76842900	1.02205600	2.87743600
H	0.03081300	1.77579500	2.81383300
H	-1.66562100	1.41295300	2.37297200
H	-1.00250200	0.86215900	3.94243000
O	0.87667800	-0.66916000	2.92753300
H	1.19031100	-1.49900000	2.54576800
H	-0.08768000	-0.09365200	1.17233200

UB3LYP-D3/def2-SVP
Zero-point correction= 0.107626 (Hartree/Particle)
Thermal correction to Energy= 0.112993
Thermal correction to Enthalpy= 0.113937
Thermal correction to Gibbs Free Energy= 0.080328
Sum of electronic and zero-point Energies= -194.113419
Sum of electronic and thermal Energies= -194.108052
Sum of electronic and thermal Enthalpies= -194.107108
Sum of electronic and thermal Free Energies= -194.140717
HF=-194.2210453
UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP
HF=-194.4528413

***i*-PrO• radical**

C	-5.13058700	7.55985900	2.88656500
H	-5.81784400	8.41401000	2.63935000
C	-5.77313200	6.77285300	4.04052900
H	-5.13077100	5.91902800	4.31035800
H	-5.89933800	7.40383700	4.93426300
H	-6.75423600	6.38234700	3.73297100
C	-3.76037400	8.16076900	3.24052200
H	-3.05238300	7.35227800	3.48455000
H	-3.36006700	8.72248400	2.38384900
H	-3.82991300	8.83111200	4.11151900
O	-5.11915900	6.86616100	1.71190100

UB3LYP-D3/def2-SVP
Zero-point correction= 0.093445 (Hartree/Particle)
Thermal correction to Energy= 0.098592
Thermal correction to Enthalpy= 0.099536
Thermal correction to Gibbs Free Energy= 0.065606
Sum of electronic and zero-point Energies= -193.456335
Sum of electronic and thermal Energies= -193.451188
Sum of electronic and thermal Enthalpies= -193.450244
Sum of electronic and thermal Free Energies= -193.484174
HF=-193.5497804
UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP
HF=-193.7778365

α-hydroxyl alkyl radical

C	-0.34939700	-0.30481200	2.42508900
C	-1.34963600	-1.41110900	2.31994400
H	-2.26954800	-1.06696100	1.82264000
H	-0.95658300	-2.26440500	1.73667100
H	-1.64256600	-1.80981600	3.31766900
C	-0.75292500	1.05718400	2.87638100
H	0.05892300	1.78058100	2.69844500
H	-1.65414700	1.39928400	2.34443800
H	-0.97782800	1.08488700	3.96574000
O	0.91965300	-0.64143600	2.83655700
H	1.11097600	-1.54838400	2.56315200

UB3LYP-D3/def2-SVP
Zero-point correction= 0.093595 (Hartree/Particle)
Thermal correction to Energy= 0.099271
Thermal correction to Enthalpy= 0.100216
Thermal correction to Gibbs Free Energy= 0.065236
Sum of electronic and zero-point Energies= -193.472582
Sum of electronic and thermal Energies= -193.466906
Sum of electronic and thermal Enthalpies= -193.465962
Sum of electronic and thermal Free Energies= -193.500942
HF=-193.5661776
UB3LYP-D3/def2-TZVPP//UB3LYP-D3/def2-SVP
HF=-193.7952184

^{3}II

C	-6.68733300	1.08108100	-0.63480500
C	-5.80015500	1.76945000	-1.48029600
C	-4.77717600	2.54963300	-0.95331000
C	-4.58877300	2.63449700	0.45235900
C	-5.50596600	1.94866800	1.29779300
C	-6.53526600	1.18521200	0.75434500
H	-7.49246500	0.47632200	-1.05837700
H	-5.92202600	1.70603700	-2.56475800
H	-4.12503900	3.11367300	-1.62184100
H	-5.37512600	2.00676600	2.37977300
H	-7.22158500	0.65545100	1.42005800
C	-3.54530400	3.45156200	1.04081200
O	-3.78471900	3.88884200	2.26502500
C	-2.27477000	3.85335100	0.46979700
C	-1.61706100	3.08099400	-0.52534300
C	-1.61792300	5.01608500	0.96367000
C	-0.39022500	3.48930000	-1.03601300
H	-2.07049000	2.15345300	-0.87810200
C	-0.38161500	5.40168000	0.45348200
H	-2.10992300	5.61803700	1.72966700
C	0.23880700	4.65022400	-0.55362200
H	0.09482300	2.88921600	-1.81034100
H	0.10063300	6.30476800	0.83654700
H	1.20629900	4.95881100	-0.95626300

UB3LYP-D3/def2-SVP-CPCM(benzene)

Zero-point correction= 0.188417 (Hartree/Particle)
Thermal correction to Energy= 0.199452
Thermal correction to Enthalpy= 0.200396
Thermal correction to Gibbs Free Energy= 0.149624
Sum of electronic and zero-point Energies= -575.949841
Sum of electronic and thermal Energies= -575.938806
Sum of electronic and thermal Enthalpies= -575.937862
Sum of electronic and thermal Free Energies= -575.988634
HF=-576.1382581
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-576.7686266

^{3}II-TS-III^{CH}

C	-6.40711800	2.44799600	-1.53908900
C	-5.31390000	3.16043300	-2.06077400
C	-4.23898800	3.50813100	-1.24969300
C	-4.21397500	3.13011900	0.12026200
C	-5.33451100	2.42203200	0.63868500
C	-6.40744100	2.08658900	-0.18481000
H	-5.31204300	3.46124100	-3.11163400
H	-3.41924400	4.09888600	-1.66156700
H	-5.33603300	2.13181300	1.69038200
H	-7.25435900	1.53784400	0.23471300
C	-3.13395400	3.51181000	1.00530600
C	-1.75565600	3.80086600	0.65661400
C	-1.12245900	3.22351600	-0.47750900
C	-0.97880300	4.63709500	1.50842900
C	0.20314700	3.51991700	-0.77082500
H	-1.67797100	2.53137100	-1.11224200
C	0.35256800	4.91151600	1.20970100
H	-1.45211300	5.08204200	2.38502600
C	0.95251400	4.36470200	0.06735200
H	0.66996500	3.07702500	-1.65448600
H	0.92829000	5.56763500	1.86763900
O	-3.40392200	3.60374700	2.29847900
C	-5.81692500	5.48377000	2.23607100
H	-5.10958100	4.65585000	2.49891800
C	-5.06818400	6.43692200	1.30659100
H	-5.71405200	7.28802800	1.03478800
H	-4.15629300	6.82133000	1.78954800
H	-4.76617500	5.92226400	0.38044700
C	-6.26417700	6.14073500	3.53340700
H	-6.94816300	6.97818800	3.31741400
H	-6.79866300	5.41464500	4.16458400
H	-5.40005500	6.52791900	4.09415500
O	-6.96719100	4.93888100	1.61912800
H	-6.69787400	4.49865000	0.79994600
H	1.99620700	4.58599500	-0.16760700
H	-7.25094100	2.18563300	-2.18103500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.296734 (Hartree/Particle)
Thermal correction to Energy= 0.314065
Thermal correction to Enthalpy= 0.315009
Thermal correction to Gibbs Free Energy= 0.249122
Sum of electronic and zero-point Energies= -770.077952
Sum of electronic and thermal Energies= -770.060621
Sum of electronic and thermal Enthalpies= -770.059677
Sum of electronic and thermal Free Energies= -770.125563
HF=-770.3746855
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-771.2324942

III

C	-6.64857200	1.07193100	-0.62088900
C	-5.76941300	1.75096200	-1.47722400
C	-4.75580400	2.55556400	-0.96426900
C	-4.58022900	2.70538600	0.43709400
C	-5.48680100	2.01581700	1.28733800
C	-6.50012400	1.21496000	0.76406700
H	-7.44236400	0.44249800	-1.02990100
H	-5.88753500	1.66348700	-2.56049600
H	-4.11275200	3.10961500	-1.64919000
H	-5.36493400	2.08041700	2.37169800
H	-7.17309500	0.68612500	1.44417600
C	-3.56948500	3.57256400	1.01134400
C	-2.28395300	3.91302200	0.45150000
C	-1.65403100	3.13374400	-0.55720600
C	-1.57169900	5.03811000	0.95160000
C	-0.40332500	3.48522100	-1.05746100
H	-2.13783800	2.22737200	-0.92293900
C	-0.32156300	5.37916800	0.44401800
H	-2.02709800	5.64215100	1.73703000
C	0.27222200	4.61254700	-0.56875100
H	0.05909000	2.86373200	-1.82895700
H	0.19813300	6.25607000	0.83962100
H	1.25357800	4.88395000	-0.96520400
O	-3.81953400	4.11957700	2.23624600
H	-4.77382500	4.12608300	2.40137100

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.201941 (Hartree/Particle)
Thermal correction to Energy= 0.213014
Thermal correction to Enthalpy= 0.213958
Thermal correction to Gibbs Free Energy= 0.163854
Sum of electronic and zero-point Energies= -576.610737
Sum of electronic and thermal Energies= -576.599665
Sum of electronic and thermal Enthalpies= -576.598720
Sum of electronic and thermal Free Energies= -576.648824
HF=-576.8126784
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-577.4453796

IV

C	-0.34885400	-0.30409300	2.42103500
C	-1.34898600	-1.41058500	2.31775600
H	-2.27071900	-1.06497100	1.82498400

H	-0.95670200	-2.26334300	1.73426700
H	-1.63716000	-1.80807100	3.31705900
C	-0.75302600	1.05727200	2.87559700
H	0.05601000	1.78447000	2.69826900
H	-1.65625900	1.39868600	2.34685200
H	-0.97683100	1.08175600	3.96540600
O	0.92231100	-0.64068800	2.82990300
H	1.10713700	-1.55542100	2.57559900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.093480 (Hartree/Particle)
Thermal correction to Energy= 0.099157
Thermal correction to Enthalpy= 0.100102
Thermal correction to Gibbs Free Energy= 0.065120
Sum of electronic and zero-point Energies= -193.474990
Sum of electronic and thermal Energies= -193.469313
Sum of electronic and thermal Enthalpies= -193.468368
Sum of electronic and thermal Free Energies= -193.503350
HF=-193.5684701
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-193.7976445

^{3}II-TS-III^{OH}

C	-6.42184900	1.69666000	-0.48325500
C	-5.39409300	2.08682700	-1.35311100
C	-4.36466000	2.91332000	-0.90895100
C	-4.31945900	3.36394300	0.44023000
C	-5.38704900	2.98103400	1.29886500
C	-6.41029100	2.15789700	0.84328400
H	-7.22984000	1.05182400	-0.83674000
H	-5.40664900	1.75829000	-2.39569900
H	-3.60075200	3.24596600	-1.61311700
H	-5.38689700	3.33929600	2.32869800
H	-7.20970000	1.86400100	1.52871400
C	-3.27964500	4.24749000	0.94119100
C	-1.92077300	4.34960800	0.44334600
C	-1.27735400	3.30228400	-0.26959000
C	-1.16143700	5.51931800	0.72548600
C	0.03252500	3.44424800	-0.71752400
H	-1.80442600	2.36329900	-0.44481600
C	0.14943200	5.64850400	0.27583100
H	-1.63102500	6.32322200	1.29424000
C	0.75647200	4.61839800	-0.45614200
H	0.50451500	2.62366900	-1.26453400
H	0.70624600	6.56370400	0.49445900
H	1.78537200	4.72208900	-0.80884700
O	-3.58127100	5.03997600	1.97501200
C	-5.82345800	6.33122500	0.30111400
H	-5.70888200	5.32457000	-0.17788300
C	-7.27931700	6.75411000	0.07629200
H	-7.46015500	7.73611700	0.54102900
H	-7.48861500	6.82889800	-1.00103700
H	-7.96365300	6.01973700	0.52503600
C	-4.78883800	7.27107400	-0.31958500
H	-4.87602200	8.27525900	0.12559500
H	-3.76854600	6.89924800	-0.14379200
H	-4.94358600	7.35375800	-1.40601800
O	-5.62183800	6.13564500	1.66154600
H	-4.57557400	5.73782500	1.88181100

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.291414 (Hartree/Particle)
Thermal correction to Energy= 0.308593
Thermal correction to Enthalpy= 0.309538
Thermal correction to Gibbs Free Energy= 0.243963
Sum of electronic and zero-point Energies= -770.076278
Sum of electronic and thermal Energies= -770.059098
Sum of electronic and thermal Enthalpies= -770.058154
Sum of electronic and thermal Free Energies= -770.123728
HF=-770.3676917
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-771.2216196

IV^{OH}

C	-5.12962200	7.55885800	2.88721800
H	-5.81701600	8.41403300	2.64138500
C	-5.77265300	6.77188600	4.04015100
H	-5.12976700	5.91877900	4.31111100
H	-5.89843800	7.40517900	4.93187100
H	-6.75500100	6.38307800	3.73385400
C	-3.76005700	8.15982100	3.24016700
H	-3.05222000	7.35177100	3.48634200
H	-3.36017900	8.72295700	2.38406700
H	-3.83276500	8.83080300	4.10996600
O	-5.12008600	6.86757200	1.71024400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.093336 (Hartree/Particle)
Thermal correction to Energy= 0.098478
Thermal correction to Enthalpy= 0.099423
Thermal correction to Gibbs Free Energy= 0.065502
Sum of electronic and zero-point Energies= -193.458356
Sum of electronic and thermal Energies= -193.453213
Sum of electronic and thermal Enthalpies= -193.452269
Sum of electronic and thermal Free Energies= -193.486189
HF=-193.5516914
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-193.7800433

Figure A2.2

1

C	-1.07437600	-2.81445400	-5.07040200
C	0.40516500	-2.64218800	-5.47606500
C	0.80125100	-1.31441400	-4.81681900
C	-0.41379400	-0.42353700	-5.08433800
C	-1.62250300	-1.37110900	-4.87497000
H	-1.64686000	-3.38602300	-5.81684200
H	-1.14156300	-3.37443000	-4.12330000
H	0.48867800	-2.53338200	-6.56915300

H	1.03875200	-3.48989100	-5.17241900
H	0.92233900	-1.44554700	-3.72749500
H	1.72397100	-0.86631400	-5.21516300
H	-0.45320900	0.45580800	-4.41125200
H	-2.04119100	-1.23692900	-3.86516200
H	-2.42660500	-1.12689800	-5.58513500
O	-0.30946900	0.02283800	-6.43221800
C	-1.18615900	1.06155700	-6.78300400
H	-1.03139900	1.96350200	-6.15523100
H	-0.98772700	1.32848000	-7.83205000
H	-2.25302600	0.77343000	-6.69788200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.172366 (Hartree/Particle)
Thermal correction to Energy= 0.179853
Thermal correction to Enthalpy= 0.180797
Thermal correction to Gibbs Free Energy= 0.139975
Sum of electronic and zero-point Energies= -310.690566
Sum of electronic and thermal Energies= -310.683079
Sum of electronic and thermal Enthalpies= -310.682135
Sum of electronic and thermal Free Energies= -310.722957
HF=-310.8629322
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-311.2154922
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-310.540565261743

1-TS-2

C	-7.11444500	3.56213900	-0.72452600
C	-6.19945400	4.64490000	-0.71232800
C	-4.97689800	4.52826500	-0.07682600
C	-4.59880400	3.32450200	0.59141600
C	-5.53065300	2.24234000	0.56420100
C	-6.74971300	2.35458600	-0.07859200
H	-6.47535500	5.58572000	-1.19290600
H	-4.31210800	5.39269900	-0.04580100
H	-5.25603100	1.30236800	1.04490300
H	-7.43854400	1.50733900	-0.09560900
C	-3.37146900	3.20087700	1.32490100
C	-2.15556900	3.96926600	1.07983600
C	-1.79327200	4.45400800	-0.20575000
C	-1.24585800	4.18962300	2.14333700
C	-0.61875300	5.15964800	-0.39705600
H	-2.43976100	4.25231800	-1.06139000
C	-0.06032400	4.89462100	1.95726600
H	-1.49928100	3.80724400	3.13302600
C	0.26321200	5.39479400	0.68183000
H	-0.33852700	5.53583300	-1.38303500
H	0.60124600	5.05678000	2.80806700
O	-3.24204800	2.30005700	2.29357400
H	-4.42261400	2.26885800	3.15114500
C	-8.38125900	3.68929700	-1.36870100
N	-9.41609200	3.79502600	-1.89204400
O	1.37935400	6.09432900	0.39056000
C	2.32983500	6.35368900	1.40891900
H	3.14247400	6.92187300	0.93815700
H	1.89522000	6.95561800	2.22622400
H	2.73930900	5.41873600	1.82987300
C	-6.96125700	6.36809400	2.70824100
C	-6.32103600	7.08822600	3.92327600
C	-5.44047700	6.02104400	4.62758700
C	-5.52087400	4.77612900	3.73553800
C	-6.89260800	4.87607700	3.05423000
H	-7.98516600	6.70780600	2.49257700
H	-6.36441500	6.54899900	1.79906600
H	-7.09813400	7.45575000	4.61105700
H	-5.73773500	7.96690500	3.60942300
H	-4.40123500	6.34477900	4.78522100
H	-5.85146800	5.75090600	5.61318500
H	-4.73491000	4.80552400	2.95948900
H	-6.99695900	4.22744200	2.17324700
H	-7.67056500	4.60004600	3.78780000
O	-5.30440500	3.60618300	4.52782300
C	-5.36500200	2.39852900	3.88701300
H	-6.23594300	2.27247100	3.22044800
H	-5.27383300	1.58665400	4.62289300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.391099 (Hartree/Particle)
Thermal correction to Energy= 0.414518
Thermal correction to Enthalpy= 0.415463
Thermal correction to Gibbs Free Energy= 0.334072
Sum of electronic and zero-point Energies= -1093.245207
Sum of electronic and thermal Energies= -1093.221788
Sum of electronic and thermal Enthalpies= -1093.220844
Sum of electronic and thermal Free Energies= -1093.302234
HF=-1093.6363062
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-1094.8530292

1-TS-8

C	-6.32119800	1.63833200	-1.35192700
C	-5.11813300	2.05398200	-1.97692300
C	-4.15255600	2.73818400	-1.26111900
C	-4.33767000	3.03940500	0.12055900
C	-5.55133700	2.61092600	0.73644000
C	-6.51641900	1.92901700	0.01975800
H	-4.96416000	1.84463000	-3.03752100
H	-3.25420600	3.08355100	-1.77549200
H	-5.71057900	2.82641000	1.79273100
H	-7.43929000	1.61549400	0.51147000
C	-3.39366200	3.81432100	0.87060600
C	-1.97724800	4.01064700	0.57438200
C	-1.17186800	2.99534200	-0.01478100
C	-1.33759200	5.21363800	0.98300900
C	0.17113200	3.20831800	-0.24993300
H	-1.62170800	2.03747000	-0.28047800
C	0.01683900	5.42648100	0.76208200
H	-1.93845000	5.98879400	1.45985800
C	0.78750200	4.42745300	0.13363600
H	0.79364200	2.44430500	-0.71977600
H	0.46546200	6.37125600	1.06796600
O	-3.73651300	4.38605600	2.00227000

H	-5.47502800	5.24154700	1.66247700
C	-7.32130400	0.94461600	-2.09795000
N	-8.13643200	0.38008300	-2.70819800
O	2.09855700	4.52814100	-0.13831200
C	2.81311100	5.69705300	0.23520000
H	3.85194100	5.53742100	-0.07960800
H	2.41305300	6.59161700	-0.27205900
H	2.78336600	5.85458400	1.32684900
C	-5.75623100	7.56162700	3.31476500
C	-5.86469200	6.23459900	4.11628500
C	-6.84221000	5.37169100	3.31019600
C	-6.47023600	5.71017900	1.87045300
C	-6.27121500	7.24199200	1.88574400
H	-6.37069500	8.35120300	3.77459600
H	-4.72122600	7.93593900	3.30358400
H	-6.18380700	6.38870500	5.15799000
H	-4.88488100	5.73158600	4.14246100
H	-6.76877100	4.29465200	3.52534800
H	-7.88951600	5.67886000	3.47959200
H	-5.59010700	7.59013900	1.09513500
H	-7.25476000	7.70662300	1.70264400
O	-7.42234900	5.21568900	0.97006600
C	-7.15301600	5.45959900	-0.39350100
H	-6.15440000	5.08308400	-0.68397300
H	-7.91100900	4.92231600	-0.98092100
H	-7.20743200	6.53625500	-0.64151000

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.393080 (Hartree/Particle)
Thermal correction to Energy= 0.417175
Thermal correction to Enthalpy= 0.418120
Thermal correction to Gibbs Free Energy= 0.334082
Sum of electronic and zero-point Energies= -1093.245652
Sum of electronic and thermal Energies= -1093.221557
Sum of electronic and thermal Enthalpies= -1093.220613
Sum of electronic and thermal Free Energies= -1093.304650
HF=-1093.6387328
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-1094.8563468
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-1092.474197175937

2-p

C	-1.09466100	-2.78296700	-4.96691000
C	0.36354200	-2.67937100	-5.47188800
C	0.86207900	-1.34947100	-4.88786500
C	-0.34327200	-0.42713500	-5.05907800
C	-1.54960300	-1.31933200	-4.69645200
H	-1.74454500	-3.29486500	-5.69255500
H	-1.13670900	-3.37020900	-4.03561900
H	0.37909000	-2.61149400	-6.57118300
H	0.98384900	-3.54114500	-5.18188300
H	1.07891700	-1.45358700	-3.81092900
H	1.75904600	-0.94562000	-5.38088200
H	-0.28607700	0.48723000	-4.44233100
H	-1.80546600	-1.17319400	-3.63534900
H	-2.43419900	-1.02581000	-5.28105700
O	-0.37795200	-0.04242800	-6.44217700
C	-1.21178600	0.96582600	-6.78217600
H	-2.01529100	1.25021400	-6.09325500
H	-1.31744100	1.11486600	-7.85881700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.158523 (Hartree/Particle)
Thermal correction to Energy= 0.166124
Thermal correction to Enthalpy= 0.167068
Thermal correction to Gibbs Free Energy= 0.125576
Sum of electronic and zero-point Energies= -310.044064
Sum of electronic and thermal Energies= -310.036463
Sum of electronic and thermal Enthalpies= -310.035519
Sum of electronic and thermal Free Energies= -310.077010
HF=-310.2025867
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-310.5538272
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-309.878042729023

8-t

C	-1.08419300	-2.74749900	-4.78575200
C	0.39928700	-2.87111300	-5.18486300
C	0.91116900	-1.41319000	-5.24041400
C	-0.33940000	-0.61098500	-5.47573400
C	-1.55994900	-1.49086200	-5.53757900
H	-1.67355400	-3.64525900	-5.02828600
H	-1.16903800	-2.57972700	-3.69820800
H	0.46678700	-3.32175300	-6.18992000
H	0.97753800	-3.51179600	-4.50125600
H	1.41298400	-1.12388700	-4.29551800
H	1.65212100	-1.24631600	-6.04395900
H	-2.46912500	-1.04235200	-5.10119900
H	-1.81082000	-1.74497000	-6.59242900
O	-0.20535100	0.54868400	-6.17879900
C	-1.36058900	1.35130700	-6.32565000
H	-1.77531400	1.64573500	-5.34373700
H	-2.15294000	0.83701500	-6.89902900
H	-1.06073600	2.25583700	-6.87341900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.158871 (Hartree/Particle)
Thermal correction to Energy= 0.166431
Thermal correction to Enthalpy= 0.167375
Thermal correction to Gibbs Free Energy= 0.126491
Sum of electronic and zero-point Energies= -310.048458
Sum of electronic and thermal Energies= -310.040898
Sum of electronic and thermal Enthalpies= -310.039954
Sum of electronic and thermal Free Energies= -310.080838
HF=-310.2073291

UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-310.5578877
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-309.880088701526

2-TS-3

C	-1.55081400	1.52052900	-0.33976900
C	-2.53334200	2.49591300	-0.13285100
C	-2.18397900	3.74352600	0.40298600
C	-0.82985800	3.96371000	0.71151400
C	0.09219200	2.95058000	0.47924300
C	-1.80483200	0.15631900	-0.87045700
C	-3.05268000	-0.30757300	-1.30105700
C	-3.18729100	-1.61763100	-1.77935200
C	-2.03302200	-2.41894100	-1.80626300
C	-0.82305500	-1.89407300	-1.36377800
H	-3.57550800	2.28765800	-0.37741700
H	-0.49632300	4.91576000	1.12874400
H	1.15798400	3.03112200	0.68171400
H	-3.92351300	0.34807200	-1.27012000
H	-2.07547900	-3.44681500	-2.17245200
H	0.10527000	-2.47151100	-1.37287700
N	-0.26187100	1.76718500	-0.03499400
N	-0.71756700	-0.64212200	-0.90727800
Br	2.83696100	-0.73735200	-1.36686800
Ni	0.98661000	0.15606200	-0.13648300
C	0.93688500	-0.38460900	1.77134600
C	-0.09361300	-0.02392500	2.66206000
C	1.96273800	-1.20605300	2.28577500
C	-0.11184200	-0.44468000	3.99260400
H	-0.91596100	0.61035800	2.31431000
C	1.97287200	-1.63999800	3.61178700
H	2.77905700	-1.51080400	1.62369100
H	-0.92398400	-0.14911000	4.66191600
H	2.78167800	-2.27327400	3.98530500
C	0.92926900	-1.25962900	4.47997200
C	-3.21355100	4.81101900	0.65367400
H	-4.20667700	4.51958600	0.28413600
H	-3.29524200	5.01915100	1.73330000
H	-2.92226700	5.75507200	0.16617800
C	-4.51168100	-2.15744100	-2.24505800
H	-4.82972600	-2.99825900	-1.60691100
H	-5.29920100	-1.39121900	-2.22190400
H	-4.43349600	-2.54640800	-3.27294600
C	0.92427300	-1.69836500	5.84514200
N	0.91768300	-2.05328000	6.95242200
C	2.36219900	4.37015900	-1.76127700
C	2.62958500	5.43873400	-0.67836600
C	4.04045300	5.10070800	-0.17445800
C	4.04126800	3.57380200	-0.12338700
C	3.23409500	3.14492500	-1.36719800
H	1.29386700	4.11736800	-1.84144500
H	2.67000600	4.75078800	-2.74828500
H	1.91364500	5.33296400	0.15314800
H	2.53966700	6.46862000	-1.05640400
H	4.79775900	5.42869000	-0.90644200
H	4.29430500	5.54254300	0.80073800
H	5.05564000	3.13927000	-0.10437100
H	3.92548300	2.86941900	-2.17779000
H	2.65487700	2.23561400	-1.15363000
O	3.38277100	3.19925200	1.10435500
C	3.34058800	1.88131200	1.39739800
H	2.87515500	1.62725800	2.34639700
H	3.89959700	1.16263200	0.79140600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.463636 (Hartree/Particle)
Thermal correction to Energy= 0.495852
Thermal correction to Enthalpy= 0.496796
Thermal correction to Gibbs Free Energy= 0.392317
Sum of electronic and zero-point Energies= -5289.218415
Sum of electronic and thermal Energies= -5289.186199
Sum of electronic and thermal Enthalpies= -5289.185255
Sum of electronic and thermal Free Energies= -5289.289734
HF=-5289.6820518
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5291.5331462
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5286.500967659608

3-Ni^{III}

C	-2.15600500	1.68384200	0.16901800
C	-3.10824200	2.58737400	0.65618900
C	-2.72789400	3.87855800	1.04122900
C	-1.36812500	4.20380000	0.92515100
C	-0.47289800	3.25616400	0.43685600
C	-2.48663100	0.29683700	-0.24723400
C	-3.76854300	-0.26104900	-0.15296100
C	-3.99080600	-1.58478600	-0.54997500
C	-2.88716200	-2.30237800	-1.03883200
C	-1.64370800	-1.68364200	-1.11162600
H	-4.15387100	2.29107300	0.73910400
H	-1.00068000	5.18946800	1.21859500
H	0.59555100	3.46573800	0.37287100
H	-4.59981800	0.32832900	0.23391200
H	-2.99377400	-3.33961100	-1.36358900
H	-0.76212200	-2.19580300	-1.50280700
N	-0.85390800	2.02790300	0.06011200
N	-1.45121100	-0.41740900	-0.72632400
Br	1.11502000	-0.46576900	-2.83031300
Ni	0.40708700	0.48764100	-0.65881600
C	0.91427700	-0.45008800	0.94036300
C	0.54272900	-0.01275300	2.22070400
C	1.58776500	-1.67644200	0.81824700
C	0.82735900	-0.77294700	3.35465500
H	0.03751600	0.94869900	2.34101900
C	1.88551900	-2.45090400	1.94064300
H	1.89247700	-2.02141600	-0.17433100
H	0.53573400	-0.42164500	4.34739000
H	2.41609500	-3.40034700	1.83593900
C	1.50571800	-2.00165600	3.22157700
C	-3.72981000	4.88118100	1.54358100
H	-4.68923400	4.40946000	1.79916800
H	-3.34901000	5.40942500	2.43125000
H	-3.92256400	5.64496000	0.77123000
C	-5.35014500	-2.22252500	-0.46064200

H	-5.31638000	-3.11642800	0.18313600
H	-6.10287900	-1.53218000	-0.05468400
H	-5.68675800	-2.55643200	-1.45561000
C	1.80887800	-2.78606500	4.38323500
N	2.05355800	-3.41971000	5.32665800
C	4.75554000	3.62586400	1.51208400
C	4.02082100	3.67918600	2.87241600
C	3.10075000	2.42396200	2.89946500
C	3.32840100	1.69826600	1.56523600
C	4.73575700	2.13672600	1.14048800
H	4.18729500	4.18797900	0.75376000
H	5.76953800	4.05236600	1.55075000
H	3.45568800	4.61556900	2.99734800
H	4.74672100	3.63639500	3.70021800
H	3.36811700	1.75165000	3.72867700
H	2.03428000	2.66529200	3.01153500
H	3.22006400	0.60681700	1.64984400
H	5.47791000	1.57541100	1.73481500
H	4.93599800	1.93222300	0.07736800
O	2.36071000	2.19167300	0.62608300
C	2.13175100	1.42906700	-0.50302700
H	2.94228800	0.72157900	-0.73344000
H	1.95296700	2.10384900	-1.36032100

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.466990 (Hartree/Particle)
Thermal correction to Energy= 0.498696
Thermal correction to Enthalpy= 0.499640
Thermal correction to Gibbs Free Energy= 0.395346
Sum of electronic and zero-point Energies= -5289.245585
Sum of electronic and thermal Energies= -5289.213879
Sum of electronic and thermal Enthalpies= -5289.212934
Sum of electronic and thermal Free Energies= -5289.317229
HF=-5289.7125743
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5291.5601546
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5286.556091820541

3-TS-5

C	-1.98080600	1.65923900	0.28274100
C	-2.89469600	2.61165400	0.75023300
C	-2.44839900	3.86061400	1.19839800
C	-1.06522100	4.09621900	1.15992300
C	-0.21203900	3.10356700	0.68697500
C	-2.38024100	0.31560200	-0.21181300
C	-3.68963800	-0.17944100	-0.16082800
C	-3.97509100	-1.46255700	-0.64340200
C	-2.90533600	-2.20319200	-1.17221900
C	-1.62974900	-1.64830600	-1.19356500
H	-3.96164600	2.38838800	0.76225200
H	-0.64916200	5.04686600	1.50048400
H	0.87018300	3.24316600	0.67902600
H	-4.49271500	0.42538100	0.26091200
H	-3.06348300	-3.20937200	-1.56653700
H	-0.76827400	-2.17733600	-1.60871700
N	-0.65453300	1.91433000	0.25503200
N	-1.37619600	-0.42188600	-0.72323700
Br	1.44849800	-0.61537400	-2.61441900
Ni	0.51237300	0.34018500	-0.50955200
C	1.18003200	-0.58244500	1.02384300
C	0.71055000	-0.22014200	2.30047400
C	1.63428400	-1.90266400	0.82597900
C	0.63611700	-1.15067300	3.33214700
H	0.41181100	0.81331200	2.48247900
C	1.57163000	-2.84243800	1.85107300
H	2.02516200	-2.18455800	-0.15463100
H	0.25120100	-0.85882000	4.31200000
H	1.91541700	-3.86529000	1.68090100
C	1.06289700	-2.47784700	3.11600600
C	-3.40346300	4.91246100	1.69192600
H	-4.42951300	4.52754400	1.77720100
H	-3.09043000	5.29436400	2.67657200
H	-3.41660900	5.77270400	1.00218800
C	-5.36540600	-2.03545600	-0.59946300
H	-5.38546500	-2.95508400	0.00787500
H	-6.08944600	-1.32594600	-0.17469300
H	-5.70319700	-2.31208200	-1.61137200
C	0.98830100	-3.44072100	4.17376000
N	0.92494300	-4.22064000	5.03406200
C	4.86024600	3.40328800	1.95757100
C	3.83497200	3.72407600	3.08563900
C	3.18931800	2.36710000	3.46431200
C	3.46356600	1.45516500	2.27057800
C	4.87731000	1.86532300	1.84343200
H	4.52138000	3.83851600	1.00521300
H	5.86035400	3.81435000	2.16182300
H	3.07220900	4.43105800	2.72482900
H	4.31354200	4.19471500	3.95809600
H	3.68053500	1.93345300	4.34981400
H	2.11295400	2.43260900	3.68030200
H	3.36914100	0.38371600	2.51115300
H	5.59725900	1.42246000	2.55206400
H	5.13835200	1.49911400	0.83868600
O	2.51615000	1.79735400	1.24752200
C	2.38158000	0.91637400	0.19161500
H	3.22451000	0.22758200	0.05386900
H	2.26241200	1.50250500	-0.74023600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.466489 (Hartree/Particle)
Thermal correction to Energy= 0.497612
Thermal correction to Enthalpy= 0.498556
Thermal correction to Gibbs Free Energy= 0.396971
Sum of electronic and zero-point Energies= -5289.236738
Sum of electronic and thermal Energies= -5289.205616
Sum of electronic and thermal Enthalpies= -5289.204672
Sum of electronic and thermal Free Energies= -5289.306257
HF=-5289.7032278
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5291.5511818
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)

HF=-5286.544615891514

5-p

C	1.02189900	0.33713300	0.19588000
C	-0.00211400	0.85933400	0.99974600
C	0.95771600	-1.00741900	-0.20005800
C	-1.07105800	0.06106100	1.40091400
H	0.05363500	1.90331500	1.31319100
C	-0.10820200	-1.81684400	0.18693600
H	1.75515600	-1.42941100	-0.81806000
H	-1.86313100	0.47378300	2.02881800
H	-0.15026000	-2.86225700	-0.12472300
C	-1.13246800	-1.28559900	0.99422700
C	-2.23034200	-2.11459000	1.40471800
N	-3.11871500	-2.78534600	1.73673000
C	4.99525900	3.48211700	1.51139800
C	4.19227700	4.08633900	2.67761600
C	2.86958700	3.27363900	2.71512800
C	3.07802200	2.05904500	1.78268200
C	4.59807700	2.00178900	1.55570900
H	4.65827300	3.91447100	0.55471700
H	6.08010600	3.65048800	1.59392500
H	4.02303900	5.16803700	2.56501700
H	4.74926600	3.94506400	3.61885900
H	2.61982100	2.94690000	3.73572700
H	2.01395100	3.85380100	2.33949600
H	2.68076100	1.12433600	2.21693000
H	5.07354700	1.50337300	2.41881100
H	4.87273500	1.43166100	0.65470200
O	2.39130200	2.33835300	0.55410800
C	2.16204800	1.22554300	-0.27339500
H	3.07398500	0.61224700	-0.40796000
H	1.90796100	1.62898900	-1.26932800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.252982 (Hartree/Particle)
Thermal correction to Energy= 0.266401
Thermal correction to Enthalpy= 0.267345
Thermal correction to Gibbs Free Energy= 0.210324
Sum of electronic and zero-point Energies= -633.688727
Sum of electronic and thermal Energies= -633.675308
Sum of electronic and thermal Enthalpies= -633.674364
Sum of electronic and thermal Free Energies= -633.731385
HF=-633.9417087
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-634.6448457
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-633.255193089977

2-TS-4

C	-5.45596100	1.51515200	-0.16937200
H	-5.57323900	2.38423100	0.48018500
H	-6.29692500	0.82325100	-0.24121300
C	-4.23247600	1.18409300	-0.65478200
H	-4.06207800	0.26441200	-1.21921000
C	-3.08714700	2.08583700	-0.48621600
O	-3.11584500	3.19520700	0.02072800
O	-1.94908000	1.54757400	-0.97987300
C	-0.77342900	2.34754300	-0.87195800
H	-0.54097200	2.56808000	0.18188700
H	0.03945300	1.76538900	-1.32401900
H	-0.89671700	3.30412800	-1.40414600
C	-6.53907600	7.25987000	-1.86803200
C	-7.24237700	7.03213500	-0.51090700
C	-6.28079100	6.10444300	0.24544200
C	-5.82060100	5.12753500	-0.83285300
C	-5.64168000	6.00724900	-2.08761900
H	-7.25914500	7.40870600	-2.68686300
H	-5.91566000	8.16742800	-1.82569000
H	-8.19823600	6.50563700	-0.66349700
H	-7.45929100	7.96784600	0.02669000
H	-5.40210400	6.66481300	0.60772600
H	-6.73068000	5.58462500	1.10457000
H	-4.91393000	4.56475400	-0.56074400
H	-4.58134400	6.28733500	-2.18393200
H	-5.90327700	5.44401700	-2.99602600
O	-6.90287000	4.18072400	-1.01498300
C	-6.64308800	3.08660800	-1.74106600
H	-5.80693700	3.10091500	-2.44815100
H	-7.52390100	2.47746000	-1.95766400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.255574 (Hartree/Particle)
Thermal correction to Energy= 0.270260
Thermal correction to Enthalpy= 0.271204
Thermal correction to Gibbs Free Energy= 0.210363
Sum of electronic and zero-point Energies= -616.207306
Sum of electronic and thermal Energies= -616.192620
Sum of electronic and thermal Enthalpies= -616.191676
Sum of electronic and thermal Free Energies= -616.252517
HF=-616.46288
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-617.1675969
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-615.865960028599

4-E

C	-5.00876600	2.21248300	-0.04435200
H	-4.56198600	2.84622800	0.74067200
H	-5.89715600	1.71530200	0.37274100
C	-4.00360400	1.22283000	-0.50109000
H	-4.27450700	0.19131200	-0.73818700
C	-2.62975300	1.63931500	-0.72321200
O	-2.21454200	2.77642100	-0.55234900
O	-1.84264100	0.62581700	-1.15032400
C	-0.47581500	0.95227800	-1.39635600
H	0.01059500	1.32769500	-0.48206200
H	0.00809100	0.02569100	-1.72937300
H	-0.38986100	1.72696900	-2.17483300
C	-6.84266700	7.01077900	-1.62774500
C	-7.83369600	6.60091300	-0.50298700
C	-6.94667200	6.01157700	0.60788100

C	-5.83663200	5.30673700	-0.17006900
C	-5.49627100	6.31861600	-1.27882000
H	-7.21463900	6.69577900	-2.61438000
H	-6.71636500	8.10377200	-1.67413800
H	-8.51267300	5.81610100	-0.86954500
H	-8.45574500	7.43846600	-0.15211800
H	-6.49838300	6.81277700	1.21946800
H	-7.47550800	5.32105700	1.28200200
H	-4.96010000	5.06145200	0.45734100
H	-4.77120200	7.04758700	-0.88195100
H	-5.01879000	5.83115900	-2.14211900
O	-6.40023100	4.11091300	-0.71439400
C	-5.47639200	3.16099600	-1.18341700
H	-4.58769200	3.63859300	-1.63413000
H	-5.97838600	2.57307900	-1.96855700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.259309 (Hartree/Particle)
Thermal correction to Energy= 0.273656
Thermal correction to Enthalpy= 0.274601
Thermal correction to Gibbs Free Energy= 0.213876
Sum of electronic and zero-point Energies= -616.242902
Sum of electronic and thermal Energies= -616.228554
Sum of electronic and thermal Enthalpies= -616.227610
Sum of electronic and thermal Free Energies= -616.288334
HF=-616.5022106
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-617.2035479
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-615.909977375188

4-TS-6

Ni	-5.16858100	0.66612900	0.36112800
C	-6.18537800	0.94585700	-1.31385400
C	-5.59406900	0.91289800	-2.59205600
C	-7.58563100	1.09867400	-1.26124400
C	-6.34539800	1.03153100	-3.76286700
H	-4.51033600	0.79479000	-2.68582400
C	-8.36133400	1.22373900	-2.41362300
H	-8.07913100	1.12737200	-0.28534700
C	-7.74229600	1.19164800	-3.67945700
H	-5.86180900	1.00612600	-4.74265900
H	-9.44477700	1.34958200	-2.34572700
Br	-6.50030700	0.61267300	2.38255600
C	-2.59150100	-0.37243400	-0.53349500
C	-1.28520000	-0.43644700	-1.03119800
C	-0.60119000	0.73685200	-1.37550700
C	-1.29171600	1.94855900	-1.22125600
C	-2.59148500	1.94265700	-0.72344700
C	-3.39975800	-1.56930900	-0.18439200
C	-2.94787300	-2.88855200	-0.30988500
C	-3.79439300	-3.95549500	0.01656800
C	-5.08678700	-3.63961900	0.46794000
C	-5.46847300	-2.30683900	0.57715800
H	-0.79333100	-1.40079000	-1.15958700
H	-0.82780600	2.89882200	-1.49281900
H	-3.16641900	2.86752600	-0.63271000
H	-1.93761300	-3.09385100	-0.66413600
H	-5.79309600	-4.42780400	0.73679600
H	-6.45391300	-2.00864000	0.94243700
N	-3.21820200	0.81298600	-0.36754600
N	-4.64426500	-1.30331600	0.25688600
C	-3.34668700	-5.38629400	-0.10268100
C	0.81414400	0.70621500	-1.88201300
H	1.50524700	1.05375600	-1.09539500
H	1.12199100	-0.30637400	-2.17890900
H	0.94038300	1.38061700	-2.74283700
H	-3.35451000	-5.87548000	0.88517500
H	-2.33279900	-5.46696000	-0.51896800
H	-4.03477200	-5.95559900	-0.74801300
C	-8.52492500	1.32916400	-4.87324600
N	-9.15708800	1.44455400	-5.84213600
C	-4.62545600	3.73338000	1.91776900
H	-3.78829500	3.20867300	1.43075000
H	-4.84247800	3.19831400	2.85211400
C	-5.80649300	3.69783200	1.01771200
H	-6.79927500	3.45807900	1.39784300
C	-5.68798800	4.12043200	-0.36689700
O	-4.62641300	4.38512600	-0.92714600
O	-6.87546800	4.19499700	-0.98878900
C	-6.84920300	4.49134300	-2.38538800
H	-6.26948600	3.72893100	-2.92597600
H	-7.89250500	4.47483000	-2.72117000
H	-6.40065400	5.48020500	-2.56762100
C	-1.00434100	6.60304200	1.22502800
C	-0.33858400	6.57953100	2.63304200
C	-0.59550500	5.15783500	3.19379900
C	-1.78139500	4.63092000	2.38356200
C	-1.47368400	5.15743200	0.97385500
H	-1.87394800	7.27847700	1.22685800
H	-0.32402300	6.96063300	0.43707900
H	-0.79150100	7.34010400	3.28613600
H	0.73868800	6.80156700	2.58470000
H	0.27249200	4.50169700	3.01859800
H	-0.81599500	5.14309700	4.27141900
H	-1.85526900	3.52705800	2.41396100
H	-0.65252600	4.54477400	0.56457500
H	-2.31598000	5.07679800	0.27108900
O	-2.94873500	5.21253100	2.96609300
C	-4.14698400	5.17259900	2.22686400
H	-4.05675800	5.73320200	1.27938500
H	-4.90018000	5.68601800	2.84405800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.565454 (Hartree/Particle)
Thermal correction to Energy= 0.604067
Thermal correction to Enthalpy= 0.605011
Thermal correction to Gibbs Free Energy= 0.485994
Sum of electronic and zero-point Energies= -5595.419741
Sum of electronic and thermal Energies= -5595.381128
Sum of electronic and thermal Enthalpies= -5595.380184
Sum of electronic and thermal Free Energies= -5595.499201
HF=-5595.9851949

UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5598.1840201

6-Ni^{III}

Ni	-4.95841400	1.02748800	0.29690100
C	-6.17901800	0.94010300	-1.17703800
C	-5.75947400	0.91302700	-2.51109600
C	-7.53470800	0.77166000	-0.86825800
C	-6.68447400	0.71397500	-3.53741100
H	-4.70750400	1.06458500	-2.76000100
C	-8.46909000	0.57132300	-1.88371900
H	-7.86050300	0.80793300	0.17466900
C	-8.04796400	0.54246400	-3.22865400
H	-6.35805300	0.69445700	-4.57972400
H	-9.52714800	0.44343500	-1.64414500
Br	-5.90516700	0.78098700	2.59982100
C	-2.56649700	-0.37555700	-0.74220000
C	-1.29153800	-0.64859000	-1.25071900
C	-0.48654800	0.38795700	-1.73924100
C	-1.03199100	1.67901700	-1.71477900
C	-2.30457500	1.88194800	-1.18698400
C	-3.49580600	-1.43506300	-0.27810200
C	-3.21254000	-2.80528400	-0.35283900
C	-4.16873700	-3.74663900	0.04382800
C	-5.39963300	-3.25403700	0.50619400
C	-5.60906400	-1.88185700	0.57069000
H	-0.91828200	-1.67218400	-1.27566900
H	-0.47503600	2.53154300	-2.10904100
H	-2.76954600	2.86935300	-1.19852300
H	-2.24964800	-3.14773500	-0.73105400
H	-6.19368800	-3.93473500	0.81976300
H	-6.54100500	-1.45863700	0.94732800
N	-3.04968400	0.88549800	-0.68737900
N	-4.67775900	-0.99686200	0.19415600
C	-3.89836800	-5.22455600	-0.01471800
C	0.90077300	0.13234000	-2.25900300
H	1.05762600	-0.92764200	-2.50495500
H	1.10729300	0.73819200	-3.15425700
H	1.64689700	0.41506400	-1.49683100
H	-3.86443700	-5.64716200	1.00322100
H	-2.94357000	-5.44883700	-0.51066800
H	-4.70455200	-5.74777700	-0.55284100
C	-9.00335100	0.34486900	-4.28020000
N	-9.77623700	0.18544700	-5.13340200
C	-4.17234700	3.54669400	1.20994500
H	-3.20829100	3.45946500	0.69165400
H	-4.09754000	2.96718400	2.13997300
C	-5.30296100	3.00648500	0.34349500
H	-6.27308000	3.06297600	0.85135000
C	-5.39649800	3.66952200	-0.98587400
O	-4.45086400	4.03168100	-1.66871000
O	-6.66730000	3.85356300	-1.38263300
C	-6.86102900	4.37793300	-2.69588000
H	-6.42912700	3.69981800	-3.44779300
H	-7.94603300	4.45223500	-2.83827500
H	-6.39125200	5.36796100	-2.79960200
C	-2.08591300	8.32290800	2.44128800
C	-1.34472500	7.35372000	3.40538400
C	-1.00728700	6.12120100	2.54690500
C	-2.19864700	6.02171300	1.59483300
C	-2.42631800	7.48590000	1.17845600
H	-2.99558000	8.72411100	2.91289800
H	-1.45980400	9.18975000	2.17785400
H	-2.01900200	7.04678300	4.21902000
H	-0.45408900	7.80618700	3.86777200
H	-0.09156100	6.29270900	1.95582100
H	-0.87264000	5.19702700	3.12888900
H	-1.99987700	5.36558300	0.72680900
H	-1.74165500	7.73000900	0.34954200
H	-3.44952700	7.65019400	0.80825400
O	-3.29978600	5.52055100	2.34955300
C	-4.38074100	5.02338300	1.58937300
H	-4.53877100	5.63107800	0.67810400
H	-5.28709300	5.11904400	2.20933400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.567850 (Hartree/Particle)
Thermal correction to Energy= 0.606460
Thermal correction to Enthalpy= 0.607404
Thermal correction to Gibbs Free Energy= 0.487516
Sum of electronic and zero-point Energies= -5595.438640
Sum of electronic and thermal Energies= -5595.400030
Sum of electronic and thermal Enthalpies= -5595.399086
Sum of electronic and thermal Free Energies= -5595.518974
HF=-5596.0064898
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5598.2017761
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5592.585545900476

6-TS-7

Ni	-5.15189000	0.69847000	0.14339900
C	-6.32841700	0.79110300	-1.37597400
C	-5.77006400	0.57592600	-2.65486600
C	-7.64500400	0.34499000	-1.13242200
C	-6.47245500	-0.11983700	-3.63192300
H	-4.77949100	0.96435000	-2.88685400
C	-8.35174000	-0.35387200	-2.10433800
H	-8.09375500	0.52755100	-0.15458400
C	-7.77179600	-0.60017900	-3.36642400
H	-6.01856000	-0.29582200	-4.60959600
H	-9.36085500	-0.71373300	-1.89208300
Br	-6.52552600	0.74716200	2.27274000
C	-2.61680800	-0.56211100	-0.65527400
C	-1.29915500	-0.75292300	-1.08973800
C	-0.58469400	0.29966500	-1.67334600
C	-1.25937600	1.52098600	-1.81896300
C	-2.56623900	1.64373400	-1.35720900
C	-3.45111300	-1.65556700	-0.09247500
C	-3.03955000	-2.99321500	-0.02900500
C	-3.90782100	-3.97419600	0.46454500
C	-5.18133300	-3.55330200	0.87952900
C	-5.51964800	-2.20651600	0.80018100
H	-0.82140700	-1.72628200	-0.97891300
H	-0.77616400	2.37640700	-2.29564400
H	-3.12397700	2.56981300	-1.50424200
H	-2.04688700	-3.28246800	-0.37392400

H	-5.90855200	-4.26995000	1.26711900
H	-6.48772200	-1.82950400	1.13667100
N	-3.22738600	0.63822900	-0.76515600
N	-4.67403000	-1.28221300	0.32884000
C	-3.50157300	-5.41959900	0.55510500
C	0.84116100	0.13641600	-2.12179000
H	1.52105900	0.64189400	-1.41512200
H	1.13574400	-0.92128500	-2.17545800
H	1.00060100	0.59779800	-3.10853500
H	-2.52339000	-5.60195200	0.08816500
H	-4.24796800	-6.06643200	0.06730500
H	-3.44275300	-5.73576200	1.60986500
C	-8.49572500	-1.31807400	-4.37169600
N	-9.08106800	-1.90212400	-5.18933000
C	-4.94051100	3.18906800	0.43210100
H	-4.14243100	3.63868400	-0.16964100
H	-4.44596000	2.48484000	1.12711700
C	-6.00377900	2.57597200	-0.51078300
H	-6.99739600	2.63404800	-0.05696600
C	-5.99785700	3.28733600	-1.83032200
O	-4.99823100	3.63807500	-2.42874100
O	-7.23478300	3.47892500	-2.30612900
C	-7.33628700	4.02828000	-3.62223900
H	-6.85583900	3.35977900	-4.35339500
H	-8.40843900	4.11454600	-3.83543000
H	-6.85357500	5.01578600	-3.67456500
C	-4.52068600	7.72421100	3.07925400
C	-3.00070300	7.50565500	3.21535100
C	-2.67353500	6.32367000	2.25982000
C	-3.96879500	6.03233600	1.47165800
C	-4.80350500	7.31463000	1.62879800
H	-5.06195000	7.03925200	3.75180600
H	-4.83646700	8.75168800	3.31754500
H	-2.69391000	7.30825100	4.25383600
H	-2.46503000	8.41335500	2.89113600
H	-1.85155700	6.57694200	1.57297000
H	-2.38266700	5.41026900	2.79860700
H	-3.76667200	5.79217200	0.41151500
H	-4.42701500	8.08315700	0.93025200
H	-5.86932300	7.15439400	1.40365400
O	-4.62085100	4.92888300	2.10236800
C	-5.58617000	4.26236000	1.31961200
H	-6.16193500	4.97175500	0.69325100
H	-6.29267300	3.77197200	2.00683500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.567385 (Hartree/Particle)
Thermal correction to Energy= 0.605264
Thermal correction to Enthalpy= 0.606208
Thermal correction to Gibbs Free Energy= 0.489032
Sum of electronic and zero-point Energies= -5595.421864
Sum of electronic and thermal Energies= -5595.383986
Sum of electronic and thermal Enthalpies= -5595.383042
Sum of electronic and thermal Free Energies= -5595.500218
HF=-5595.9892496
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5598.184924

7-p

C	-5.36514900	1.58989600	0.30362900
C	-4.40423700	0.96895000	-0.51293700
C	-6.27953000	0.78847500	1.00283800
C	-4.35477400	-0.41761500	-0.62923600
H	-3.69279100	1.58307300	-1.06954700
C	-6.24089800	-0.60093400	0.89778100
H	-7.03304100	1.25779800	1.63990400
C	-5.27503100	-1.21436600	0.07893200
H	-3.60621700	-0.89034900	-1.26776500
H	-6.95707400	-1.21518100	1.44673900
C	-5.22980000	-2.64482600	-0.03598800
N	-5.19330200	-3.80198200	-0.12913400
C	-4.17023900	3.61379800	1.24502200
H	-3.25952800	3.42056800	0.65757400
H	-4.08138700	3.04348100	2.18263700
C	-5.38556800	3.10494100	0.45377200
H	-6.31519500	3.38503700	0.97224200
C	-5.43607100	3.73007900	-0.93761800
O	-4.46638800	4.07969900	-1.57124300
O	-6.69022600	3.80224500	-1.39762400
C	-6.85610700	4.30112500	-2.73114100
H	-6.32381200	3.66179600	-3.45156600
H	-7.93404900	4.28647300	-2.93089500
H	-6.46450000	5.32619500	-2.81306500
C	-1.71557300	8.29185900	2.19220500
C	-0.98767100	7.29664700	3.13820300
C	-0.77166200	6.03211700	2.28827400
C	-2.02600800	5.98007300	1.41748000
C	-2.20529400	7.44625700	0.98435100
H	-2.55455500	8.78317900	2.70773900
H	-1.04052000	9.09433300	1.85589100
H	-1.63813500	7.04540100	3.98968000
H	-0.04911600	7.70089900	3.54715500
H	0.11068900	6.14325000	1.63549400
H	-0.64675300	5.11286900	2.88013300
H	-1.92301100	5.29788900	0.55359600
H	-1.58057500	7.63262400	0.09562300
H	-3.24516200	7.66066100	0.69454000
O	-3.10143600	5.55213700	2.25568400
C	-4.25492800	5.10527200	1.57837000
H	-4.42836800	5.69137300	0.65606000
H	-5.11586300	5.28945700	2.24392100

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.352803 (Hartree/Particle)
Thermal correction to Energy= 0.373610
Thermal correction to Enthalpy= 0.374554
Thermal correction to Gibbs Free Energy= 0.297408
Sum of electronic and zero-point Energies= -939.879399
Sum of electronic and thermal Energies= -939.858592
Sum of electronic and thermal Enthalpies= -939.857648
Sum of electronic and thermal Free Energies= -939.934795
HF=-940.2322024
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-941.2855468

DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-939.282471940178

8-TS-9

C	-5.05595800	1.65760700	-0.36457600
H	-5.10928300	2.32132500	0.50047300
H	-5.97531800	1.16237000	-0.67993800
C	-3.83408400	1.21250800	-0.77675100
H	-3.72377000	0.44986900	-1.55118400
C	-2.60190300	1.77773300	-0.22441200
O	-2.52632500	2.64171500	0.63411800
O	-1.50051200	1.22142800	-0.78668300
C	-0.24386400	1.70199700	-0.31685000
H	-0.12979400	1.52324200	0.76417500
H	0.52597000	1.15203400	-0.87307800
H	-0.14136500	2.78401100	-0.49756100
C	-4.37828100	5.07376100	-0.86235100
C	-5.80231300	5.49000800	-0.44051300
C	-6.69038500	4.25952400	-0.74673600
C	-5.88301700	3.45995300	-1.74135600
C	-4.60686000	4.17902900	-2.09106500
H	-3.72875000	5.93508900	-1.08047400
H	-3.89120900	4.48354800	-0.07134900
H	-6.13433000	6.34253600	-1.05650900
H	-5.85922000	5.80829800	0.61138300
H	-6.91745300	3.67365900	0.16176000
H	-7.66544300	4.53031700	-1.18738400
H	-3.76470400	3.50122900	-2.30794100
H	-4.77343000	4.79548500	-2.99904800
O	-6.60540000	2.76673600	-2.65046700
C	-5.90658300	2.09840300	-3.68981300
H	-5.18797400	1.37066800	-3.27887100
H	-5.36266700	2.80749600	-4.33658500
H	-6.65854500	1.56947700	-4.29024700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.256251 (Hartree/Particle)
Thermal correction to Energy= 0.270699
Thermal correction to Enthalpy= 0.271644
Thermal correction to Gibbs Free Energy= 0.213502
Sum of electronic and zero-point Energies= -616.215569
Sum of electronic and thermal Energies= -616.201121
Sum of electronic and thermal Enthalpies= -616.200177
Sum of electronic and thermal Free Energies= -616.258318
HF=-616.4718201
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-617.1755658
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-615.871806437968

9-E

C	-5.17530200	2.29310100	-0.37436500
H	-4.92201000	2.92031900	0.49510600
H	-6.04828300	1.67420100	-0.11787800
C	-4.01957200	1.42152700	-0.68128500
H	-4.16075200	0.41208500	-1.07297300
C	-2.65786500	1.86288900	-0.44639000
O	-2.33919100	2.94756400	0.02047900
O	-1.74700000	0.92846200	-0.80884500
C	-0.37769800	1.27733900	-0.61525300
H	-0.16905200	1.48285800	0.44669000
H	0.21168900	0.41737600	-0.95708800
H	-0.11348100	2.17456100	-1.19734300
C	-4.61112000	5.33947200	-0.81751800
C	-6.04773900	5.30708200	-0.21425100
C	-6.78244700	4.16609200	-0.94915700
C	-5.67324900	3.25921600	-1.51721300
C	-4.61405100	4.29459400	-1.94632300
H	-4.33298000	6.33699700	-1.18984000
H	-3.86218400	5.05548200	-0.06444900
H	-6.57464200	6.26447400	-0.34463700
H	-6.00955400	5.11984700	0.87045400
H	-7.49318600	3.61406400	-0.31516000
H	-7.34483300	4.54906300	-1.81500300
H	-3.62024500	3.86401600	-2.12968200
H	-4.96698400	4.74442500	-2.88960600
O	-6.22565900	2.49678100	-2.57663500
C	-5.34596900	1.98734700	-3.55128500
H	-4.50704700	1.41492400	-3.11157400
H	-4.91153600	2.78068700	-4.18732400
H	-5.92882900	1.30921200	-4.19248300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.259201 (Hartree/Particle)
Thermal correction to Energy= 0.273278
Thermal correction to Enthalpy= 0.274223
Thermal correction to Gibbs Free Energy= 0.217384
Sum of electronic and zero-point Energies= -616.242975
Sum of electronic and thermal Energies= -616.228898
Sum of electronic and thermal Enthalpies= -616.227953
Sum of electronic and thermal Free Energies= -616.284792
HF=-616.502176
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-617.2017578
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-615.908986194114

9-TS-11

Ni	-5.34392600	0.60469500	0.37472200
C	-6.41506800	0.78774600	-1.28061800
C	-5.85742500	0.71606200	-2.57242500
C	-7.81698600	0.90958300	-1.19641000
C	-6.64195400	0.76735800	-3.72622000
H	-4.77376300	0.62074800	-2.69047400
C	-8.62578400	0.96690400	-2.33133900
H	-8.28516200	0.96744300	-0.20947100
C	-8.04001000	0.89579000	-3.61133000
H	-6.18383500	0.71277000	-4.71701100
H	-9.70993900	1.06908300	-2.23902800
Br	-6.64348600	0.57549400	2.41951400
C	-2.74400800	-0.37999500	-0.51632700

C	-1.43838100	-0.41691000	-1.01889400
C	-0.80366500	0.76395700	-1.42566800
C	-1.54263100	1.95315900	-1.32980200
C	-2.83937900	1.92015800	-0.82512000
C	-3.50185100	-1.58865100	-0.10094200
C	-3.00195300	-2.89443500	-0.17391000
C	-3.80301300	-3.97627600	0.21265100
C	-5.10043900	-3.68843000	0.66814000
C	-5.53078800	-2.36711500	0.72319000
H	-0.90835700	-1.36601000	-1.10069500
H	-1.11840000	2.90621600	-1.65262100
H	-3.45346800	2.82354400	-0.78151900
H	-1.98972700	-3.07758500	-0.53466800
H	-5.77311100	-4.48930100	0.98201600
H	-6.52184900	-2.08975100	1.08952700
N	-3.41724100	0.78592600	-0.40621700
N	-4.74961100	-1.34887800	0.34635300
C	-3.30221100	-5.39314900	0.15277100
C	0.60961700	0.76504700	-1.93891200
H	0.96419500	-0.24989600	-2.16774200
H	0.69952800	1.38327500	-2.84540300
H	1.28658700	1.19934500	-1.18385200
H	-3.25828700	-5.82814600	1.16484500
H	-2.29948200	-5.45674000	-0.29255400
H	-3.98692500	-6.02275100	-0.43762200
C	-8.85757900	0.96245900	-4.78758500
N	-9.51876200	1.02003900	-5.74219600
C	-4.79950400	3.73716500	1.81725100
H	-3.92723000	3.37715500	1.25147600
H	-4.94102400	3.06596100	2.67512900
C	-6.00254900	3.65831800	0.95531300
H	-6.96084400	3.35850700	1.37861900
C	-5.97860800	4.00888900	-0.45192900
O	-4.96572700	4.25109300	-1.10361100
O	-7.21065500	4.04259300	-0.99029400
C	-7.28543800	4.26205600	-2.39910200
H	-6.73611800	3.47624500	-2.93780800
H	-8.34940000	4.21960200	-2.65949900
H	-6.86222600	5.24294300	-2.66595500
C	-2.64067900	5.80388600	0.85956400
C	-1.97982800	5.04832700	2.05207700
C	-3.05964100	4.98557700	3.15130300
C	-4.40385800	5.13806100	2.41258400
C	-4.04950400	6.19177200	1.34281400
H	-2.06249700	6.68767000	0.55015200
H	-2.72296800	5.15191900	-0.02241600
H	-1.07146700	5.55344000	2.41392000
H	-1.66988800	4.03613900	1.74565500
H	-3.01890400	4.07167700	3.76329200
H	-2.97887400	5.84447500	3.83577900
H	-4.77540000	6.25782800	0.52188900
H	-4.02773200	7.16922100	1.85339100
O	-5.37525300	5.55716400	3.35342800
C	-6.54959600	6.15821900	2.86030200
H	-7.06383600	5.53283600	2.10590600
H	-6.35985400	7.14712700	2.40284700
H	-7.22850200	6.29454400	3.71515200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.564791 (Hartree/Particle)
Thermal correction to Energy= 0.603366
Thermal correction to Enthalpy= 0.604311
Thermal correction to Gibbs Free Energy= 0.487290
Sum of electronic and zero-point Energies= -5595.419726
Sum of electronic and thermal Energies= -5595.381150
Sum of electronic and thermal Enthalpies= -5595.380206
Sum of electronic and thermal Free Energies= -5595.497227
HF=-5595.9845168
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5598.1818225

11-Ni^{III}

Ni	-5.08930900	1.07561400	0.45185900
C	-6.23015100	1.10087000	-1.08607200
C	-5.73172100	1.11865200	-2.39252200
C	-7.60558200	0.95975100	-0.86399100
C	-6.59866500	0.98943600	-3.47887100
H	-4.66280000	1.25206600	-2.56960200
C	-8.48286100	0.82991100	-1.94030800
H	-7.99127000	0.96078000	0.15898600
C	-7.98240000	0.84462300	-3.25794900
H	-6.21144900	1.00394900	-4.50023500
H	-9.55645700	0.72349800	-1.76924000
Br	-6.14384200	0.66320300	2.68218400
C	-2.63785100	-0.32921400	-0.44922000
C	-1.31863000	-0.60652100	-0.82523700
C	-0.44799300	0.43277100	-1.17582900
C	-0.97360500	1.73205200	-1.15749200
C	-2.29360100	1.93778000	-0.76478500
C	-3.62923000	-1.38936000	-0.14175600
C	-3.36658900	-2.76031000	-0.26516400
C	-4.37718000	-3.69708800	-0.02223600
C	-5.63968300	-3.19926500	0.33857300
C	-5.82683000	-1.82783300	0.45995700
H	-0.96104800	-1.63564700	-0.85291300
H	-0.36433700	2.58916800	-1.45178200
H	-2.74306500	2.93146100	-0.78882700
H	-2.37679200	-3.10583800	-0.56252400
H	-6.47536100	-3.87553900	0.52952700
H	-6.78462400	-1.40268400	0.76209400
N	-3.10508700	0.93806900	-0.39079500
N	-4.84421100	-0.94807500	0.23156300
C	-4.13090800	-5.17613800	-0.13445900
C	0.98453200	0.17121200	-1.54921500
H	1.15464000	-0.88352600	-1.80837600
H	1.29422300	0.79917800	-2.39836900
H	1.64655800	0.42140600	-0.70271000
H	-4.19036200	-5.64888000	0.86008800
H	-3.14187800	-5.39749500	-0.55959500
H	-4.89850200	-5.65379100	-0.76350700
C	-8.87810500	0.71885400	-4.37135200
N	-9.60250600	0.61755900	-5.27447600
C	-4.30642800	3.51516500	1.55324600
H	-3.35595400	3.50751400	1.00824200
H	-4.20642100	2.79956400	2.38206000
C	-5.41082200	3.06373300	0.60310900
H	-6.41258800	3.10532600	1.03713300
C	-5.40843000	3.75441500	-0.71294000
O	-4.42108200	4.03957300	-1.37259700

O	-6.65020100	4.05553000	-1.13642400
C	-6.76308200	4.62336800	-2.44163700
H	-6.33697800	3.94394900	-3.19512100
H	-7.83609800	4.76054400	-2.62269600
H	-6.23931700	5.59003800	-2.49609800
C	-3.63501700	6.54122100	0.56414700
C	-2.42413300	6.00159900	1.37997900
C	-3.02996000	5.39460900	2.65460100
C	-4.43727200	4.91508100	2.24661700
C	-4.89720400	6.06778300	1.31957500
H	-3.61732600	7.63911700	0.48434900
H	-3.62086800	6.14219900	-0.45902500
H	-1.68438000	6.78336500	1.61053700
H	-1.88990100	5.22998200	0.80151600
H	-2.42594200	4.58642400	3.09650800
H	-3.17105600	6.16423700	3.43036100
H	-5.72829200	5.80367500	0.65102400
H	-5.26797200	6.86193200	1.98749800
O	-5.19464200	4.84186000	3.44520900
C	-6.56149300	4.50054000	3.35614500
H	-6.71151400	3.42624200	3.15250200
H	-7.09592300	5.09003700	2.58716600
H	-7.01330700	4.72890700	4.33397200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.567945 (Hartree/Particle)
Thermal correction to Energy= 0.606123
Thermal correction to Enthalpy= 0.607068
Thermal correction to Gibbs Free Energy= 0.493115
Sum of electronic and zero-point Energies= -5595.438606
Sum of electronic and thermal Energies= -5595.400427
Sum of electronic and thermal Enthalpies= -5595.399483
Sum of electronic and thermal Free Energies= -5595.513435
HF=-5596.0065505
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5598.1985432

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Ni	-4.99023200	0.49010200	0.35554300
C	-6.25996800	0.85726200	-1.02652300
C	-5.79500200	0.71450400	-2.35350300
C	-7.58768900	0.47321900	-0.73414100
C	-6.59755700	0.14095500	-3.33215700
H	-4.79582600	1.05830200	-2.61642700
C	-8.39409300	-0.10141600	-1.70900800
H	-7.96292500	0.59680100	0.28290600
C	-7.90749000	-0.28077800	-3.02141500
H	-6.21390200	0.01438600	-4.34692500
H	-9.40973800	-0.41660300	-1.46003400
Br	-6.15509300	0.26505700	2.56439300
C	-2.58370300	-0.79434300	-0.75487400
C	-1.29222000	-1.00127900	-1.25609700
C	-0.52083000	0.07826500	-1.70096400
C	-1.11645300	1.34725800	-1.64708300
C	-2.40028000	1.48193200	-1.12841000
C	-3.47638900	-1.90789800	-0.34021900
C	-3.16316200	-3.26256700	-0.51311600
C	-4.08816400	-4.24960300	-0.15214900
C	-5.31424000	-3.81747800	0.37834600
C	-5.55264300	-2.45608700	0.53541000
H	-0.87950700	-2.00884600	-1.30460100
H	-0.58982900	2.23173600	-2.01164600
H	-2.90034100	2.45124700	-1.12586200
H	-2.20585400	-3.55840000	-0.94216900
H	-6.08116200	-4.53722500	0.67235800
H	-6.47874100	-2.07400800	0.97004300
N	-3.11378500	0.44599200	-0.66217600
N	-4.65460800	-1.52798000	0.18614300
C	-3.78920600	-5.71416500	-0.32033300
C	0.88185900	-0.10445900	-2.21038000
H	1.03870500	0.45686500	-3.14447300
H	1.60557000	0.28616000	-1.47492500
H	1.11974000	-1.16235000	-2.39023700
H	-4.58285700	-6.20990700	-0.90177200
H	-3.75020500	-6.21374400	0.66175600
H	-2.82908800	-5.88189300	-0.82855700
C	-8.73416800	-0.87227300	-4.02909300
N	-9.40318700	-1.35423500	-4.84931700
C	-4.71419700	3.04273000	0.94153500
H	-3.73120600	3.07182400	0.46234600
H	-4.64656000	2.37835200	1.81242900
C	-5.79415600	2.53804100	-0.03736700
H	-6.76876500	2.59804000	0.44796900
C	-5.76016600	3.32341100	-1.30851600
O	-4.74990900	3.58148600	-1.93619800
O	-6.98114100	3.71106200	-1.70799200
C	-7.05729500	4.38544200	-2.96722500
H	-6.68860900	3.73278200	-3.77314900
H	-8.11642800	4.62189000	-3.12351600
H	-6.45572200	5.30702200	-2.95355200
C	-3.47903200	5.82391000	0.26900000
C	-2.72025100	5.34758100	1.54482200
C	-3.80993600	4.79612300	2.48926600
C	-5.00445600	4.44339900	1.57421600
C	-4.96855000	5.63824100	0.59590800
H	-3.24846000	6.86690600	0.00422700
H	-3.21367300	5.20748100	-0.60287500
H	-2.15652600	6.16450700	2.02018600
H	-1.98367000	4.56840700	1.29182700
H	-3.48023200	3.93912700	3.09586600
H	-4.16422200	5.57263100	3.18504500
H	-5.60201800	5.52818600	-0.29313000
H	-5.34431200	6.51648000	1.14550400
O	-6.18024000	4.34903500	2.36766000
C	-7.40147000	4.84135700	1.86043300
H	-7.60881100	4.51366200	0.82663900
H	-7.45591000	5.94618100	1.88324700
H	-8.19696900	4.44616300	2.51004800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.567151 (Hartree/Particle)
Thermal correction to Energy= 0.605067
Thermal correction to Enthalpy= 0.606011
Thermal correction to Gibbs Free Energy= 0.491438
Sum of electronic and zero-point Energies= -5595.417217
Sum of electronic and thermal Energies= -5595.379302

Sum of electronic and thermal Enthalpies= -5595.378357
Sum of electronic and thermal Free Energies= -5595.492930
HF=-5595.9843682
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5598.1780991

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C	-5.37398500	1.60452200	0.24931100
C	-4.32837700	1.02707400	-0.49144500
C	-6.36563100	0.76935300	0.78605200
C	-4.27140700	-0.34989000	-0.69024000
H	-3.55907900	1.66887400	-0.92517600
C	-6.32010700	-0.61091000	0.59696500
H	-7.18664000	1.20491700	1.36064100
C	-5.26878000	-1.18080500	-0.14417400
H	-3.45676600	-0.78901100	-1.26909300
H	-7.09689300	-1.25098700	1.01934600
C	-5.21532600	-2.60140200	-0.34554900
N	-5.17223700	-3.75059800	-0.50840300
C	-4.25917900	3.52850500	1.44737300
H	-3.34272900	3.54123200	0.83967700
H	-4.11450300	2.75120200	2.21286300
C	-5.41183800	3.10492100	0.50839200
H	-6.38772000	3.34507500	0.94437200
C	-5.32895300	3.83120500	-0.82931500
O	-4.30061700	4.07577900	-1.41881500
O	-6.54356100	4.14127400	-1.29910100
C	-6.59066000	4.78925200	-2.57740900
H	-6.10088900	4.17022100	-3.34365100
H	-7.65321400	4.92214400	-2.81252400
H	-6.08422600	5.76517300	-2.53243000
C	-3.85860100	6.66829400	0.58855200
C	-2.54828800	6.13825700	1.23677400
C	-2.99205500	5.43151100	2.52499900
C	-4.39290600	4.87255600	2.21184600
C	-5.01666400	6.03635700	1.39817600
H	-3.91714600	7.76676400	0.62626000
H	-3.90703400	6.38046100	-0.47081000
H	-1.81753400	6.93649100	1.43587400
H	-2.05627500	5.42408500	0.55737200
H	-2.29759500	4.64867500	2.86839400
H	-3.11425500	6.15158900	3.35005200
H	-5.87231200	5.74691500	0.77122500
H	-5.40165700	6.75175200	2.14189600
O	-5.03490600	4.68405000	3.47308200
C	-6.35170300	4.19260100	3.48600300
H	-6.41260500	3.12242600	3.20777900
H	-7.02898300	4.76369400	2.82177100
H	-6.72504100	4.28941700	4.51678700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.352979 (Hartree/Particle)
Thermal correction to Energy= 0.373378
Thermal correction to Enthalpy= 0.374322
Thermal correction to Gibbs Free Energy= 0.302359
Sum of electronic and zero-point Energies= -939.876772
Sum of electronic and thermal Energies= -939.856373
Sum of electronic and thermal Enthalpies= -939.855429
Sum of electronic and thermal Free Energies= -939.927392
HF=-940.2297509
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-941.2811298
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-939.279919150347

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C	-2.10150800	1.64941300	0.26099100
C	-3.08908500	2.61834000	0.47808200
C	-2.74570700	3.88827600	0.95623900
C	-1.38819600	4.12025400	1.21871200
C	-0.45812000	3.11276200	0.97693200
C	-2.41314300	0.27398200	-0.20479100
C	-3.71780300	-0.22092900	-0.34338200
C	-3.92866800	-1.54481500	-0.74430400
C	-2.79013000	-2.32911700	-0.98961800
C	-1.52630300	-1.76844600	-0.84049100
H	-4.13486000	2.38994300	0.27290800
H	-1.04903400	5.08024900	1.61386500
H	0.59916500	3.24725900	1.20262100
H	-4.57598900	0.41524000	-0.12736600
H	-2.88497900	-3.37316100	-1.29565100
H	-0.61541500	-2.33687700	-1.03615200
N	-0.79536300	1.90855500	0.49371300
N	-1.34444700	-0.49818600	-0.46332400
Br	1.35107600	-0.69018800	-2.27747500
Ni	0.56145400	0.32246600	-0.09943700
C	0.76620800	-0.80599900	1.44038400
C	0.10862000	-0.50364100	2.64348500
C	1.41234400	-2.04630800	1.32280800
C	0.09244100	-1.40659500	3.70600400
H	-0.39057700	0.46239700	2.75764400
C	1.41136100	-2.96335700	2.37524000
H	1.91942800	-2.29927200	0.38776200
H	-0.42194200	-1.16077000	4.63821000
H	1.91907600	-3.92555200	2.27373000
C	0.74878200	-2.64802600	3.57846200
C	-3.77951300	4.96002500	1.16556900
H	-4.79692300	4.54539000	1.20614200
H	-3.58858100	5.51982300	2.09381200
H	-3.74471300	5.68666500	0.33596300
C	-5.31159100	-2.11240800	-0.91171600
H	-5.41832700	-3.05397100	-0.35002100
H	-6.08754000	-1.41263300	-0.57047100
H	-5.50361900	-2.34724900	-1.97187900
C	0.73917000	-3.58263700	4.66614000
N	0.72928400	-4.33863000	5.54921000
C	3.74103300	2.00389200	-1.44133400
C	4.58084000	1.28395800	-0.37488600
C	3.55556500	0.33272600	0.26166500
C	2.29850500	1.19982200	0.39355700
C	2.37675200	2.24799200	-0.75959600
H	4.19768400	2.93790600	-1.80439600
H	3.59931600	1.33469000	-2.30349900
H	4.95126100	2.00441800	0.37645700
H	5.45423900	0.75757000	-0.79133600

H	3.34363800	-0.48523900	-0.43783500
H	3.87466500	-0.12076700	1.20754400
H	1.55286100	2.18911800	-1.48754600
H	2.33464300	3.24499600	-0.29772200
O	2.20467100	1.92112200	1.59353700
C	2.79352800	1.44788700	2.78829200
H	3.89098900	1.57435100	2.77561500
H	2.55515700	0.39322600	2.98912700
H	2.38003600	2.06017500	3.60292900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.467264 (Hartree/Particle)
Thermal correction to Energy= 0.498858
Thermal correction to Enthalpy= 0.499802
Thermal correction to Gibbs Free Energy= 0.400013
Sum of electronic and zero-point Energies= -5289.240829
Sum of electronic and thermal Energies= -5289.209234
Sum of electronic and thermal Enthalpies= -5289.208290
Sum of electronic and thermal Free Energies= -5289.308080
HF=-5289.7080926
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5291.5529724
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5286.551105933105

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C	-2.07560700	1.56251000	0.29180000
C	-3.04376600	2.54435200	0.53901500
C	-2.68303100	3.76980100	1.11034900
C	-1.32955700	3.94362000	1.43615500
C	-0.42009100	2.92814700	1.15634300
C	-2.40482500	0.22107000	-0.25455500
C	-3.71524900	-0.23841300	-0.44478900
C	-3.94435900	-1.53672000	-0.91424900
C	-2.81643500	-2.33106400	-1.17581300
C	-1.54424200	-1.80674100	-0.97285800
H	-4.08783700	2.35912900	0.28654200
H	-0.98021900	4.86286800	1.91119700
H	0.62880400	3.02174700	1.43708100
H	-4.56490100	0.40466500	-0.21511300
H	-2.92608700	-3.35563200	-1.53794200
H	-0.63895900	-2.38032800	-1.18280000
N	-0.77123500	1.77102200	0.57706200
N	-1.34347200	-0.56046300	-0.52710100
Br	1.63664100	-0.99459100	-2.01231800
Ni	0.51735100	0.18847400	-0.05191900
C	0.96885700	-0.73073200	1.57040100
C	0.22939900	-0.37941000	2.71950200
C	1.35174800	-2.08116500	1.42093000
C	-0.16048300	-1.33273100	3.65315100
H	-0.03489200	0.66598200	2.87967700
C	0.97640800	-3.04494500	2.35266400
H	1.91588300	-2.38144900	0.53711300
H	-0.75083400	-1.04084100	4.52477700
H	1.26763000	-4.08791600	2.20862900
C	0.20842600	-2.68350500	3.47916700
C	-3.69332400	4.85626600	1.35643300
H	-4.72313100	4.47262500	1.32491700
H	-3.52649000	5.33986000	2.33110300
H	-3.60217000	5.64076700	0.58590800
C	-5.33455600	-2.07040600	-1.12784500
H	-5.49712800	-2.98075900	-0.52835700
H	-6.10410600	-1.33446800	-0.85506300
H	-5.48306200	-2.35087500	-2.18346300
C	-0.19076100	-3.67156400	4.43537900
N	-0.51811400	-4.47244400	5.21268400
C	3.89156700	1.59073200	-0.70739000
C	4.67535100	0.87167900	0.39888100
C	3.62696200	-0.10499600	0.94353500
C	2.35395100	0.73637100	1.05362600
C	2.47168900	1.77158200	-0.12984600
H	4.33463100	2.55241100	-1.00839200
H	3.83735100	0.94394700	-1.59554400
H	4.98807500	1.58284400	1.18346600
H	5.57931600	0.36281800	0.02953100
H	3.44395400	-0.87731400	0.18456000
H	3.89816100	-0.61182800	1.87775200
H	1.72233000	1.70039300	-0.93910200
H	2.35044200	2.76370800	0.32156300
O	2.25176400	1.53114300	2.20862000
C	2.84762400	1.11450300	3.42315800
H	3.94774500	1.20275200	3.38608500
H	2.57937400	0.08219400	3.69777000
H	2.46761100	1.79099500	4.20199300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.467154 (Hartree/Particle)
Thermal correction to Energy= 0.497834
Thermal correction to Enthalpy= 0.498778
Thermal correction to Gibbs Free Energy= 0.401853
Sum of electronic and zero-point Energies= -5289.226602
Sum of electronic and thermal Energies= -5289.195922
Sum of electronic and thermal Enthalpies= -5289.194978
Sum of electronic and thermal Free Energies= -5289.291903
HF=-5289.693756
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5291.5383976
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5286.534882413162

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C	1.20128900	0.13500800	-0.22879400
C	-0.03709700	0.54712200	0.29595600
C	1.25112000	-1.06420500	-0.95596400
C	-1.19137900	-0.20406900	0.09855800
H	-0.07992500	1.47048400	0.87565200
C	0.10320900	-1.82933900	-1.16258700
H	2.19518900	-1.41905500	-1.37056300
H	-2.14508400	0.13047400	0.51145800
H	0.15907100	-2.76129500	-1.72835900
C	-1.12950900	-1.40373100	-0.63696600
C	-2.31389200	-2.18791800	-0.84446500

N	-3.27243300	-2.82216800	-1.01258100
C	3.90061800	2.75524200	-0.94598100
C	4.73670100	1.62647500	-0.27846200
C	3.80294200	0.40664500	-0.25407400
C	2.41567000	1.03633300	-0.02028700
C	2.45069900	2.21615400	-1.01532200
H	3.94970300	3.67964900	-0.35259600
H	4.27573000	2.99979300	-1.95158100
H	4.99808400	1.90943000	0.75221600
H	5.67797300	1.41759000	-0.80858100
H	3.81029400	-0.08953800	-1.23649600
H	4.07109400	-0.35405300	0.49382000
H	2.21312100	1.83586200	-2.02077400
H	1.68646300	2.96059200	-0.74870300
O	2.34653800	1.66131300	1.26797900
C	2.54149300	0.83385600	2.39470400
H	3.59533000	0.51941500	2.50978400
H	1.90868000	-0.07291600	2.36641800
H	2.26176600	1.42430400	3.27965900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.252314 (Hartree/Particle)
Thermal correction to Energy= 0.266028
Thermal correction to Enthalpy= 0.266972
Thermal correction to Gibbs Free Energy= 0.210948
Sum of electronic and zero-point Energies= -633.687992
Sum of electronic and thermal Energies= -633.674278
Sum of electronic and thermal Enthalpies= -633.673334
Sum of electronic and thermal Free Energies= -633.729358
HF=-633.940306
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-634.6429569
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-633.256640685927

Figure A2.3
S5-A

C	-2.46340100	-0.59251200	-0.48881700
C	-2.51467900	0.82711600	-0.88588300
C	-3.10075600	1.76044400	0.05367700
C	-3.54466800	1.35600500	1.28396400
C	-3.52900400	-0.03883600	1.65417300
C	-3.02981100	-0.97811300	0.76314000
Br	-2.95641800	1.26230500	-2.81649000
H	-3.16957600	2.81335900	-0.23118800
H	-2.39939600	-1.36867200	-1.26147000
H	-3.08878800	-2.04076200	1.01553000
H	-3.93261400	2.08888700	1.99473000
C	1.94835900	0.23185200	0.18919500
C	0.81124500	-1.62530900	0.99833800
C	1.96154500	-2.12594200	1.59944600
C	3.16825800	-1.41484500	1.49069000
C	3.14022700	-0.21429900	0.76904400
C	1.80742400	1.49028100	-0.58463600
C	0.30708200	2.84583600	-1.73072600
C	1.30814500	3.75771000	-2.05005300
C	2.62468500	3.52935900	-1.61669600
C	2.85917700	2.36553200	-0.87287800
H	-0.14561100	-2.14702700	1.06781900
H	1.91548900	-3.06663300	2.15248800
H	4.05302800	0.37369200	0.66674300
H	-0.72418200	2.98269100	-2.06425600
H	1.06003700	4.64422600	-2.63793700
H	3.86795900	2.14477900	-0.52189800
N	0.79932200	-0.47695000	0.30601300
N	0.54470700	1.73923500	-1.01040900
Ni	-0.75568200	0.38985400	-0.50029700
C	3.72801800	4.49755900	-1.94583200
H	3.83151700	4.61288500	-3.03712300
H	3.50215100	5.49648600	-1.53814600
H	4.69584600	4.17063100	-1.54011900
C	4.42998600	-1.92890300	2.12839900
H	4.29014700	-2.06395500	3.21323500
H	4.69960800	-2.91453500	1.71478900
H	5.27698600	-1.24624200	1.97149300
C	-4.03352100	-0.44771000	2.92663100
N	-4.44077600	-0.77435500	3.96751500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.302883 (Hartree/Particle)
Thermal correction to Energy= 0.325980
Thermal correction to Enthalpy= 0.326925
Thermal correction to Gibbs Free Energy= 0.245137
Sum of electronic and zero-point Energies= -4979.097238
Sum of electronic and thermal Energies= -4979.074141
Sum of electronic and thermal Enthalpies= -4979.073196
Sum of electronic and thermal Free Energies= -4979.154984
HF=-4979.400121
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4980.9091328

^{3}A

C	-2.71387700	-0.43424100	1.31146300
C	-2.43585700	-0.79537200	-0.05354700
C	-2.82870900	0.09390700	-1.10464600
C	-3.40038100	1.30954400	-0.81013100
C	-3.64630200	1.69231300	0.54921000
C	-3.30119700	0.81865300	1.58459800
Br	-2.26840200	-2.69109000	-0.49282200
H	-2.65872700	-0.20188000	-2.14093600
H	-2.64663800	-1.17983000	2.10853000
H	-3.51314300	1.09117000	2.62038000
H	-3.66793000	1.99531500	-1.61583300
C	2.10150300	-0.07428300	0.21473200
C	1.46419000	-2.29973600	0.63026900
C	2.74222800	-2.77034100	0.40474600
C	3.77337800	-1.84599400	0.06358500
C	3.42825700	-0.50690700	-0.02910700
C	1.63991700	1.29222600	0.13817500
C	-0.21732200	2.71510100	0.32439700
C	0.54223000	3.83891500	0.06278200
C	1.93798000	3.69381800	-0.18088900
C	2.46323500	2.41188000	-0.13440200

H	0.64474400	-2.97967800	0.88133100
H	2.95299000	-3.83865100	0.48590400
H	4.18976100	0.22600800	-0.30134900
H	-1.28866000	2.79718200	0.51702200
H	0.06918700	4.82291100	0.04820600
H	3.53056000	2.26236300	-0.30643000
N	1.13172300	-0.99458300	0.55492300
N	0.28826500	1.46602400	0.36077700
Ni	-0.65749000	-0.23577400	0.72070600
C	2.78773500	4.90121600	-0.46885600
H	3.84161900	4.63283800	-0.63317600
H	2.42427200	5.43266100	-1.36503000
H	2.74235900	5.62219100	0.36528900
C	5.17345200	-2.33442500	-0.18961800
H	5.85676100	-1.51069800	-0.44304100
H	5.57528000	-2.85392500	0.69724000
H	5.19226400	-3.06372500	-1.01768800
C	-4.22373000	2.96575500	0.84234300
N	-4.68186500	4.01017200	1.07359800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.301656 (Hartree/Particle)
Thermal correction to Energy= 0.324727
Thermal correction to Enthalpy= 0.325671
Thermal correction to Gibbs Free Energy= 0.245423
Sum of electronic and zero-point Energies= -4979.079636
Sum of electronic and thermal Energies= -4979.056565
Sum of electronic and thermal Enthalpies= -4979.055621
Sum of electronic and thermal Free Energies= -4979.135869
HF=-4979.3812918
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4980.8866644

S5-A-TS-C

C	-2.64005700	-0.54508300	0.15987300
C	-2.29019200	0.75567100	-0.29228400
C	-3.03674500	1.87421800	0.13316500
C	-4.03812000	1.70730900	1.07432900
C	-4.34524400	0.41582900	1.58952000
C	-3.64653200	-0.70731800	1.12416600
Br	-2.19408500	0.67428600	-2.96577300
H	-2.79943300	2.87214300	-0.24269700
H	-2.23422700	-1.44115600	-0.32870800
H	-3.92598800	-1.70436200	1.47272300
H	-4.59029000	2.57303200	1.44751800
C	2.18068600	0.11610100	0.19256200
C	1.23348000	-1.86669800	0.95086700
C	2.46122000	-2.33584300	1.40388900
C	3.60871500	-1.53980900	1.24690200
C	3.44444100	-0.29324200	0.62970800
C	1.89849600	1.40471500	-0.48240100
C	0.23006700	2.70366800	-1.45306400
C	1.14736900	3.69025600	-1.80162000
C	2.50361700	3.53349500	-1.47555900
C	2.86866000	2.35571700	-0.80975100
H	0.32090900	-2.45633200	1.06412500
H	2.52167200	-3.31644600	1.88056000
H	4.30784100	0.35863600	0.49408100
H	-0.82278100	2.76080100	-1.73573400
H	0.80033800	4.57709800	-2.33600400
H	3.91451200	2.18143500	-0.55509000
N	1.09237100	-0.67214600	0.35792000
N	0.59349200	1.59481800	-0.79388300
Ni	-0.58869800	0.18753700	-0.20968300
C	3.51702500	4.58574400	-1.83227300
H	3.43813000	4.85901200	-2.89636000
H	3.33849000	5.50443000	-1.24917900
H	4.54492200	4.25003200	-1.63403900
C	4.95512900	-2.02592800	1.70735100
H	4.88771800	-2.49304600	2.70198500
H	5.33574800	-2.79718000	1.01601500
H	5.69381500	-1.21345500	1.74756200
C	-5.38236900	0.26264800	2.56457900
N	-6.21893900	0.14093800	3.36340200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.302888 (Hartree/Particle)
Thermal correction to Energy= 0.325633
Thermal correction to Enthalpy= 0.326577
Thermal correction to Gibbs Free Energy= 0.244763
Sum of electronic and zero-point Energies= -4979.085645
Sum of electronic and thermal Energies= -4979.062900
Sum of electronic and thermal Enthalpies= -4979.061956
Sum of electronic and thermal Free Energies= -4979.143770
HF=-4979.3885333
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4980.9004576

^{3}S5-A-TS-C'

C	-2.82043500	0.01708900	1.44451400
C	-2.38693800	-0.48829200	0.17546900
C	-2.82760900	0.16355300	-1.01788400
C	-3.51573100	1.35272400	-0.93641100
C	-3.86064500	1.91834300	0.33156100
C	-3.52045500	1.22315600	1.50995500
Br	-2.28606100	-2.63359700	0.10026700
H	-2.55984800	-0.25921100	-1.98830400
H	-2.66887300	-0.56540000	2.35717500
H	-3.81604800	1.62668000	2.48121100
H	-3.79204100	1.88625600	-1.84884100
C	2.18779100	-0.16513000	0.22972100
C	1.60430300	-2.40497800	0.56986800
C	2.88877400	-2.83635700	0.28594800
C	3.88344800	-1.88795600	-0.05519800
C	3.50577800	-0.54704900	-0.08121200
C	1.69793100	1.21571600	0.23774400
C	-0.15737600	2.58062000	0.63007700
C	0.55207200	3.72717300	0.31054600
C	1.90987300	3.62008800	-0.07300000
C	2.46765600	2.34345800	-0.10465900
H	0.80344700	-3.10771500	0.81459200
H	3.12287900	-3.90244600	0.32147100
H	4.24283100	0.21364300	-0.34245000
H	-1.21033100	2.62283900	0.91857500

H	0.05722200	4.69964800	0.35344900
H	3.50968900	2.21957200	-0.40292500
N	1.24900000	-1.10622300	0.54922900
N	0.38903000	1.35295100	0.59992200
Ni	-0.55753700	-0.37583000	0.78292800
C	2.70167800	4.84681000	-0.43482000
H	3.73901000	4.60195000	-0.70463000
H	2.23865500	5.37260300	-1.28654100
H	2.72249100	5.56033700	0.40575200
C	5.28470400	-2.33022100	-0.37654500
H	5.93923500	-1.47976700	-0.61562700
H	5.72668000	-2.87753100	0.47288300
H	5.28926200	-3.02081600	-1.23651700
C	-4.54928200	3.16435600	0.39945800
N	-5.09906700	4.19048200	0.45195300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.301013 (Hartree/Particle)
Thermal correction to Energy= 0.323919
Thermal correction to Enthalpy= 0.324863
Thermal correction to Gibbs Free Energy= 0.243852
Sum of electronic and zero-point Energies= -4979.076134
Sum of electronic and thermal Energies= -4979.053228
Sum of electronic and thermal Enthalpies= -4979.052283
Sum of electronic and thermal Free Energies= -4979.133294
HF=-4979.3771464
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4980.8842376

S5-B

Ni	-0.76352600	0.14588400	-0.13676500
C	-2.52743400	0.94611100	-0.63052600
C	-1.49878000	3.18418500	-2.06579200
C	-2.81927200	2.29887600	-0.20954100
C	-1.81433700	0.76698900	-1.88669000
C	-1.30418100	1.89541500	-2.56195500
C	-2.30132800	3.37006400	-0.88439200
H	-3.44544500	2.45142400	0.67086100
H	-1.88302700	-0.17930600	-2.43062200
H	-0.76380900	1.75186800	-3.50056700
H	-2.49134200	4.38446500	-0.52685400
N	0.76694000	1.48985100	0.07053400
C	3.06951600	3.01014800	0.60893100
C	0.67071700	2.74877600	0.51330500
C	1.99387000	0.94716800	-0.09041500
C	3.15569400	1.68576300	0.16746600
C	1.78150100	3.53900700	0.78887100
N	0.78370900	-0.99097300	-0.77429500
C	3.08411500	-2.54456600	-1.17654400
C	0.68722900	-2.26247700	-1.18763500
C	2.00363600	-0.46066300	-0.54723700
C	3.16729300	-1.21817700	-0.74301000
C	1.79779700	-3.06789500	-1.40304800
H	-0.34089200	3.12875800	0.65249800
H	4.13669100	1.23176500	0.02545200
H	1.64011100	4.56254500	1.14248700
H	-0.32684800	-2.63906700	-1.34766600
H	4.14633200	-0.77755400	-0.55354400
H	1.66422000	-4.09644100	-1.74514100
Br	-4.01948800	-0.32966100	-0.29770400
C	-0.84454100	-0.39474500	1.79703400
C	4.30997000	-3.39095300	-1.38760100
H	4.32333000	-3.81321600	-2.40541100
H	5.23540600	-2.81695000	-1.23822200
H	4.31731600	-4.24239300	-0.68694800
C	4.29517800	3.84199000	0.87194500
H	5.21520200	3.24173700	0.82919100
H	4.37894800	4.64883700	0.12462300
H	4.23846200	4.32445100	1.86056700
C	-1.36566200	-1.82222700	1.89057200
H	-2.39693000	-1.90650800	1.51692300
H	-0.72659200	-2.51088500	1.31393000
H	-1.36143300	-2.17861400	2.94542400
C	-1.66260600	0.57254800	2.63262400
H	-1.28739000	1.60349300	2.52461000
H	-2.72202200	0.55954700	2.33421700
H	-1.61331100	0.31276300	3.71390900
C	-0.92827100	4.31140300	-2.72855000
N	-0.45595000	5.23606300	-3.25636900
O	0.52566700	-0.36789500	2.23298200
H	0.55362700	-0.69580400	3.14805900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.399318 (Hartree/Particle)
Thermal correction to Energy= 0.428577
Thermal correction to Enthalpy= 0.429521
Thermal correction to Gibbs Free Energy= 0.336571
Sum of electronic and zero-point Energies= -5172.611482
Sum of electronic and thermal Energies= -5172.582223
Sum of electronic and thermal Enthalpies= -5172.581279
Sum of electronic and thermal Free Energies= -5172.674229
HF=-5173.0107998
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.735179

S5-B-TS-D

Ni	-0.69767400	0.07356700	-0.23701200
C	-2.22105800	1.15602500	-0.76263800
C	-1.95762100	3.76236900	-1.84844000
C	-2.83276100	2.27489200	-0.12043500
C	-1.62863800	1.36085100	-2.05393100
C	-1.45559600	2.65020900	-2.55098600
C	-2.68060700	3.54400800	-0.63900300
H	-3.38854100	2.12822600	0.80498200
H	-1.34229000	0.50981600	-2.67766200
H	-0.95534200	2.79767700	-3.51092600
H	-3.10512400	4.39999100	-0.10909900
N	0.88466400	1.39224900	-0.10100900
C	3.18834900	2.90469800	0.39875000
C	0.79057000	2.68618300	0.21856900
C	2.09805400	0.81060000	-0.16657300
C	3.26603400	1.54552300	0.07383900
C	1.90701000	3.47612600	0.47222900
N	0.86276300	-1.15578700	-0.74762500

C	3.13791100	-2.78060600	-0.93971500
C	0.75224500	-2.44906900	-1.07939400
C	2.08425000	-0.63378300	-0.50801800
C	3.23530200	-1.42827400	-0.59433100
C	1.85210600	-3.29078200	-1.19187600
H	-0.22060000	3.09308400	0.27098800
H	4.24276300	1.06520400	0.01019000
H	1.77735000	4.53061400	0.72501900
H	-0.26408600	-2.81141600	-1.25612300
H	4.21573000	-0.99756600	-0.39008800
H	1.70926800	-4.33669600	-1.47163300
Br	-3.44547900	-0.68401700	-0.81897200
C	-0.85336600	-0.36719700	1.72500400
C	4.35108400	-3.66485300	-1.03528900
H	4.40542300	-4.14637000	-2.02501200
H	5.28200600	-3.10434400	-0.87026200
H	4.29893700	-4.47355300	-0.28769400
C	4.41928600	3.73056900	0.65672500
H	5.33636900	3.12613700	0.61247500
H	4.50419800	4.54050400	-0.08642900
H	4.36639900	4.20945500	1.64778000
C	-1.26193000	-1.82644300	1.87408300
H	-2.27346900	-2.00746700	1.48515000
H	-0.55988000	-2.49150000	1.34795200
H	-1.25217200	-2.12228000	2.94636500
C	-1.76836900	0.55942600	2.49756500
H	-1.47624500	1.61256100	2.36107700
H	-2.81351900	0.44038100	2.17490200
H	-1.72614200	0.33716500	3.58593500
C	-1.77582700	5.08413300	-2.35351700
N	-1.61553100	6.16530900	-2.75586900
O	0.49756800	-0.20629400	2.18094000
H	0.54288600	-0.52223200	3.09911300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.398889 (Hartree/Particle)
Thermal correction to Energy= 0.427891
Thermal correction to Enthalpy= 0.428835
Thermal correction to Gibbs Free Energy= 0.335984
Sum of electronic and zero-point Energies= -5172.604623
Sum of electronic and thermal Energies= -5172.575622
Sum of electronic and thermal Enthalpies= -5172.574678
Sum of electronic and thermal Free Energies= -5172.667529
HF=-5173.0035128
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.7280516

S5-D

Ni	-0.69767400	0.07356700	-0.23701200
C	-2.22105800	1.15602500	-0.76263800
C	-1.95762100	3.76236900	-1.84844000
C	-2.83276100	2.27489200	-0.12043500
C	-1.62863800	1.36085100	-2.05393100
C	-1.45559600	2.65020900	-2.55098600
C	-2.68060700	3.54400800	-0.63900300
H	-3.38854100	2.12822600	0.80498200
H	-1.34229000	0.50981600	-2.67766200
H	-0.95534200	2.79767700	-3.51092600
H	-3.10512400	4.39999100	-0.10909900
N	0.88466400	1.39224900	-0.10100900
C	3.18834900	2.90469800	0.39875000
C	0.79057000	2.68618300	0.21856900
C	2.09805400	0.81060000	-0.16657300
C	3.26603400	1.54552300	0.07383900
C	1.90701000	3.47612600	0.47222900
N	0.86276300	-1.15578700	-0.74762500
C	3.13791100	-2.78060600	-0.93971500
C	0.75224500	-2.44906900	-1.07939400
C	2.08425000	-0.63378300	-0.50801800
C	3.23530200	-1.42827400	-0.59433100
C	1.85210600	-3.29078200	-1.19187600
H	-0.22060000	3.09308400	0.27098800
H	4.24276300	1.06520400	0.01019000
H	1.77735000	4.53061400	0.72501900
H	-0.26408600	-2.81141600	-1.25612300
H	4.21573000	-0.99756600	-0.39008800
H	1.70926800	-4.33669600	-1.47163300
Br	-3.44547900	-0.68401700	-0.81897200
C	-0.85336600	-0.36719700	1.72500400
C	4.35108400	-3.66485300	-1.03528900
H	4.40542300	-4.14637000	-2.02501200
H	5.28200600	-3.10434400	-0.87026200
H	4.29893700	-4.47355300	-0.28769400
C	4.41928600	3.73056900	0.65672500
H	5.33636900	3.12613700	0.61247500
H	4.50419800	4.54050400	-0.08642900
H	4.36639900	4.20945500	1.64778000
C	-1.26193000	-1.82644300	1.87408300
H	-2.27346900	-2.00746700	1.48515000
H	-0.55988000	-2.49150000	1.34795200
H	-1.25217200	-2.12228000	2.94636500
C	-1.76836900	0.55942600	2.49756500
H	-1.47624500	1.61256100	2.36107700
H	-2.81351900	0.44038100	2.17490200
H	-1.72614200	0.33716500	3.58593500
C	-1.77582700	5.08413300	-2.35351700
N	-1.61553100	6.16530900	-2.75586900
O	0.49756800	-0.20629400	2.18094000
H	0.54288600	-0.52223200	3.09911300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.398889 (Hartree/Particle)
Thermal correction to Energy= 0.427891
Thermal correction to Enthalpy= 0.428835
Thermal correction to Gibbs Free Energy= 0.335984
Sum of electronic and zero-point Energies= -5172.604623
Sum of electronic and thermal Energies= -5172.575622
Sum of electronic and thermal Enthalpies= -5172.574678
Sum of electronic and thermal Free Energies= -5172.667529
HF=-5173.0035128
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5174.7280516

Figure A2.4

Int-Ni^{I}

C	-6.33087500	3.78361200	-1.30672900
H	-7.00907400	3.13414300	-1.88335300
H	-6.54427000	3.65378100	-0.23378100
H	-6.54448200	4.82784600	-1.58486400
C	-4.87361500	3.44701900	-1.63741900
C	-4.63237500	1.92409400	-1.42097700
H	-5.15499000	1.61226700	-0.50121600
H	-5.16244400	1.42609700	-2.25339100
C	-3.18771100	1.41650000	-1.31918600
C	-3.92525000	4.29522200	-0.77638400
H	-2.87932600	4.12854000	-1.07434100
H	-4.15161400	5.36415200	-0.91545000
H	-4.01786400	4.05013500	0.29483200
H	-2.71947000	1.60725700	-0.34172600
O	-4.70501100	3.78341400	-3.01230900
H	-3.95083200	3.25868900	-3.35085500
C	-2.29208500	1.75007800	-2.40023200
O	-2.58764000	2.12421300	-3.54116600
O	-0.96180600	1.60853900	-2.07341700
C	-0.03307600	1.81961000	-3.12748000
H	-0.13381200	2.82809300	-3.55843200
H	0.96717000	1.69835800	-2.68880400
H	-0.17363300	1.08752700	-3.94027000
Ni	-3.31418300	-0.59086500	-1.54117800
N	-4.21275100	-2.31221700	-1.79327600
C	-5.31918100	-4.88028900	-2.12743500
C	-5.53006500	-2.47500200	-2.00921400
C	-3.42184900	-3.41377800	-1.73751600
C	-3.94992800	-4.69958400	-1.90043400
C	-6.11670500	-3.72249100	-2.17953600
N	-1.71540200	-1.79827500	-1.37934300
C	0.33990000	-3.69768400	-1.15118600
C	-0.45158200	-1.41173700	-1.15303800
C	-1.99107700	-3.11742300	-1.49455400
C	-0.98500800	-4.08514300	-1.38545000
C	0.59555300	-2.32029900	-1.03383700
H	-6.12316000	-1.55773700	-2.04433700
H	-3.29335600	-5.56927100	-1.85181500
H	-7.19278300	-3.79332900	-2.35323900
H	-0.30177800	-0.33196200	-1.08292100
H	-1.22771600	-5.14428800	-1.48128900
H	1.60869100	-1.95515200	-0.85048600
C	1.45204400	-4.70425000	-1.03171500
H	1.08280600	-5.73620300	-1.11603400
H	2.20709600	-4.54325400	-1.81875800
H	1.97040100	-4.59981700	-0.06466900
C	-5.92324200	-6.24570500	-2.31186200
H	-6.39612700	-6.33113200	-3.30418900
H	-5.17143300	-7.04242300	-2.22024800
H	-6.71271100	-6.42788100	-1.56441900

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.410115 (Hartree/Particle)
Thermal correction to Energy= 0.437143
Thermal correction to Enthalpy= 0.438087
Thermal correction to Gibbs Free Energy= 0.347981
Sum of electronic and zero-point Energies= -2581.365154
Sum of electronic and thermal Energies= -2581.338126
Sum of electronic and thermal Enthalpies= -2581.337181
Sum of electronic and thermal Free Energies= -2581.427287
HF=-2581.7752684
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-2583.192744

TS-OA-Ni$^{I/III}$

Ni	-0.70329500	-0.05368700	-0.07394300
C	-1.59198100	1.24801500	-1.29034100
C	-0.74108800	3.85771100	-1.84056800
C	-2.13598800	2.32761300	-0.56022600
C	-0.73827200	1.49168100	-2.39303400
C	-0.29127600	2.78148200	-2.63889600
C	-1.68315600	3.61450900	-0.81390200
H	-2.82863800	2.13875800	0.25725900
H	-0.38572200	0.65577200	-2.99749400
H	0.41773900	2.96668900	-3.44853700
H	-2.04570800	4.44391700	-0.20294900
N	1.07934900	0.93514400	0.19641700
C	3.58753500	2.16905500	0.38214500
C	1.20239100	2.14411600	0.75248500
C	2.17237100	0.31664700	-0.29534800
C	3.43801000	0.90737300	-0.20924400
C	2.42693800	2.79481600	0.86255600
N	0.60521300	-1.29666000	-1.12158100
C	2.59218800	-3.06419500	-2.01800700
C	0.27647600	-2.45058600	-1.71759900
C	1.91042500	-0.98891800	-0.95527100
C	2.91994600	-1.85447300	-1.39395500
C	1.22702000	-3.35390700	-2.18009800
H	0.27747200	2.60298100	1.10071400
H	4.31205700	0.39923500	-0.61736500
H	2.47201400	3.78563100	1.31898300
H	-0.79406100	-2.64036500	-1.82735300
H	3.96807500	-1.59585500	-1.24170300
H	0.90482700	-4.27991200	-2.66110400
Br	-2.83053900	-0.48554800	-1.49535800
C	3.64842600	-4.02653600	-2.48676200
H	4.66036400	-3.61276300	-2.37481400
H	3.59515700	-4.96484900	-1.91012000
H	3.49359100	-4.29094000	-3.54497100
C	4.93274600	2.83024700	0.50493800
H	4.88628900	3.88062900	0.17783700
H	5.25974400	2.83431800	1.55836000
H	5.70052800	2.31182800	-0.08671000
C	-0.25073800	5.18044100	-2.07272400
N	0.15945300	6.25405400	-2.25355200
C	-2.69559500	-1.67454000	4.18156800
H	-2.75787900	-0.57918400	4.26449300
H	-3.53371600	-2.01643800	3.55206900
H	-2.81485100	-2.09849400	5.19097400
C	-1.33930200	-2.09714400	3.59812000
C	-1.15856500	-1.57615100	2.13909300
H	-0.07984900	-1.71013700	1.92955100
H	-1.69181400	-2.26091400	1.45802900
C	-1.61226800	-0.15256400	1.80116400
C	-1.21014100	-3.62311600	3.60805100
H	-0.26279700	-3.92613400	3.13375400
H	-1.20098300	-3.98862500	4.64697400

H	-2.04372200	-4.10409600	3.07232300
H	-2.69232200	-0.06053200	1.63368000
O	-0.28415900	-1.61725700	4.42569400
H	-0.11070700	-0.68887500	4.16956800
C	-1.11222900	0.91759100	2.62523500
O	-0.11480100	0.90366500	3.35614500
O	-1.83564900	2.07691700	2.51045600
C	-1.43349000	3.16368100	3.33486900
H	-0.41115700	3.50015900	3.09817500
H	-2.14471000	3.97760700	3.14080500
H	-1.45820700	2.88698000	4.40079100

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.499946 (Hartree/Particle)
Thermal correction to Energy= 0.535671
Thermal correction to Enthalpy= 0.536616
Thermal correction to Gibbs Free Energy= 0.426376
Sum of electronic and zero-point Energies= -5478.831364
Sum of electronic and thermal Energies= -5478.795638
Sum of electronic and thermal Enthalpies= -5478.794694
Sum of electronic and thermal Free Energies= -5478.904934
HF=-5479.3313099
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5481.404544

Int-Ni^{III}

Ni	-0.47554500	0.22648600	-0.79759300
C	-1.47757100	1.86254500	-0.92937900
C	-2.43704600	4.46038100	-1.48527500
C	-2.06326000	2.63744600	0.07894400
C	-1.38413800	2.40446700	-2.22572600
C	-1.84856600	3.68843200	-2.50605200
C	-2.54305100	3.92213800	-0.19092000
H	-2.11777000	2.27757100	1.10459200
H	-0.94668300	1.82103000	-3.03855800
H	-1.76440700	4.09416600	-3.51654100
H	-2.99164200	4.51573700	0.60874400
N	1.31699600	1.27873200	-0.45612900
C	3.76498200	2.38931800	0.36478400
C	1.45174900	2.60241600	-0.29316000
C	2.38252900	0.48103100	-0.22399700
C	3.61034900	1.00977500	0.19016400
C	2.64569900	3.19394800	0.10231000
N	0.90175100	-1.29007900	-0.85006700
C	2.87641000	-3.27397800	-0.62031900
C	0.62958600	-2.56697700	-1.15291400
C	2.15252200	-0.96179000	-0.46212900
C	3.15203100	-1.93156100	-0.33565300
C	1.57778600	-3.57871800	-1.05414900
H	0.56442400	3.20522600	-0.48338000
H	4.45381700	0.34763100	0.38297400
H	2.69598500	4.27904300	0.21206600
H	-0.39032400	-2.76187600	-1.49004800
H	4.15425300	-1.64720900	-0.01649800
H	1.29745400	-4.60206100	-1.31154700
Br	-2.06664500	-0.86607100	-2.29672000
C	3.91636200	-4.34645200	-0.45496900
H	4.92967100	-3.92734300	-0.37848400
H	3.71834800	-4.92263800	0.46485500
H	3.88926100	-5.05791800	-1.29436100
C	5.05937400	2.98554700	0.84221000
H	5.29394400	3.91246500	0.29718300
H	4.98064300	3.24888600	1.91084400
H	5.89943000	2.28571000	0.72957200
C	-2.91599900	5.78422800	-1.76198100
N	-3.29837300	6.85865100	-1.98475800
C	-2.72898500	-1.24540300	3.42041500
H	-2.14761500	-0.34243800	3.66216300
H	-3.62968400	-0.93421700	2.86668300
H	-3.04071700	-1.70634300	4.37036400
C	-1.88588900	-2.24334600	2.61257100
C	-1.49181600	-1.69029200	1.20891300
H	-0.66152500	-2.32815000	0.88341900
H	-2.31892800	-1.85645800	0.50474100
C	-1.12194400	-0.21915900	1.13273100
C	-2.65381600	-3.55461800	2.42571800
H	-2.07441700	-4.24763000	1.79560400
H	-2.81155100	-4.03399700	3.40448400
H	-3.63323100	-3.38302000	1.95323900
H	-1.99776200	0.41716000	1.26422500
O	-0.71316800	-2.58782000	3.35321300
H	-0.01917000	-1.93916800	3.14510000
C	-0.01129000	0.21482100	1.98537900
O	0.91599200	-0.49340600	2.37040300
O	-0.06317500	1.52457000	2.31583500
C	0.99993600	2.02227600	3.12769300
H	1.97320400	1.87486100	2.63683900
H	0.80476100	3.09318000	3.26319200
H	1.01942400	1.51133000	4.10248500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.503286 (Hartree/Particle)
Thermal correction to Energy= 0.538985
Thermal correction to Enthalpy= 0.539929
Thermal correction to Gibbs Free Energy= 0.432391
Sum of electronic and zero-point Energies= -5478.863057
Sum of electronic and thermal Energies= -5478.827358
Sum of electronic and thermal Enthalpies= -5478.826414
Sum of electronic and thermal Free Energies= -5478.933952
HF=-5479.3663432
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5481.4389015

TS-RD-Ni$^{III/II}$

Ni	-0.68079000	0.38993000	-0.72548200
C	-1.50599000	2.07991500	-1.04050200
C	-2.37015300	4.68221300	-1.71497600
C	-2.13460000	2.89259000	-0.08630400
C	-1.33356100	2.58278000	-2.34447900
C	-1.74866200	3.86904000	-2.68372400
C	-2.56389200	4.18081700	-0.41452600
H	-2.25970300	2.54875200	0.93916700
H	-0.87232000	1.95871200	-3.11437100
H	-1.60186900	4.24722900	-3.69788000

H	-3.04595200	4.80604300	0.34054900
N	1.10288600	1.21458300	-0.18913900
C	3.59738900	2.12021100	0.73787700
C	1.36109800	2.52651800	-0.07576200
C	2.06992900	0.32550400	0.14482000
C	3.31539400	0.75614900	0.61136200
C	2.58257700	3.01617800	0.36974100
N	0.50316100	-1.31546900	-0.59323700
C	2.18796800	-3.47725600	-0.01251800
C	0.13301800	-2.56600300	-0.88520900
C	1.72234200	-1.09891500	-0.05473700
C	2.57908800	-2.15817000	0.24813000
C	0.94361100	-3.66545500	-0.62419300
H	0.55152400	3.20159300	-0.34954500
H	4.07701700	0.02422400	0.87827500
H	2.73331400	4.09537300	0.43572000
H	-0.85387800	-2.67123800	-1.34192700
H	3.54929800	-1.96767500	0.70660700
H	0.58694500	-4.66656000	-0.87392000
Br	-2.53485600	-0.59891400	-1.80399500
C	3.04416500	-4.63930600	0.40074700
H	4.11238400	-4.37777400	0.41805300
H	2.75837800	-4.94534400	1.42210300
H	2.89870500	-5.50747200	-0.25855700
C	4.91490200	2.60793900	1.27161700
H	5.25260200	3.50870500	0.73734800
H	4.81038900	2.88063600	2.33581100
H	5.69612800	1.83801000	1.19905000
C	-2.79808500	6.00948300	-2.05062400
N	-3.14015100	7.08682100	-2.32103000
C	-1.36308300	-2.16472200	4.10571200
H	-0.95470100	-1.17031700	4.33479500
H	-2.43529400	-2.16717500	4.35910000
H	-0.84915900	-2.89502600	4.75007100
C	-1.13653800	-2.53486600	2.62899700
C	-1.86793500	-1.55048300	1.67749600
H	-1.81887500	-1.97214300	0.66383600
H	-2.94324000	-1.58752100	1.92681800
C	-1.49358200	-0.08212600	1.61603400
C	-1.67533300	-3.94434900	2.36234500
H	-1.49054200	-4.22850100	1.31495300
H	-1.15500900	-4.66715400	3.00941700
H	-2.75631000	-4.00912600	2.55917300
H	-2.33806300	0.58343000	1.43869800
O	0.25633500	-2.60295000	2.34527100
H	0.61032000	-1.70355800	2.50794500
C	-0.40704200	0.54086100	2.33043700
O	0.62989600	0.01008500	2.74659600
O	-0.59791100	1.87404100	2.51595900
C	0.39874800	2.56929300	3.25827000
H	1.39586000	2.43619000	2.81477200
H	0.11396800	3.62886000	3.23341700
H	0.43169600	2.21164400	4.29978600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.501335 (Hartree/Particle)
Thermal correction to Energy= 0.536611
Thermal correction to Enthalpy= 0.537555
Thermal correction to Gibbs Free Energy= 0.431860
Sum of electronic and zero-point Energies= -5478.861120
Sum of electronic and thermal Energies= -5478.825845
Sum of electronic and thermal Enthalpies= -5478.824900
Sum of electronic and thermal Free Energies= -5478.930595
HF=-5479.3624551
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5481.4335244

TS-RE-Ni$^{III/I}$

Ni	-0.47941900	0.55153000	-1.20022800
C	-1.91851100	1.88670100	-0.80308100
C	-3.33018600	4.26147000	-1.44437700
C	-1.56539900	3.12673900	-0.22469600
C	-3.04628900	1.85710400	-1.65625500
C	-3.73198700	3.02041600	-1.98324800
C	-2.23838600	4.29885300	-0.55443400
H	-0.77106700	3.15997100	0.51827700
H	-3.34965500	0.91577100	-2.11374300
H	-4.57863900	2.97701400	-2.67166300
H	-1.93192300	5.24843600	-0.11014700
N	1.38087300	1.44203200	-0.56620900
C	3.89340300	2.41492100	0.22950600
C	1.66933800	2.74719600	-0.64252900
C	2.33383900	0.58391400	-0.14005000
C	3.58958100	1.04973400	0.27346800
C	2.89731500	3.27493200	-0.25905800
N	0.82099100	-1.14947800	-0.79272200
C	2.40147600	-3.21210300	0.24287900
C	0.44365300	-2.42199000	-0.92542900
C	1.98354300	-0.86162900	-0.18314000
C	2.79668800	-1.87152200	0.34320000
C	1.19615200	-3.47941100	-0.42194400
H	0.87663200	3.39067300	-1.02824700
H	4.34723200	0.34498600	0.61548900
H	3.07437800	4.34910000	-0.34428700
H	-0.49108100	-2.59008000	-1.46293200
H	3.73262700	-1.62649700	0.84552600
H	0.83436000	-4.50286800	-0.53862100
Br	-1.05501500	-0.25635600	-3.44652000
C	3.22576900	-4.32561400	0.82945000
H	3.41049700	-5.11291700	0.08161000
H	4.19462200	-3.96655900	1.20469200
H	2.68734300	-4.79817700	1.66775800
C	5.22892600	2.94631900	0.67112900
H	5.91232700	2.14075200	0.97397200
H	5.70521500	3.52129200	-0.13919100
H	5.10643900	3.63470700	1.52343900
C	-4.03086300	5.46384100	-1.78142500
N	-4.59834500	6.44219900	-2.05137200
C	-3.47639500	-1.49528700	2.43927600
H	-2.68932500	-0.93282400	2.96342900
H	-4.35478500	-0.83924800	2.32765700
H	-3.75430800	-2.34772500	3.07782400
C	-2.98279800	-2.00867900	1.07764700
C	-2.68340300	-0.84340500	0.09077800
H	-2.19031500	-1.30060800	-0.77852300
H	-3.64352500	-0.46635200	-0.28984300
C	-1.92792000	0.39091700	0.59199600
C	-4.04334800	-2.90924300	0.43715500

H	-3.71054400	-3.23752900	-0.55976200
H	-4.18621500	-3.80425800	1.06146300
H	-5.00835200	-2.39018800	0.33471900
H	-2.61308600	1.08842400	1.07739500
O	-1.83799500	-2.83738600	1.23897300
H	-1.10544500	-2.25988500	1.52667800
C	-0.76935600	0.25531700	1.52551100
O	-0.20767000	-0.77348600	1.87285600
O	-0.41025700	1.44483400	2.04260800
C	0.67828400	1.44607900	2.96975200
H	1.60069900	1.08869200	2.48875200
H	0.79946500	2.48734300	3.29134700
H	0.45638200	0.80037200	3.83209400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.503556 (Hartree/Particle)
Thermal correction to Energy= 0.538728
Thermal correction to Enthalpy= 0.539672
Thermal correction to Gibbs Free Energy= 0.432440
Sum of electronic and zero-point Energies= -5478.848752
Sum of electronic and thermal Energies= -5478.813581
Sum of electronic and thermal Enthalpies= -5478.812637
Sum of electronic and thermal Free Energies= -5478.919869
HF=-5479.3523084
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5481.4219747

Figure A2.5
Ni-ArBr

C	-2.46340100	-0.59251200	-0.48881700
C	-2.51467900	0.82711600	-0.88588300
C	-3.10075600	1.76044400	0.05367700
C	-3.54466800	1.35600500	1.28396400
C	-3.52900400	-0.03883600	1.65417300
C	-3.02981100	-0.97811300	0.76314000
Br	-2.95641800	1.26230500	-2.81649000
H	-3.16957600	2.81335900	-0.23118800
H	-2.39939600	-1.36867200	-1.26147000
H	-3.08878800	-2.04076200	1.01553000
H	-3.93261400	2.08888700	1.99473000
C	1.94835900	0.23185200	0.18919500
C	0.81124500	-1.62530900	0.99833800
C	1.96154500	-2.12594200	1.59944600
C	3.16825800	-1.41484500	1.49069000
C	3.14022700	-0.21429900	0.76904400
C	1.80742400	1.49028100	-0.58463600
C	0.30708200	2.84583600	-1.73072600
C	1.30814500	3.75771000	-2.05005300
C	2.62468500	3.52935900	-1.61669600
C	2.85917700	2.36553200	-0.87287800
H	-0.14561100	-2.14702700	1.06781900
H	1.91548900	-3.06663300	2.15248800
H	4.05302800	0.37369200	0.66674300
H	-0.72418200	2.98269100	-2.06425600
H	1.06003700	4.64422600	-2.63793700
H	3.86795900	2.14477900	-0.52189800
N	0.79932200	-0.47695000	0.30601300
N	0.54470700	1.73923500	-1.01040900
Ni	-0.75568200	0.38985400	-0.50029700
C	3.72801800	4.49755900	-1.94583200
H	3.83151700	4.61288500	-3.03712300
H	3.50215100	5.49648600	-1.53814600
H	4.69584600	4.17063100	-1.54011900
C	4.42998600	-1.92890300	2.12839900
H	4.29014700	-2.06395500	3.21323500
H	4.69960800	-2.91453500	1.71478900
H	5.27698600	-1.24624200	1.97149300
C	-4.03352100	-0.44771000	2.92663100
N	-4.44077600	-0.77435500	3.96751500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.302883 (Hartree/Particle)
Thermal correction to Energy= 0.325980
Thermal correction to Enthalpy= 0.326925
Thermal correction to Gibbs Free Energy= 0.245137
Sum of electronic and zero-point Energies= -4979.097238
Sum of electronic and thermal Energies= -4979.074141
Sum of electronic and thermal Enthalpies= -4979.073196
Sum of electronic and thermal Free Energies= -4979.154984
HF=-4979.400121
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-4980.9091328

Ni(0)-ole

C	-4.22144400	1.12899900	-1.31466100
H	-4.92838800	1.28005800	-0.48500100
H	-4.61875300	1.47634800	-2.28094000
C	-2.81528300	1.37016400	-1.05517900
H	-2.44452300	1.56769200	-0.04108700
C	-1.92179500	1.80769100	-2.12535100
O	-2.19803500	2.02061600	-3.29347500
O	-0.62290700	1.92152600	-1.68116000
C	0.33721500	2.27820800	-2.66722700
H	0.08704200	3.24090300	-3.14088800
H	1.30300600	2.35574300	-2.14946100
H	0.39774800	1.51623400	-3.46211200
Ni	-3.22251800	-0.50937000	-1.37915000
N	-4.23304200	-2.15723200	-1.65247500
C	-5.46642900	-4.66975800	-1.96218900
C	-5.56549100	-2.25926100	-1.79008200
C	-3.48761300	-3.29313700	-1.66742000
C	-4.07874600	-4.55204500	-1.81859700
C	-6.21372100	-3.47958600	-1.94604100
N	-1.69790800	-1.75505900	-1.36567800
C	0.29612100	-3.73609800	-1.38624900
C	-0.40300700	-1.42424000	-1.23229900
C	-2.03141900	-3.06087100	-1.51573100
C	-1.05761300	-4.06546200	-1.52780900
C	0.61280600	-2.37474400	-1.23782700
H	-6.11386200	-1.31569000	-1.77241000
H	-3.45836000	-5.44923400	-1.82491700
H	-7.30035700	-3.50169900	-2.05533200
H	-0.19855000	-0.35570100	-1.12634400
H	-1.34831800	-5.10971400	-1.65010000

H	1.65082900	-2.05316000	-1.12608600
C	1.37440500	-4.78571000	-1.39583600
H	0.96042900	-5.79824200	-1.50484400
H	2.08015500	-4.61097600	-2.22455800
H	1.96086400	-4.75080400	-0.46315000
C	-6.13931900	-6.00565500	-2.12525400
H	-6.71937500	-6.03844900	-3.06197300
H	-5.41366600	-6.83124700	-2.14011200
H	-6.84997600	-6.18653800	-1.30198300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.310043 (Hartree/Particle)
Thermal correction to Energy= 0.331310
Thermal correction to Enthalpy= 0.332254
Thermal correction to Gibbs Free Energy= 0.256705
Sum of electronic and zero-point Energies= -2387.828530
Sum of electronic and thermal Energies= -2387.807263
Sum of electronic and thermal Enthalpies= -2387.806319
Sum of electronic and thermal Free Energies= -2387.881867
HF=-2388.1385729
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-2389.33305

A-Ni-TS-D

C	-6.54572400	3.30099200	-1.59621800
H	-6.99543400	2.39288400	-2.03223200
H	-6.72923800	3.30162600	-0.51108700
H	-7.08359200	4.16925400	-2.03289100
C	-5.08352100	3.36169900	-1.90220200
C	-4.24860500	1.23957600	-1.21062700
H	-4.93599700	1.16818500	-0.36481100
H	-4.66666800	1.15311200	-2.21348000
C	-2.82244600	1.39937400	-1.00136700
C	-4.21847600	4.30265100	-1.12098600
H	-3.14948400	4.08262500	-1.27167700
H	-4.38412300	5.35170900	-1.44425300
H	-4.43043700	4.23809100	-0.04277900
H	-2.42990900	1.54388000	0.01120600
O	-4.82983100	3.26712200	-3.24395300
H	-3.88677300	2.99244100	-3.35166000
C	-1.97234800	1.86453400	-2.06591300
O	-2.31615500	2.24616200	-3.19349100
O	-0.64080200	1.85011200	-1.73937500
C	0.25745800	2.29566400	-2.74798900
H	0.01518500	3.31839200	-3.07763500
H	1.26044100	2.27345700	-2.30067300
H	0.22704600	1.63735500	-3.63164400
Ni	-3.14894300	-0.50883100	-1.42138200
N	-4.18947800	-2.14218100	-1.63269000
C	-5.45251500	-4.63335100	-1.99423400
C	-5.52446200	-2.22710500	-1.76233000
C	-3.45593200	-3.28463100	-1.68559500
C	-4.06302700	-4.53368100	-1.86322700
C	-6.18791600	-3.43490900	-1.94037800
N	-1.64058600	-1.76174400	-1.49852400
C	0.31439200	-3.77778500	-1.34656700
C	-0.34016300	-1.44749600	-1.37509300
C	-1.99883600	-3.06937600	-1.54666300
C	-1.04424400	-4.09079900	-1.46791700
C	0.65700500	-2.41376100	-1.30296300
H	-6.06444700	-1.27867900	-1.71604600
H	-3.45109300	-5.43573000	-1.90854600
H	-7.27602700	-3.44335500	-2.03652000
H	-0.11976000	-0.37765400	-1.33606500
H	-1.35672700	-5.13578000	-1.49570100
H	1.70081700	-2.10468900	-1.21061300
C	1.37176700	-4.84490100	-1.25736900
H	0.94500900	-5.85386000	-1.34994700
H	2.12650800	-4.71471400	-2.05012200
H	1.90570700	-4.78506400	-0.29442400
C	-6.14167500	-5.95640500	-2.19088600
H	-6.69325600	-5.97069200	-3.14545000
H	-5.42892200	-6.79336900	-2.19387700
H	-6.88019300	-6.13475800	-1.39206000

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.404731 (Hartree/Particle)
Thermal correction to Energy= 0.432230
Thermal correction to Enthalpy= 0.433174
Thermal correction to Gibbs Free Energy= 0.343645
Sum of electronic and zero-point Energies= -2581.306020
Sum of electronic and thermal Energies= -2581.278521
Sum of electronic and thermal Enthalpies= -2581.277577
Sum of electronic and thermal Free Energies= -2581.367106
HF=-2581.7107507
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-2583.1288357

Aryl bromide

C	-2.58328000	-0.56943900	-0.52231500
C	-2.59004200	0.79107000	-0.85270000
C	-3.06887200	1.75169900	0.04499000
C	-3.54695300	1.34604200	1.28973600
C	-3.54670800	-0.01811600	1.63692200
C	-3.06174900	-0.97272800	0.72288500
Br	-1.93644300	1.34339500	-2.55297200
H	-3.06794900	2.80828200	-0.22623400
H	-2.20587100	-1.30691800	-1.23201000
H	-3.06042900	-2.03105300	0.98991900
H	-3.92251800	2.08799500	1.99667200
C	-4.03961900	-0.43474900	2.91931100
N	-4.43826100	-0.77190400	3.95658100

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.089176 (Hartree/Particle)
Thermal correction to Energy= 0.096652
Thermal correction to Enthalpy= 0.097596
Thermal correction to Gibbs Free Energy= 0.055610
Sum of electronic and zero-point Energies= -2897.446746
Sum of electronic and thermal Energies= -2897.439270
Sum of electronic and thermal Enthalpies= -2897.438325

Sum of electronic and thermal Free Energies= -2897.480312
HF=-2897.5359214
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-2898.2072775

Figure A2.6

A^{THF}

C	-0.46538100	-4.57313000	1.28576000
O	-0.76317900	-3.23490900	1.29172500
C	-1.26398900	-5.31883800	2.31915800
H	0.54298100	-4.81325500	0.94149200
C	-1.94341900	-3.03990500	2.08162700
C	-1.90664500	-4.16404800	3.12075900
H	-0.64700400	-5.98512800	2.94556900
H	-2.04467900	-5.95610000	1.85777500
H	-1.90791800	-2.02594600	2.50599600
H	-2.83728000	-3.11954400	1.43349300
H	-1.25467300	-3.87509900	3.96070400
H	-2.90132900	-4.40360600	3.52383200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.102514 (Hartree/Particle)
Thermal correction to Energy= 0.107359
Thermal correction to Enthalpy= 0.108303
Thermal correction to Gibbs Free Energy= 0.074371
Sum of electronic and zero-point Energies= -231.529057
Sum of electronic and thermal Energies= -231.524212
Sum of electronic and thermal Enthalpies= -231.523267
Sum of electronic and thermal Free Energies= -231.557199
HF=-231.6315705
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-231.8968378

A-TS-B'^{THF}

C	-2.35127400	1.57579800	0.13470500
C	-3.36690000	2.44464100	0.54996200
C	-3.04715400	3.69247000	1.09956100
C	-1.68515400	4.01617600	1.20806900
C	-0.72291400	3.10565300	0.78134500
C	-2.60038300	0.23684600	-0.45945600
C	-3.87154400	-0.31002700	-0.67136800
C	-4.00249000	-1.58493200	-1.23684100
C	-2.82140600	-2.26573300	-1.57743600
C	-1.59030900	-1.66351100	-1.33963600
H	-4.41289400	2.15456400	0.44895200
H	-1.36998800	4.97433600	1.62674600
H	0.34773600	3.31723700	0.85693400
H	-4.76557000	0.25049800	-0.39741700
H	-2.85949200	-3.26069800	-2.02586300
H	-0.64281400	-2.14675900	-1.59124800
N	-1.04952500	1.91576900	0.25770000
N	-1.48903900	-0.44717800	-0.79425200
Br	1.82365200	-0.31289400	-1.90965800
Ni	0.26869200	0.40178400	-0.21185900
C	0.47047400	-0.45812700	1.56347300
C	-0.21048000	-0.05202000	2.72909700
C	1.28210100	-1.60712800	1.67027900
C	-0.08482000	-0.73161000	3.94129600
H	-0.85782400	0.83044200	2.69955100
C	1.42628700	-2.30800800	2.86840100
H	1.82207000	-1.95949600	0.78566100
H	-0.61923900	-0.39049800	4.83171100
H	2.06532500	-3.19299700	2.92404400
C	0.74135300	-1.87098800	4.01990400
C	-4.10988600	4.65239700	1.55865700
H	-5.12140200	4.25188500	1.40307900
H	-3.98794700	4.88006800	2.63009900
H	-4.02767500	5.60844300	1.01653500
C	-5.34959000	-2.21385300	-1.46516800
H	-5.47327100	-3.09864000	-0.81885300
H	-6.17094700	-1.51584700	-1.25046700
H	-5.44780100	-2.56031200	-2.50617700
C	0.87870600	-2.57927700	5.25907500
N	0.98748200	-3.15253900	6.26483300
C	2.75026900	2.00133200	1.67264100
H	2.02199400	1.77464200	2.45071900
C	4.31144100	1.96661400	-0.09317200
C	3.14687000	2.91395300	-0.38912200
H	5.18851700	2.53413700	0.25684500
H	4.59623800	1.38523200	-0.98114800
H	3.44728000	3.91031300	-0.74490100
H	2.44639500	2.45908000	-1.11098800
O	2.45626100	3.07404300	0.86829700
C	3.74583800	1.08379800	1.03915200
H	4.52212800	0.73803900	1.74283700
H	3.25978300	0.18251800	0.62185000

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.407387 (Hartree/Particle)
Thermal correction to Energy= 0.437069
Thermal correction to Enthalpy= 0.438013
Thermal correction to Gibbs Free Energy= 0.340081
Sum of electronic and zero-point Energies= -5210.702801
Sum of electronic and thermal Energies= -5210.673120
Sum of electronic and thermal Enthalpies= -5210.672175
Sum of electronic and thermal Free Energies= -5210.770108
HF=-5211.1101884
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5212.8744598

B'^{THF}

C	-2.23868400	1.72194100	0.28388800
C	-3.31599900	2.53499900	0.65882600
C	-3.09441300	3.83943700	1.11490100
C	-1.76333100	4.28153600	1.15962300
C	-0.74008000	3.41922200	0.77802300
C	-2.40498300	0.34403300	-0.24544900
C	-3.64402900	-0.30068100	-0.35606300
C	-3.71859500	-1.59885600	-0.87439500
C	-2.51363100	-2.20043700	-1.27013700
C	-1.31873600	-1.50178500	-1.12986600
H	-4.33682700	2.15973300	0.58886900

H	-1.51998800	5.29501900	1.48565400
H	0.30245600	3.74090400	0.77839500
H	-4.55773300	0.20040400	-0.03647400
H	-2.50232400	-3.21103000	-1.68413200
H	-0.35829000	-1.92696800	-1.43004600
N	-0.96552900	2.16430900	0.36442900
N	-1.26671100	-0.26144200	-0.63271000
Br	1.78541600	-0.24290100	-1.99171700
Ni	0.51256100	0.68560200	-0.05895800
C	0.57728400	-0.38459400	1.54282300
C	-0.06467600	-0.00853400	2.73274000
C	1.17786700	-1.65264200	1.47689400
C	-0.12720700	-0.87273700	3.82654600
H	-0.52838100	0.97925600	2.81266300
C	1.12912700	-2.53065600	2.55993100
H	1.69021000	-1.95420300	0.55887500
H	-0.63475700	-0.57089800	4.74592800
H	1.59833900	-3.51544100	2.49724000
C	0.47027100	-2.14625400	3.74551600
C	-4.22577600	4.73292900	1.54286200
H	-5.20580800	4.30518100	1.28858500
H	-4.19505000	4.89110800	2.63396000
H	-4.14242800	5.72487800	1.07178800
C	-5.02769100	-2.32862000	-1.00173400
H	-5.01962300	-3.24477400	-0.38882100
H	-5.87719000	-1.70837600	-0.68285800
H	-5.19775400	-2.64178600	-2.04448700
C	0.40877700	-3.04298300	4.86307800
N	0.35554900	-3.76911900	5.76931500
C	1.98398800	1.67541500	0.78592400
H	1.56747200	2.06170600	1.72985100
C	4.29887800	2.04357200	0.26431000
C	3.38474900	2.70551900	-0.76591200
H	4.63997400	2.78835700	1.00221400
H	5.18604000	1.58244200	-0.19407700
H	3.65444500	3.74285500	-1.01413200
H	3.31590500	2.10967200	-1.69067800
O	2.09778600	2.73829200	-0.12453100
C	3.35618300	1.01654900	0.91985200
H	3.59938900	0.80377600	1.97082300
H	3.37871700	0.06871000	0.36583200

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.411204 (Hartree/Particle)
Thermal correction to Energy= 0.440054
Thermal correction to Enthalpy= 0.440998
Thermal correction to Gibbs Free Energy= 0.346230
Sum of electronic and zero-point Energies= -5210.730737
Sum of electronic and thermal Energies= -5210.701887
Sum of electronic and thermal Enthalpies= -5210.700943
Sum of electronic and thermal Free Energies= -5210.795712
HF=-5211.1419416
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5212.9026238

B'-TS-F^{THF}

C	-2.39459400	1.61380000	0.17291300
C	-3.41615400	2.48809100	0.56669500
C	-3.11018900	3.78148100	1.00465000
C	-1.75467000	4.14842200	1.01740500
C	-0.79114500	3.23008100	0.61279200
C	-2.63939100	0.23248800	-0.31468900
C	-3.89983100	-0.37886300	-0.32645100
C	-4.04233500	-1.68771500	-0.80195500
C	-2.88166100	-2.33399600	-1.25757300
C	-1.66118700	-1.66767800	-1.21428900
H	-4.45763100	2.16850600	0.52661300
H	-1.44839900	5.14634400	1.33881900
H	0.27248000	3.47639600	0.59595300
H	-4.77572800	0.15603100	0.04145600
H	-2.92561400	-3.35503400	-1.64302300
H	-0.73182100	-2.12652700	-1.56114600
N	-1.09852700	1.98954200	0.20882700
N	-1.54351200	-0.41602400	-0.75555300
Br	1.55523800	-0.60466800	-2.18638600
Ni	0.25709900	0.48319900	-0.33993900
C	0.65459900	-0.39517500	1.33152700
C	-0.10168500	-0.08099300	2.48245400
C	1.14664600	-1.71283600	1.20777400
C	-0.41305800	-1.04508000	3.43426800
H	-0.46686400	0.93917100	2.62301300
C	0.84686700	-2.68626000	2.15592100
H	1.73956100	-1.97882200	0.33124700
H	-1.01997800	-0.78405500	4.30421200
H	1.21886100	-3.70550600	2.02912300
C	0.05502700	-2.36680500	3.27867700
C	-4.17851700	4.74528700	1.44320200
H	-4.04061300	5.01787700	2.50249700
H	-4.12242100	5.67968300	0.86184000
H	-5.18643000	4.32316500	1.32532300
C	-5.37521300	-2.38516700	-0.81884800
H	-6.19047800	-1.72145100	-0.49778400
H	-5.60736400	-2.75828000	-1.82926200
H	-5.36050900	-3.26067600	-0.14890200
C	-0.26617000	-3.36749700	4.25114800
N	-0.53136300	-4.17939100	5.04050100
C	1.89297900	1.14108500	0.89108800
H	1.62317400	1.65160700	1.82553600
C	4.15511000	1.63294500	0.29117900
C	3.20995400	2.21900900	-0.75372900
H	4.41308900	2.39063400	1.04950800
H	5.08844800	1.25251600	-0.14923800
H	3.39386400	3.27784400	-0.98958500
H	3.20715400	1.62560100	-1.68161400
O	1.90558600	2.13972100	-0.14081900
C	3.28438200	0.52347500	0.89809800
H	3.58809500	0.20705700	1.90523300
H	3.29831600	-0.35282500	0.23439300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.410835 (Hartree/Particle)
Thermal correction to Energy= 0.438944
Thermal correction to Enthalpy= 0.439888
Thermal correction to Gibbs Free Energy= 0.347875
Sum of electronic and zero-point Energies= -5210.715185
Sum of electronic and thermal Energies= -5210.687076

Sum of electronic and thermal Enthalpies= -5210.686132
Sum of electronic and thermal Free Energies= -5210.778145
HF=-5211.1260197
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5212.8856316

p^{CC-THF}

C	0.84204500	0.01525200	0.41737500
C	0.08919200	-0.37815500	1.53556300
C	0.69640600	-0.69022100	-0.78522700
C	-0.78127000	-1.46244400	1.46476100
H	0.18419400	0.17405700	2.47455800
C	-0.17401300	-1.77530600	-0.87197000
H	1.26817100	-0.36777300	-1.65621400
H	-1.36219200	-1.76335800	2.33866100
H	-0.28457300	-2.31938600	-1.81206800
C	-0.91801300	-2.17177800	0.25527500
C	-1.81582600	-3.28880600	0.17240900
N	-2.54118100	-4.19380500	0.10638900
C	1.82559500	1.15838900	0.53803800
H	1.34869000	1.96620300	1.12905100
C	4.12427900	1.78205100	0.60674400
C	3.59686300	1.88615000	-0.82650700
H	4.02933000	2.75135800	1.12291700
H	5.17805300	1.47026200	0.65390700
H	3.78234700	2.86886000	-1.28974000
H	4.05031900	1.11194900	-1.47466400
O	2.18532300	1.67261000	-0.74105800
C	3.15695300	0.76080100	1.21022200
H	3.09761500	0.78721100	2.30767100
H	3.43342900	-0.26213600	0.90603400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.196255 (Hartree/Particle)
Thermal correction to Energy= 0.207196
Thermal correction to Enthalpy= 0.208141
Thermal correction to Gibbs Free Energy= 0.157979
Sum of electronic and zero-point Energies= -555.172054
Sum of electronic and thermal Energies= -555.161113
Sum of electronic and thermal Enthalpies= -555.160169
Sum of electronic and thermal Free Energies= -555.210330
HF=-555.3683091
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-555.9858873

A-TS-D^{THF}

C	-4.72123500	1.31294300	-1.81771900
H	-5.35786200	1.67963600	-1.01106000
H	-5.20804500	0.76218500	-2.62494000
C	-3.37152900	1.21932700	-1.63154800
H	-2.72057600	0.72406200	-2.35567700
C	-2.72482400	1.85877300	-0.48598100
O	-3.27779600	2.52829000	0.37330400
O	-1.38716800	1.63971700	-0.47601800
C	-0.65967200	2.23439200	0.59494400
H	-1.01577500	1.86557500	1.56995300
H	0.39168400	1.95613500	0.44771000
H	-0.76546600	3.33120100	0.58447000
C	-5.26732700	3.42440500	-2.79114100
O	-6.12450100	3.92415500	-1.87625100
C	-3.98565600	4.21004700	-2.83744100
H	-5.75587500	2.98676600	-3.66477600
C	-5.37194600	4.72702500	-0.93791500
C	-4.21664900	5.30105400	-1.76419600
H	-3.79893900	4.63089500	-3.83919700
H	-3.11837400	3.56998800	-2.59594600
H	-6.05765800	5.47805500	-0.52279100
H	-4.99884000	4.07012300	-0.13591300
H	-4.51375400	6.25027700	-2.23623800
H	-3.32755000	5.48652900	-1.14584400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.200133 (Hartree/Particle)
Thermal correction to Energy= 0.211806
Thermal correction to Enthalpy= 0.212750
Thermal correction to Gibbs Free Energy= 0.160537
Sum of electronic and zero-point Energies= -537.695389
Sum of electronic and thermal Energies= -537.683716
Sum of electronic and thermal Enthalpies= -537.682772
Sum of electronic and thermal Free Energies= -537.734985
HF=-537.895522
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-538.5136763

D^{THF}

C	-4.42989200	2.08844500	-1.59165200
H	-4.78754800	2.31809900	-0.57615600
H	-5.12816100	1.37162900	-2.05409800
C	-3.06821700	1.50852000	-1.53042000
H	-2.67278500	0.91431400	-2.35838900
C	-2.18731500	1.76937200	-0.40586500
O	-2.45922100	2.49194700	0.54261500
O	-1.00321800	1.12584200	-0.52034400
C	-0.06920700	1.33373300	0.53793800
H	-0.48582000	1.00215600	1.50219500
H	0.81969600	0.74220200	0.28590000
H	0.19558000	2.39946900	0.62550300
C	-4.52473700	3.38881800	-2.44171100
O	-5.90424300	3.71375600	-2.60832900
C	-3.87748800	4.61704200	-1.77604200
H	-4.08853700	3.18779900	-3.43608700
C	-6.21386000	4.95462400	-1.97443200
C	-5.05775200	5.23093300	-1.01298600
H	-3.51670100	5.31519500	-2.54873600
H	-3.03365400	4.35232300	-1.12517300
H	-6.29345400	5.75646000	-2.73547100
H	-7.19184100	4.86428400	-1.47409100
H	-4.92837300	6.30073700	-0.79274400
H	-5.21193700	4.70434400	-0.05728600

UB3LYP-D3/def2-SVP-CPCM(benzene)

Zero-point correction= 0.202916 (Hartree/Particle)
Thermal correction to Energy= 0.214397
Thermal correction to Enthalpy= 0.215342
Thermal correction to Gibbs Free Energy= 0.163561
Sum of electronic and zero-point Energies= -537.727976
Sum of electronic and thermal Energies= -537.716494
Sum of electronic and thermal Enthalpies= -537.715550
Sum of electronic and thermal Free Energies= -537.767331
HF=-537.9308919
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-538.5461321

D-TS-E^{THF}

Ni	-4.96066700	0.48974800	0.81189900
C	-6.23452800	0.83564500	-0.66206600
C	-5.87603700	0.78499300	-2.02311100
C	-7.58707400	1.09773800	-0.36461200
C	-6.80400100	0.99653300	-3.04285200
H	-4.83823300	0.58208300	-2.30521700
C	-8.53406900	1.32295300	-1.36288600
H	-7.90082800	1.14033600	0.68270600
C	-8.14506900	1.27684200	-2.71608900
H	-6.50070300	0.95806400	-4.09218500
H	-9.57370400	1.54166000	-1.10690100
Br	-5.92850300	0.61981400	3.01429100
C	-2.65170500	-0.59143000	-0.56507400
C	-1.50354000	-0.67614200	-1.36006400
C	-0.87438400	0.48890600	-1.81839800
C	-1.45249900	1.71485300	-1.45465400
C	-2.59629500	1.72970400	-0.66192500
C	-3.40070000	-1.77416400	-0.06673000
C	-3.01847900	-3.10251000	-0.28880500
C	-3.80109500	-4.15160500	0.20997300
C	-4.95890900	-3.80976300	0.92926700
C	-5.27796300	-2.46941100	1.11768000
H	-1.09783800	-1.64949000	-1.63662600
H	-1.02596100	2.66078400	-1.79458900
H	-3.08482500	2.67118800	-0.40555000
H	-2.11085500	-3.32841600	-0.84881900
H	-5.60813600	-4.58377900	1.34380800
H	-6.15724500	-2.15006000	1.68245700
N	-3.17404300	0.60589600	-0.21811800
N	-4.51759300	-1.48366000	0.62889700
C	-3.42463800	-5.59158700	-0.00611400
C	0.36814400	0.43707600	-2.66370600
H	0.26678600	1.08393300	-3.54915100
H	1.23445100	0.80894700	-2.09130800
H	0.59466100	-0.58466100	-2.99953100
H	-4.23592600	-6.13027000	-0.52186600
H	-3.26662600	-6.09817700	0.95995700
H	-2.50747000	-5.69215900	-0.60312100
C	-9.09890100	1.53250000	-3.75538500
N	-9.86622700	1.74844200	-4.60190800
C	-4.60637800	4.00635500	1.74003100
H	-3.67504100	4.36989700	1.27934700
H	-4.40453300	3.01944100	2.19654900
C	-5.66794900	3.85580600	0.71750300
H	-6.67704400	3.59828600	1.03862000
C	-5.43399500	4.13942300	-0.68430800
O	-4.33426800	4.36425200	-1.18124300
O	-6.56907800	4.13334800	-1.41066500
C	-6.43370000	4.39584700	-2.80500600
H	-5.74570400	3.67547600	-3.27138200
H	-7.43583600	4.28653300	-3.23640700
H	-6.05007400	5.41439200	-2.97654500
C	-5.02055500	4.96058300	2.88859500
O	-6.30093100	4.60069900	3.39885800
C	-4.06429900	4.88752900	4.08913200
H	-5.09321000	5.98364800	2.47996900
C	-6.19082400	4.00590600	4.69527200
C	-4.69637200	3.77202400	4.93268700
H	-4.07941400	5.84370400	4.63704100
H	-3.02483700	4.68295500	3.79173300
H	-6.61647900	4.69650300	5.44894600
H	-6.76947900	3.06880400	4.70892500
H	-4.42104600	3.82128600	5.99664800
H	-4.41017300	2.78049400	4.54925600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.508362 (Hartree/Particle)
Thermal correction to Energy= 0.544300
Thermal correction to Enthalpy= 0.545244
Thermal correction to Gibbs Free Energy= 0.433407
Sum of electronic and zero-point Energies= -5516.905104
Sum of electronic and thermal Energies= -5516.869167
Sum of electronic and thermal Enthalpies= -5516.868222
Sum of electronic and thermal Free Energies= -5516.980059
HF=-5517.4134662
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5519.5272694

E^{THF}

Ni	-4.96748700	0.49328900	0.58191900
C	-6.21216300	0.58613200	-0.86719800
C	-5.81812300	0.75385700	-2.19880000
C	-7.55789300	0.34742400	-0.56170000
C	-6.75914500	0.67873200	-3.22693300
H	-4.77406800	0.96105200	-2.44171800
C	-8.50782000	0.26786900	-1.57921900
H	-7.86378700	0.23432500	0.48181500
C	-8.11258600	0.43500300	-2.92197100
H	-6.45339500	0.81134700	-4.26727400
H	-9.55829100	0.08477400	-1.34210700
Br	-5.84451600	-0.12115000	2.86336500
C	-2.55181300	-0.67024300	-0.66081300
C	-1.27822600	-0.82146000	-1.21963200
C	-0.51496100	0.30330900	-1.55823600
C	-1.09979800	1.55710200	-1.33437700
C	-2.36952000	1.63693100	-0.76689400
C	-3.44025900	-1.81649300	-0.34701500
C	-3.11474200	-3.15196800	-0.61852300
C	-4.03606800	-4.17084500	-0.35184100
C	-5.27600900	-3.78979400	0.18598500

C	-5.52756400	-2.44816900	0.44671400
H	-0.87366500	-1.81689600	-1.40240000
H	-0.57686000	2.47683000	-1.60456500
H	-2.86597100	2.59909500	-0.62728700
H	-2.14628000	-3.40532900	-1.04912000
H	-6.04399600	-4.53407100	0.40612500
H	-6.46764100	-2.11309600	0.88689300
N	-3.07375800	0.55242200	-0.41386000
N	-4.62917500	-1.48909700	0.19210800
C	-3.71994600	-5.61582300	-0.62211300
C	0.87071400	0.17152600	-2.12636300
H	1.07090300	0.95211900	-2.87542900
H	1.61931800	0.28981900	-1.32419800
H	1.03060500	-0.81318900	-2.58877700
H	-4.51541300	-6.08363600	-1.22350100
H	-3.66056000	-6.17750000	0.32494300
H	-2.76445300	-5.73565200	-1.15182900
C	-9.08397300	0.36208000	-3.97484500
N	-9.86931200	0.30267800	-4.82953600
C	-4.26703500	2.86938300	1.85532800
H	-3.33515600	3.08557100	1.31508900
H	-4.05362900	2.06509800	2.57339200
C	-5.37177600	2.42934000	0.90455900
H	-6.33429500	2.38588000	1.42388500
C	-5.49557200	3.29120000	-0.30233500
O	-4.56847600	3.79615400	-0.91663500
O	-6.77371900	3.48075500	-0.67019800
C	-6.99414300	4.19844500	-1.88334700
H	-6.53521400	3.66858000	-2.73239100
H	-8.08180300	4.24710600	-2.01643700
H	-6.56873800	5.21203100	-1.82632900
C	-4.65784400	4.13985800	2.64753700
O	-5.94517400	4.02691600	3.24052500
C	-3.72016100	4.39628000	3.83492300
H	-4.70032600	4.99290000	1.94909900
C	-5.83246600	3.48281100	4.55994800
C	-4.33158500	3.49524000	4.92201700
H	-3.77995100	5.45675700	4.12773300
H	-2.66829500	4.16111400	3.61264900
H	-6.43153400	4.11450600	5.23873300
H	-6.24380100	2.45906000	4.57892900
H	-4.14647400	3.87072100	5.93910300
H	-3.91519400	2.47773700	4.86491300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.511396
(Hartree/Particle)
Thermal correction to Energy= 0.547241
Thermal correction to Enthalpy= 0.548185
Thermal correction to Gibbs Free Energy= 0.436938
Sum of electronic and zero-point Energies= -5516.924197
Sum of electronic and thermal Energies= -5516.888352
Sum of electronic and thermal Enthalpies= -5516.887408
Sum of electronic and thermal Free Energies= -5516.998655
HF=-5517.4355929
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5519.5440135

E-TS-F^{THF}

Ni	-5.00453400	-0.19034200	0.38242500
C	-6.29938100	0.17096000	-0.97651900
C	-5.84171400	0.24136900	-2.31024100
C	-7.58228100	-0.36227700	-0.72961400
C	-6.60723000	-0.26612200	-3.35337000
H	-4.87987500	0.70340200	-2.52916400
C	-8.35104300	-0.87492400	-1.76819600
H	-7.95364500	-0.39629800	0.29600600
C	-7.87058800	-0.83775800	-3.09417000
H	-6.23140800	-0.22363900	-4.37798800
H	-9.33234000	-1.30657300	-1.55946200
Br	-6.13588100	-0.73396900	2.58879200
C	-2.49136600	-1.12782600	-0.82761100
C	-1.19710400	-1.15798700	-1.36110600
C	-0.55293700	0.02872800	-1.73017600
C	-1.27567700	1.21947400	-1.56653500
C	-2.55503100	1.17834200	-1.01998900
C	-3.25656500	-2.35719800	-0.49318900
C	-2.80331600	-3.65447300	-0.76707200
C	-3.61446900	-4.75843900	-0.47897400
C	-4.87491400	-4.49948200	0.08291700
C	-5.25467900	-3.18674600	0.34150600
H	-0.68280300	-2.10935300	-1.49672500
H	-0.85211800	2.17990900	-1.86764200
H	-3.15245800	2.08754000	-0.93162700
H	-1.82398300	-3.81402700	-1.21806100
H	-5.55889600	-5.31630300	0.32296000
H	-6.21286400	-2.94015800	0.80339700
N	-3.14537800	0.03885900	-0.62966900
N	-4.46314100	-2.14434600	0.06293400
C	-3.16398700	-6.16693700	-0.75405800
C	0.84935700	0.03150400	-2.27262900
H	0.94803800	0.73463400	-3.11369400
H	1.55647500	0.35953700	-1.49171900
H	1.16029800	-0.96780700	-2.60919100
H	-3.90461900	-6.69933600	-1.37193800
H	-3.06813400	-6.73033600	0.18882600
H	-2.19434300	-6.19532200	-1.27083300
C	-8.65894200	-1.36288500	-4.16771800
N	-9.29631000	-1.79071000	-5.04127800
C	-4.92319800	2.25064100	1.24374300
H	-3.99671800	2.57514100	0.75691400
H	-4.66619200	1.46829300	1.97131100
C	-5.96236500	1.76422900	0.21203300
H	-6.93308700	1.70552900	0.70937200
C	-6.02421300	2.72029300	-0.94030300
O	-5.05498400	3.22454600	-1.47800700
O	-7.27903300	2.95699200	-1.34139400
C	-7.43654600	3.76520700	-2.50948700
H	-6.95759800	3.28296300	-3.37592000
H	-8.51672400	3.85506500	-2.67563900
H	-6.98654900	4.75888000	-2.36425800
C	-5.48117500	3.45528100	2.04378800
O	-6.79926200	3.21391900	2.52027500
C	-4.65329200	3.73294700	3.30607000
H	-5.53115600	4.33056800	1.37279900
C	-6.77836100	2.79566400	3.89146100
C	-5.30385200	2.77940600	4.32027500
H	-4.78727400	4.78238200	3.61458500
H	-3.57718100	3.55411200	3.16069200
H	-7.37200100	3.51619300	4.48352300

H	-7.23989100	1.79856200	3.97504500
H	-5.16182700	3.09619100	5.36390900
H	-4.89758700	1.76151300	4.21504600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.510849 (Hartree/Particle)
Thermal correction to Energy= 0.546077
Thermal correction to Enthalpy= 0.547021
Thermal correction to Gibbs Free Energy= 0.437937
Sum of electronic and zero-point Energies= -5516.908554
Sum of electronic and thermal Energies= -5516.873326
Sum of electronic and thermal Enthalpies= -5516.872382
Sum of electronic and thermal Free Energies= -5516.981466
HF=-5517.419403
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5519.5276346

$p^{DCF-THF}$

C	-6.41104300	0.09519600	-0.56992600
C	-5.39415600	-0.28761600	-1.46166700
C	-7.39768100	-0.84114400	-0.22666200
C	-5.36048600	-1.57198900	-1.99841100
H	-4.62515600	0.43559700	-1.74291000
C	-7.37590800	-2.13127200	-0.75372800
H	-8.19488300	-0.55516900	0.46365500
C	-6.35374100	-2.50590100	-1.64542100
H	-4.56807300	-1.85876100	-2.69229100
H	-8.14869300	-2.85195100	-0.47975000
C	-6.32512900	-3.83235100	-2.19410900
N	-6.30177100	-4.90557900	-2.63774100
C	-5.29389500	1.65945600	1.07732800
H	-4.31745700	1.59956000	0.57156400
H	-5.35203600	0.82421700	1.79425600
C	-6.41925800	1.48673600	0.04411100
H	-7.38145700	1.64486600	0.54904600
C	-6.31079700	2.52091300	-1.06961900
O	-5.27541600	3.01433200	-1.45679100
O	-7.50656600	2.79030100	-1.60636600
C	-7.52203200	3.70122500	-2.71188300
H	-6.91708600	3.31042900	-3.54418700
H	-8.57150600	3.79690500	-3.01468500
H	-7.11865600	4.68050600	-2.41315100
C	-5.37918600	2.98435900	1.83911600
O	-6.70008500	3.13576300	2.38408600
C	-4.41661100	3.05755000	3.04130100
H	-5.19685000	3.81328400	1.13321700
C	-6.64704300	3.25828600	3.80213700
C	-5.31298300	2.63789000	4.21426000
H	-4.06403600	4.09143200	3.18342500
H	-3.53235600	2.41650500	2.91026900
H	-6.69129400	4.32600900	4.09873700
H	-7.52455300	2.75042400	4.23371200
H	-4.95327000	2.99430200	5.19076000
H	-5.40197200	1.54024800	4.26304800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.296381 (Hartree/Particle)
Thermal correction to Energy= 0.314368
Thermal correction to Enthalpy= 0.315312
Thermal correction to Gibbs Free Energy= 0.247203
Sum of electronic and zero-point Energies= -861.365572
Sum of electronic and thermal Energies= -861.347585
Sum of electronic and thermal Enthalpies= -861.346641
Sum of electronic and thermal Free Energies= -861.414750
HF=-861.6619532
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-862.6289765

Table A2.2
TS-Giese Addition[4]

C	-4.90489700	1.50015100	-1.60372500
H	-5.40954500	1.94377600	-0.74258200
H	-5.51272300	0.93887800	-2.31454900
C	-3.54823500	1.38653900	-1.59837900
H	-3.00815200	0.87449200	-2.39772500
C	-2.74516600	2.01574700	-0.54935500
O	-3.17248500	2.63861300	0.40908100
O	-1.41586700	1.84636600	-0.76278700
C	-0.54505700	2.41431900	0.21287000
H	-0.75070200	2.00380300	1.21384400
H	0.47603100	2.16021700	-0.09858200
H	-0.66489000	3.50847400	0.25765400
C	-5.37848000	3.49958300	-2.94036200
O	-4.20250000	4.14408100	-2.96307100
H	-6.14090100	3.88312700	-2.24858900
C	-3.87243400	4.95207000	-1.82632500
H	-4.11185300	4.40263300	-0.90171700
H	-4.48558300	5.87235600	-1.85520800
C	-5.78427700	2.90034700	-4.24109300
H	-4.96713600	2.28546200	-4.65297800
H	-6.67842600	2.27124900	-4.12108100
H	-6.01519300	3.68378100	-4.98996400
C	-2.39303500	5.27125800	-1.88786400
H	-2.14599000	5.81382900	-2.81360000
H	-2.10405100	5.89476900	-1.02808500
H	-1.80182600	4.34359500	-1.86166700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.219439 (Hartree/Particle)
Thermal correction to Energy= 0.233119
Thermal correction to Enthalpy= 0.234063
Thermal correction to Gibbs Free Energy= 0.178063
Sum of electronic and zero-point Energies= -538.886739
Sum of electronic and thermal Energies= -538.873059
Sum of electronic and thermal Enthalpies= -538.872115
Sum of electronic and thermal Free Energies= -538.928115
HF=-539.106178
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-539.729223

DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-538.597013782666

TS-Giese Addition[6]

C	-4.69165200	1.84902800	-1.73802500
H	-5.28111000	2.60791500	-1.21981600
H	-5.21043100	1.21904700	-2.46399700
C	-3.39040500	1.66195400	-1.46198800
H	-2.79537100	0.89914000	-1.97003000
C	-2.67715100	2.50976700	-0.48526400
O	-3.15743900	3.41551200	0.16897200
O	-1.37793100	2.16018200	-0.39440400
C	-0.57987600	2.91888600	0.51388400
H	-0.96746900	2.83628600	1.54132200
H	0.43349000	2.50264900	0.45617900
H	-0.57036300	3.98362300	0.23248000
C	-4.80844000	4.00539100	-3.61692300
C	-6.19806700	4.46208500	-3.34205100
H	-4.55103400	3.30722800	-4.41491600
H	-6.90686600	3.64376800	-3.54595000
H	-6.48734500	5.30627300	-4.01318900
C	-4.19799900	5.91634700	-2.41855800
C	-5.23983500	5.49600400	-1.39134200
H	-3.29996000	6.29972100	-1.91392600
H	-4.58984500	6.71163300	-3.07967800
H	-5.58422700	6.38913800	-0.84087500
H	-4.76591600	4.80589100	-0.67437700
O	-3.78531600	4.80492100	-3.21887400
O	-6.37535000	4.86555900	-1.98548400

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.203960 (Hartree/Particle)
Thermal correction to Energy= 0.217102
Thermal correction to Enthalpy= 0.218046
Thermal correction to Gibbs Free Energy= 0.162090
Sum of electronic and zero-point Energies= -612.835400
Sum of electronic and thermal Energies= -612.822258
Sum of electronic and thermal Enthalpies= -612.821314
Sum of electronic and thermal Free Energies= -612.877269
HF=-613.0393598
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-613.7473919
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-612.502054523782

TS-Metalation[6]

C	-2.24946100	1.47118100	-0.17244200
C	-3.10493900	2.47250500	0.30153700
C	-2.59856000	3.73619500	0.63055700
C	-1.22001400	3.94119900	0.45663500
C	-0.42393400	2.90211100	-0.01500500
C	-2.69859200	0.10514000	-0.54693700
C	-4.02690200	-0.33357300	-0.49260400
C	-4.34915800	-1.64380400	-0.86907800
C	-3.29691100	-2.47164500	-1.29570100
C	-1.99927400	-1.97161400	-1.32498300
H	-4.17037400	2.27368200	0.41905500
H	-0.76476200	4.90672400	0.68722200
H	0.65152400	3.02071000	-0.16751900
H	-4.81709300	0.33943100	-0.15898400
H	-3.48669800	-3.50200700	-1.60369100
H	-1.14577000	-2.56994000	-1.65404700
N	-0.92563000	1.69782000	-0.31771400
N	-1.71460300	-0.71774500	-0.95880900
Br	1.37705200	-1.08726700	-2.54884700
Ni	0.17559600	0.01664700	-0.77813000
C	0.61229300	-0.62345800	1.04471000
C	0.01554900	-0.12406000	2.21972000
C	1.53642200	-1.67797900	1.20054900
C	0.32637200	-0.62397700	3.48528600
H	-0.71312800	0.69062400	2.15536000
C	1.86774600	-2.19763800	2.45243800
H	2.01575600	-2.09664600	0.31012800
H	-0.14736300	-0.21359400	4.38079100
H	2.59278900	-3.01019500	2.54530100
C	1.26365000	-1.66830600	3.61095400
C	-3.48410000	4.83019000	1.16027300
H	-3.32477400	5.76713400	0.60371800
H	-4.54848600	4.56327500	1.09907900
H	-3.24374700	5.03842200	2.21628100
C	-5.76291500	-2.15532300	-0.82434100
H	-6.08906300	-2.47815100	-1.82644300
H	-5.83485200	-3.03517500	-0.16464600
H	-6.46540500	-1.39215000	-0.46118700
C	1.59457500	-2.18895900	4.90558700
N	1.86012800	-2.60940000	5.95651700
C	3.00171600	1.45021900	-0.13012100
C	3.27714800	1.31477200	1.33034600
H	2.86959300	0.62767100	-0.83413800
H	3.75265900	0.34675600	1.54142900
H	2.32868100	1.34102700	1.91250100
C	3.53882600	3.75565600	-0.04877800
C	3.61212900	3.61553800	1.46405500
H	4.55836900	3.71624900	-0.47230400
H	3.05987500	4.69964300	-0.34813200
H	2.60149400	3.75776200	1.90437500
H	4.27858100	4.38697300	1.88065200
O	2.76497000	2.69618500	-0.63449000
O	4.13450000	2.35184500	1.81100000

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.412592 (Hartree/Particle)
Thermal correction to Energy= 0.442942
Thermal correction to Enthalpy= 0.443886
Thermal correction to Gibbs Free Energy= 0.343728
Sum of electronic and zero-point Energies= -5285.842586
Sum of electronic and thermal Energies= -5285.812236
Sum of electronic and thermal Enthalpies= -5285.811292
Sum of electronic and thermal Free Energies= -5285.911450
HF=-5286.2551776
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5288.1105167

DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5283.131701722762

TS-Giese Addition[7]

C	-4.56371100	1.72022600	-1.00478300
H	-4.63357000	2.66461600	-0.46224700
H	-5.49576600	1.24639500	-1.31855700
C	-3.39208000	1.02814800	-1.01219800
H	-3.31077500	0.02799100	-1.44403000
C	-2.16250400	1.62991700	-0.48622600
O	-2.04775600	2.76332500	-0.04906900
O	-1.11872300	0.76981300	-0.54576500
C	0.13058000	1.26017400	-0.06486600
H	0.06070900	1.54927900	0.99566900
H	0.85178800	0.44208700	-0.18648100
H	0.45689200	2.14142100	-0.64001900
C	-4.64218100	3.25981600	-2.89806800
C	-3.23342000	3.33701700	-3.40963300
C	-3.19274100	4.61460600	-2.53905300
H	-5.57320500	2.89029400	-3.34029700
H	-3.13963100	3.52059300	-4.49339000
H	-2.55623700	2.51706300	-3.12096600
H	-2.97443300	5.56438100	-3.04948400
H	-2.62214100	4.51846100	-1.60436700
O	-4.62985300	4.48270900	-2.28266800

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.170115 (Hartree/Particle)
Thermal correction to Energy= 0.180942
Thermal correction to Enthalpy= 0.181886
Thermal correction to Gibbs Free Energy= 0.131901
Sum of electronic and zero-point Energies= -498.401183
Sum of electronic and thermal Energies= -498.390356
Sum of electronic and thermal Enthalpies= -498.389412
Sum of electronic and thermal Free Energies= -498.439397
HF=-498.5712981
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-499.1472031
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-498.118336065888

TS-Giese Addition[8]

C	-4.67993500	1.36069500	-1.13495400
H	-4.98424400	2.12167900	-0.41604000
H	-5.46685300	0.77978300	-1.61845200
C	-3.37678000	0.98335600	-1.20559900
H	-3.04845700	0.15537100	-1.83835300
C	-2.33556800	1.72158700	-0.48044600
O	-2.50337700	2.71611400	0.20368300
O	-1.11431600	1.16688100	-0.66340000
C	-0.02582500	1.80827000	-0.00280000
H	-0.17132700	1.80974300	1.08911300
H	0.87428100	1.23692200	-0.26277100
H	0.07864100	2.85301900	-0.33626500
C	-5.15080000	2.99845200	-2.93100700
C	-5.23735700	4.45998200	-2.51299400
C	-6.74781800	4.24149000	-2.82285600
H	-4.39830500	2.50693000	-3.55875600
H	-7.17300100	4.85458700	-3.63344300
H	-7.42471000	4.24044000	-1.95332500
O	-6.47449900	2.88840300	-3.28737700
C	-4.52814900	5.40219700	-3.49400600
H	-4.82119300	6.44909000	-3.30881700
H	-3.43579200	5.32850600	-3.36976300
H	-4.77162900	5.15546300	-4.53960700
C	-4.89593600	4.81048800	-1.06425800
H	-3.84491700	4.57656200	-0.83955400
H	-5.07080900	5.88306200	-0.87890000
H	-5.51482500	4.24053600	-0.35555300

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.225588 (Hartree/Particle)
Thermal correction to Energy= 0.239375
Thermal correction to Enthalpy= 0.240319
Thermal correction to Gibbs Free Energy= 0.182969
Sum of electronic and zero-point Energies= -576.924090
Sum of electronic and thermal Energies= -576.910303
Sum of electronic and thermal Enthalpies= -576.909358
Sum of electronic and thermal Free Energies= -576.966709
HF=-577.1496777
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-577.8123863
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-576.601893362912

TS-Giese Addition[9]

C	-4.47761200	1.65410900	-1.03437200
H	-4.53546900	2.67068300	-0.64314400
H	-5.40129000	1.19523900	-1.39263600
C	-3.32158400	0.96638600	-0.99147600
H	-3.24569700	-0.06979700	-1.32963200
C	-2.08560400	1.59478500	-0.49074300
O	-1.94732700	2.77122100	-0.20419700
O	-1.07939300	0.70254200	-0.39351400
C	0.17224500	1.20499500	0.07405200
H	0.07071800	1.63888500	1.08100000
H	0.85869300	0.34957900	0.09713500
H	0.55979200	1.98435500	-0.60091200
C	-4.64914400	3.57354200	-3.12600000
O	-4.64923000	4.61544100	-2.24473300
H	-5.57791400	3.42486000	-3.69213400
C	-3.30265300	5.09763900	-2.11300800
C	-2.49885700	4.23646000	-3.10752500
H	-3.29401400	6.17112400	-2.35880600
H	-2.95438800	4.94280700	-1.08159300
H	-1.88659900	4.82452600	-3.80568500
H	-1.86250000	3.51312000	-2.57628200
O	-3.50459200	3.54709400	-3.85940500

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.175839 (Hartree/Particle)

Thermal correction to Energy= 0.187887
Thermal correction to Enthalpy= 0.188831
Thermal correction to Gibbs Free Energy= 0.134762
Sum of electronic and zero-point Energies= -573.584642
Sum of electronic and thermal Energies= -573.572595
Sum of electronic and thermal Enthalpies= -573.571650
Sum of electronic and thermal Free Energies= -573.625720
HF=-573.7604816
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-574.4271296
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-573.274376740306

TS-Metalation[9]

C	-2.45612600	1.58816400	0.03812200
C	-3.46781100	2.41729900	0.53529000
C	-3.15700500	3.69157200	1.02718300
C	-1.80992800	4.08579300	0.98629400
C	-0.85052900	3.20999800	0.48648700
C	-2.69558500	0.23220900	-0.52084200
C	-3.95269800	-0.37706600	-0.60828700
C	-4.07514800	-1.65858500	-1.16095600
C	-2.90116400	-2.28130800	-1.61744100
C	-1.68351200	-1.61948300	-1.49796200
H	-4.50354000	2.07705900	0.54092000
H	-1.50498700	5.07146600	1.34410000
H	0.20831900	3.47300500	0.44125200
H	-4.84223100	0.13982700	-0.24750200
H	-2.93427200	-3.27766100	-2.06315800
H	-0.74215000	-2.05713200	-1.84008000
N	-1.16681400	1.99087000	0.03046000
N	-1.58980900	-0.39858100	-0.96212400
Br	1.64665300	-0.09393400	-2.31193500
Ni	0.16886700	0.52299100	-0.51326100
C	0.49596200	-0.35677400	1.23432700
C	-0.07772000	0.05642800	2.45286600
C	1.27136700	-1.53376600	1.26201800
C	0.11327200	-0.64817500	3.64114500
H	-0.68674800	0.96496100	2.48369800
C	1.48173400	-2.25909700	2.43591100
H	1.73069900	-1.89011400	0.33404300
H	-0.33801600	-0.30274500	4.57484400
H	2.09180800	-3.16595400	2.43068100
C	0.90063200	-1.81769500	3.64081400
C	-4.21441100	4.60235900	1.58759600
H	-4.08030700	4.71785500	2.67617400
H	-4.13975200	5.60857700	1.14612600
H	-5.22733200	4.21523400	1.40843700
C	-5.40547900	-2.35367600	-1.25746700
H	-5.42302100	-3.23894600	-0.60030500
H	-6.23550300	-1.69490900	-0.96596300
H	-5.58615200	-2.71156700	-2.28344100
C	1.10464100	-2.55122800	4.85572500
N	1.26643000	-3.14604800	5.84169100
C	2.33060400	2.46503600	1.81363000
H	2.19945800	3.12460100	2.68401400
C	3.70799400	1.18239600	0.60409700
C	3.43201600	2.46242800	-0.18659500
H	4.76222200	0.87549100	0.60746700
H	3.07401000	0.35559300	0.24720300
H	4.30569300	3.13595100	-0.22710100
H	3.06235900	2.25612400	-1.20035100
O	2.39209800	3.09182200	0.58475600
O	3.32864400	1.54788900	1.93644600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.384646 (Hartree/Particle)
Thermal correction to Energy= 0.413824
Thermal correction to Enthalpy= 0.414768
Thermal correction to Gibbs Free Energy= 0.317332
Sum of electronic and zero-point Energies= -5246.589018
Sum of electronic and thermal Energies= -5246.559840
Sum of electronic and thermal Enthalpies= -5246.558896
Sum of electronic and thermal Free Energies= -5246.656332
HF=-5246.9736636
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5248.7864111
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5243.899080103147

TS-Giese Addition[10]

C	-4.73204200	1.33849200	-1.83477700
H	-5.34749300	1.64252000	-0.98716900
H	-5.22509200	0.74921400	-2.61048300
C	-3.37245300	1.23494700	-1.65557600
H	-2.72230000	0.76283300	-2.39566300
C	-2.72866000	1.86218500	-0.50305800
O	-3.28691100	2.52085100	0.36115800
O	-1.39079800	1.64712300	-0.49291700
C	-0.66721200	2.23247300	0.58619400
H	-1.02504200	1.85248600	1.55622900
H	0.38510200	1.95830300	0.43852500
H	-0.77613400	3.32896700	0.58649600
C	-5.21326500	3.28730600	-2.86542900
C	-3.97892700	4.16334200	-2.79407500
H	-5.48693700	2.81846000	-3.81456600
C	-5.37725100	4.84849000	-0.84329700
C	-4.22764800	5.28576900	-1.75659700
H	-3.76092600	4.58790300	-3.78882300
H	-3.09999500	3.55308900	-2.52679700
H	-5.90420400	5.68470700	-0.36278800
H	-5.03242700	4.13565700	-0.08006900
H	-4.50942600	6.21576600	-2.27527400
H	-3.32545600	5.49513000	-1.16098700
S	-6.54983800	3.96554400	-1.96046700

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.196833 (Hartree/Particle)
Thermal correction to Energy= 0.208915
Thermal correction to Enthalpy= 0.209859
Thermal correction to Gibbs Free Energy= 0.156332

Sum of electronic and zero-point Energies= -860.626752
Sum of electronic and thermal Energies= -860.614670
Sum of electronic and thermal Enthalpies= -860.613726
Sum of electronic and thermal Free Energies= -860.667252
HF=-860.8235849
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-861.4921794
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-860.011606748139

TS-Metalation[10]

C	-2.50763500	1.59081900	0.14278000
C	-3.55631900	2.39608800	0.60149200
C	-3.28968400	3.65135300	1.16286500
C	-1.94515400	4.05005900	1.23539100
C	-0.94963200	3.19935600	0.76536600
C	-2.69905600	0.24961800	-0.46724200
C	-3.94451100	-0.35656500	-0.66862400
C	-4.02098600	-1.62670300	-1.25497500
C	-2.81333100	-2.24054500	-1.62710000
C	-1.60989900	-1.58126600	-1.39813100
H	-4.58731700	2.04986200	0.52663900
H	-1.67018200	5.01820700	1.65923300
H	0.11013600	3.46658900	0.81414400
H	-4.86089900	0.15433200	-0.37226700
H	-2.80904300	-3.22735200	-2.09469800
H	-0.64440000	-2.01069500	-1.67714200
N	-1.22388600	2.00138100	0.23338900
N	-1.56021100	-0.37163900	-0.83138000
Br	1.70684400	-0.07152700	-2.00483900
Ni	0.16321800	0.56207100	-0.26924600
C	0.41426600	-0.29630200	1.50176700
C	-0.12013500	0.18122200	2.71472500
C	1.12901900	-1.51089200	1.55630500
C	0.05546500	-0.49439800	3.92340000
H	-0.68730200	1.11741300	2.72732500
C	1.31913000	-2.21010000	2.74864400
H	1.56107800	-1.91523100	0.63522500
H	-0.36330400	-0.09761100	4.85179200
H	1.88208500	-3.14681200	2.76349100
C	0.78209100	-1.70161800	3.94842200
C	-4.38920400	4.53792000	1.67906500
H	-5.38495800	4.12419900	1.46672400
H	-4.29616100	4.66785400	2.77000800
H	-4.32415200	5.54166300	1.22977800
C	-5.33852900	-2.31959900	-1.46974000
H	-5.42942100	-3.18419600	-0.79105100
H	-6.19014300	-1.65008600	-1.28395000
H	-5.41475900	-2.70804200	-2.49737700
C	0.96838600	-2.40730700	5.18283700
N	1.11707100	-2.97907500	6.18424600
C	2.98964700	1.89141100	1.83946200
H	2.35165700	1.63969200	2.68701900
C	4.59563100	1.70814300	0.01775900
C	3.67501700	2.82323400	-0.48947500
H	5.48877600	2.15169100	0.48851700
H	4.92678200	1.07757100	-0.82232100
H	4.21206400	3.67485800	-0.93062200
H	2.94511700	2.43165900	-1.21285100
C	3.79910300	0.90126500	1.05758100
H	4.45718300	0.30275500	1.71152800
H	3.13023400	0.18785900	0.53995700
S	2.74737000	3.40705400	1.00313600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.404083 (Hartree/Particle)
Thermal correction to Energy= 0.434200
Thermal correction to Enthalpy= 0.435145
Thermal correction to Gibbs Free Energy= 0.335248
Sum of electronic and zero-point Energies= -5533.639171
Sum of electronic and thermal Energies= -5533.609053
Sum of electronic and thermal Enthalpies= -5533.608109
Sum of electronic and thermal Free Energies= -5533.708005
HF=-5534.0432533
UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5535.8594203
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-5530.651681138575

TS-Giese Addition[11]

C	-4.50349200	2.29905400	-0.05032900
H	-4.25346900	3.16894900	0.56065800
H	-5.55761800	2.02530600	-0.13216800
C	-3.51584600	1.41802700	-0.38385600
H	-3.72665900	0.46780500	-0.87936900
C	-2.11004300	1.81143600	-0.25064200
O	-1.71048100	2.85958600	0.23445400
O	-1.28091500	0.89605500	-0.79231500
C	0.09200900	1.27628600	-0.90440800
H	0.51294900	1.53897900	0.07806400
H	0.61703500	0.40867900	-1.32339100
H	0.18437700	2.13919200	-1.58185900
C	-4.51956200	3.82902000	-1.87450000
C	-5.10830800	3.07739700	-3.04376600
H	-5.04787300	4.61373700	-1.33025200
C	-3.87915400	2.41233500	-3.69476100
H	-5.59154400	3.78654400	-3.74162300
H	-5.88249500	2.36001900	-2.73350500
H	-3.85523800	2.46815200	-4.79232700
H	-3.78083400	1.35071400	-3.41832000
N	-3.16932600	3.98426700	-2.12019400
H	-2.52859700	4.41892400	-1.46004500
C	-2.67477700	3.13987600	-3.09961600
O	-1.50149100	3.00791500	-3.38625600

UB3LYP-D3/def2-SVP-CPCM(benzene)
Zero-point correction= 0.194092 (Hartree/Particle)
Thermal correction to Energy= 0.206218
Thermal correction to Enthalpy= 0.207162
Thermal correction to Gibbs Free Energy= 0.154687
Sum of electronic and zero-point Energies= -591.850463

Sum of electronic and thermal Energies= -591.838336
Sum of electronic and thermal Enthalpies= -591.837392
Sum of electronic and thermal Free Energies= -591.889868
HF=-592.0445545

UB3LYP-D3/def2-TZVPP-CPCM(benzene)//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-592.7219999
DLPNO-CCSD(T)/def2-TZVPP//UB3LYP-D3/def2-SVP-CPCM(benzene)
HF=-591.496666329300

Appendix 3: Computational Methods, Results, Coordinates and Energies from Chapter 4 (Mechanistic Study of Enantioselective Three-Component Carboarylation of Alkenes Enabled by Visible-Light Dual Ni/Photoredox Catalysis)

A3.1 Methods

All optimizations were carried out without constraints at the (U)B3LYP-D3(BJ)/def2-SVP level of theory in THF solvent using the CPCM implicit solvent model with "opt=noeigen" keyword as implemented in Gaussian16. To compare energetics, we also carried out single point energy calculations using (U)B3LYP-D3(BJ)/def2-TZVPP-CPCM(THF). All structural figures were generated using CLYview. Vibrational frequencies were computed at the same level to obtain thermal corrections (at 298 K; enthalpic and free energy) and to characterize the stationary points as transition states (one and only one imaginary frequency) or minima (zero imaginary frequencies). Exhaustive conformational searches were performed for all intermediates to map out the lowest energy profile, and intrinsic reaction coordinate (IRCs) calculations were undertaken for selected transition state structures to ensure they connected the illustrated ground states.

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 enantiodetermining radical addition step.[230] 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.[355]

A3.2 Supplementary Figures

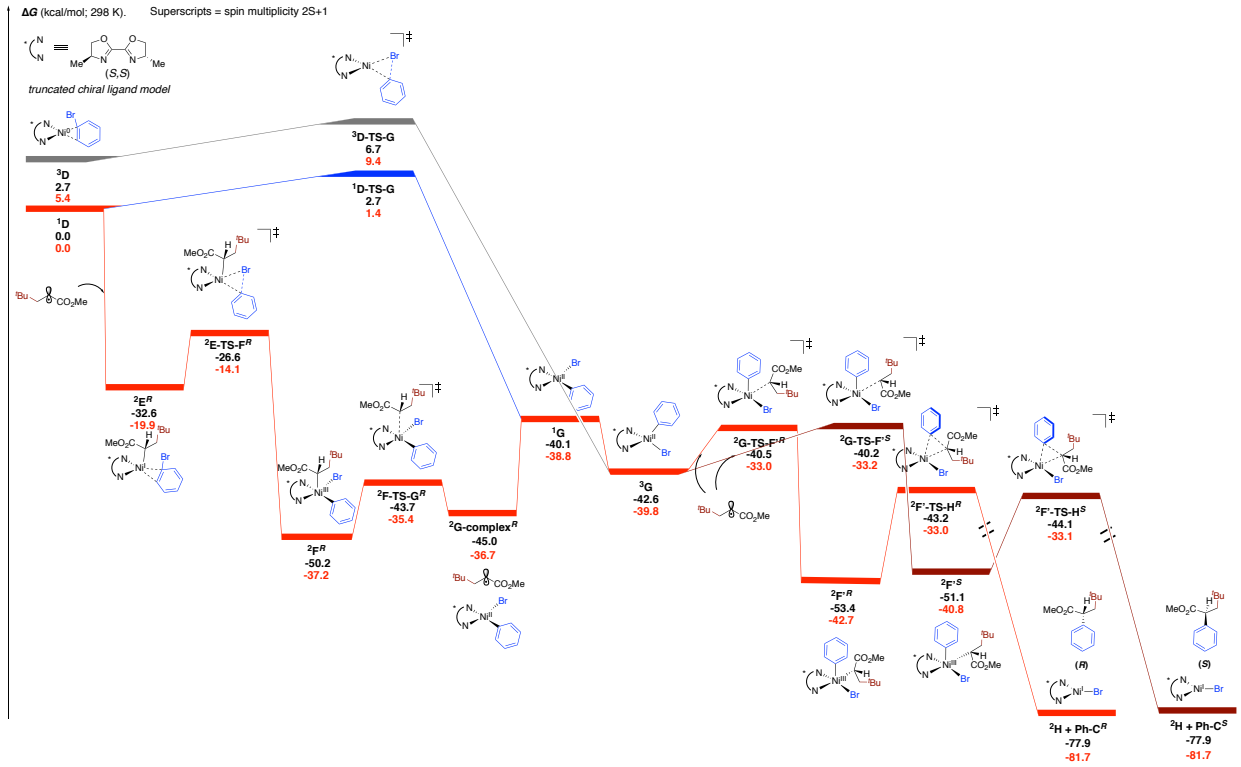


Figure A3.1 Possible mechanistic pathways that lead to the formation of three-component alkylarylation product. Free energy values given were calculated at the UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) (black) and UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) (red) levels of method.

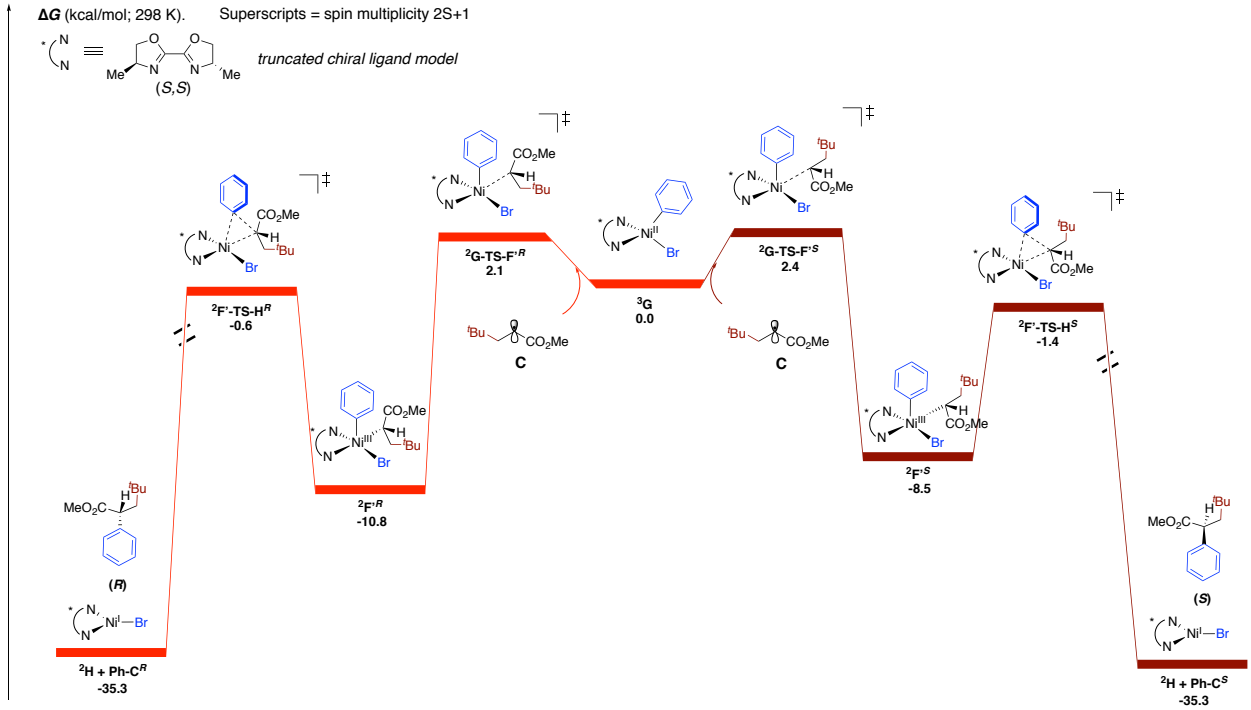


Figure A3.2 Mechanistic pathways that lead to the formation of three-component alkylarylation products with different stereochemistry. Free energy values given were calculated at the UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) level of method.

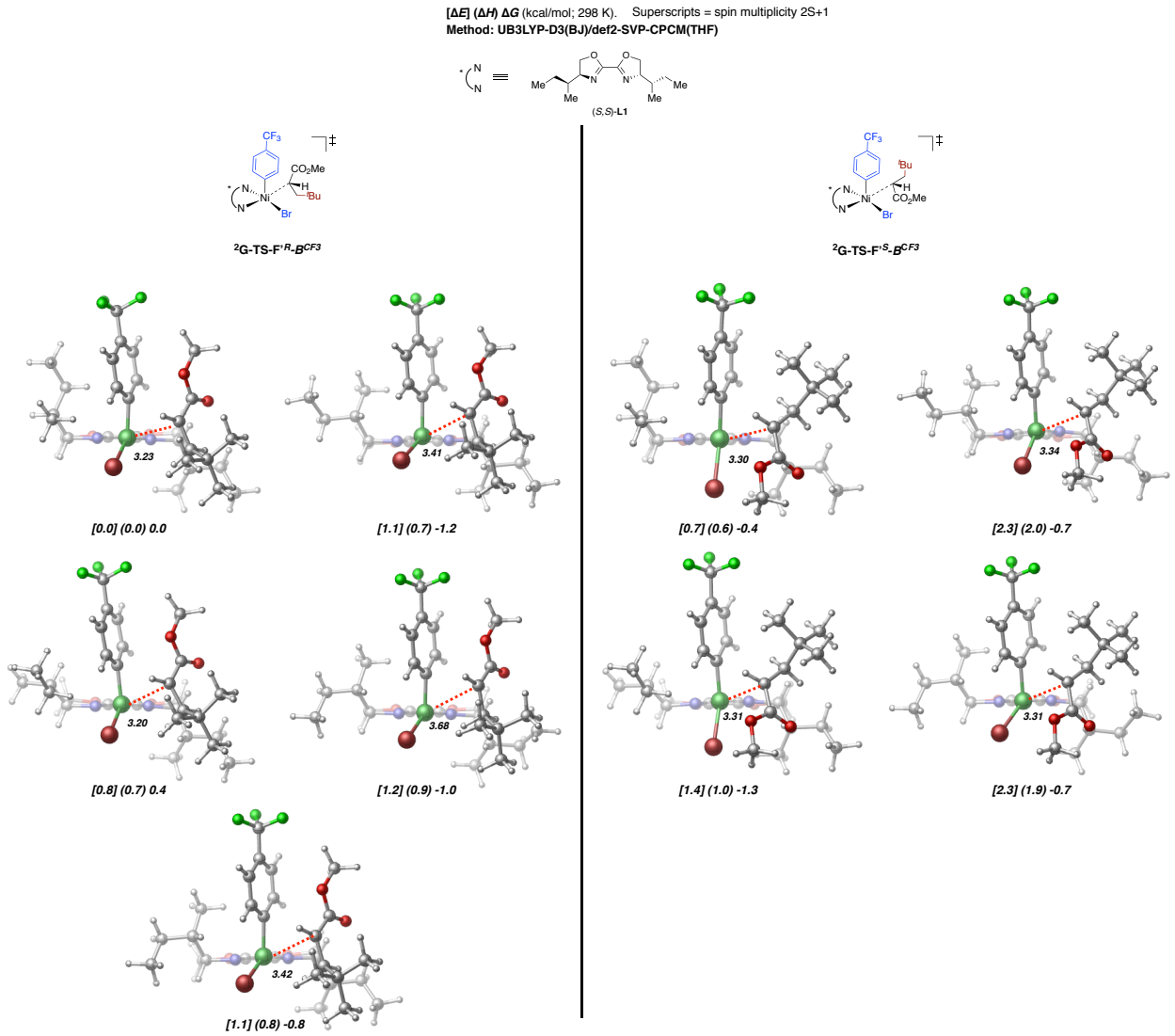


Figure A3.3 Different located conformations of the enantiodetermining radical addition step with full ligand system. Energy values given were calculated at the UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) level of method.

Table A3.1 Enantioselectivity determined by electronic energies, enthalpies and free energies.

Method	*E*		*H*		*G*	
	configuration	ee (%)	configuration	ee (%)	configuration	ee (%)
UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)	*R*	59.5	*R*	54.6	*R*	0.2

The origin of enantioselectivity of this three-component alkylarylation of olefin was explored with focus on the enantiodetermining radical addition step with full ligand (*S,S*)-*sec*-Bu-BiOx **L1** and *p*-CF_3-ArBr as the model system. In particular, nine of the lowest-energy radical

addition transition states were taken into consideration (**Figure A3.3**). Boltzmann calculation was performed based on the electronic energy, enthalpy and free energy values of these conformations. As shown in **Table A3.1**, electronic energy values obtained with the optimization method ([UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)]) predicted the correct enantiomer (*R*-product) albeit with underestimated enantiomeric ratio (~ 80:20 vs. ~95:5 in experiment).

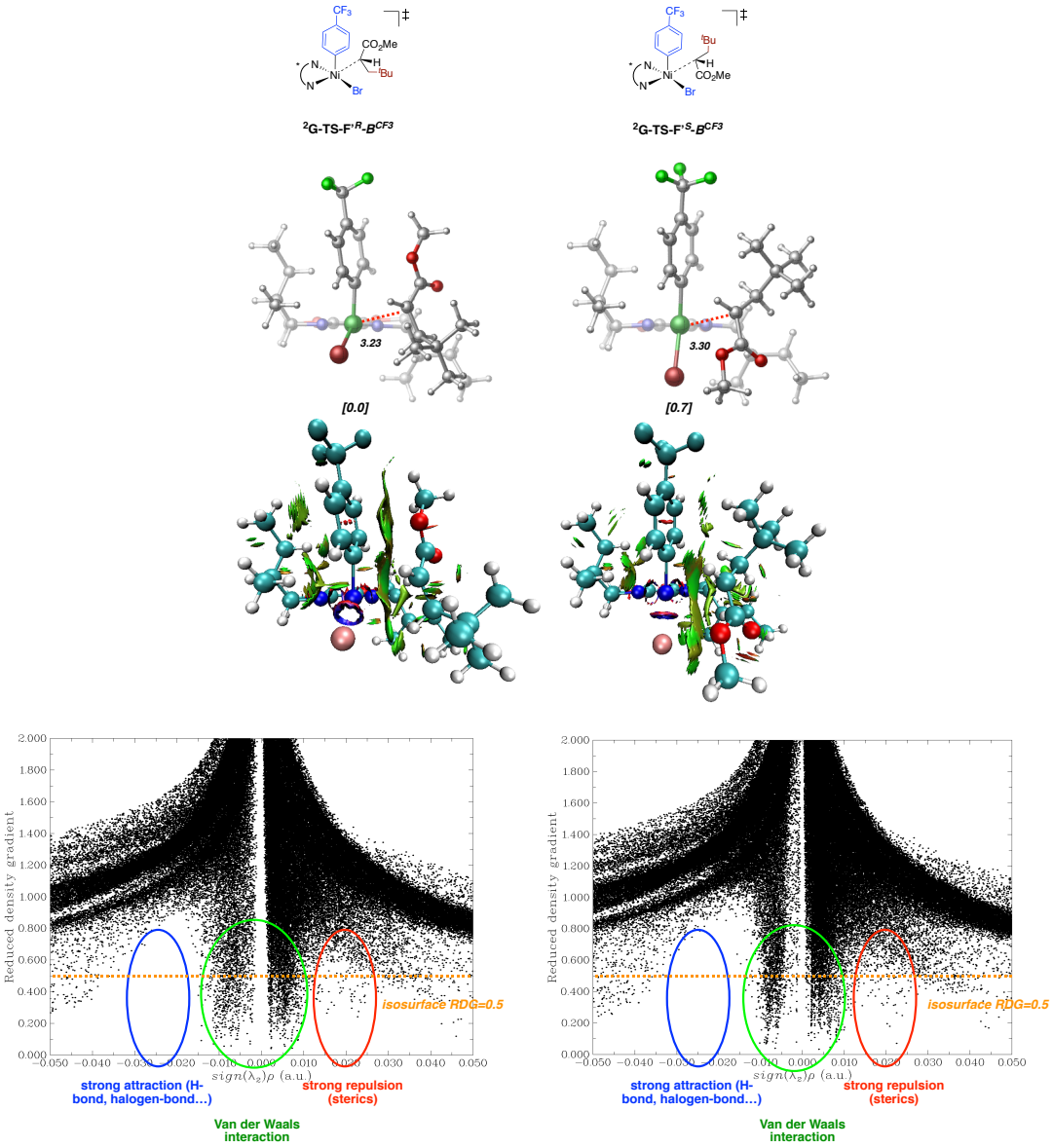
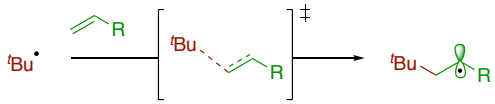


Figure A3.4 Color-filled RDG isosurface and scatter map created from NCI analysis on the lowest-energy radical addition transition states. Electronic energy values given were calculated at the UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) level of method.

From the colored-filled RDG isosurface, it could be seen that both the C-H•••π interaction (between alkyl chain and aryl ring) and the π-π interactions (between aryl ring and ester moiety) are present in the system, thus emphasizing the effect of noncovalent interactions in the entiodetermining radical addition step.



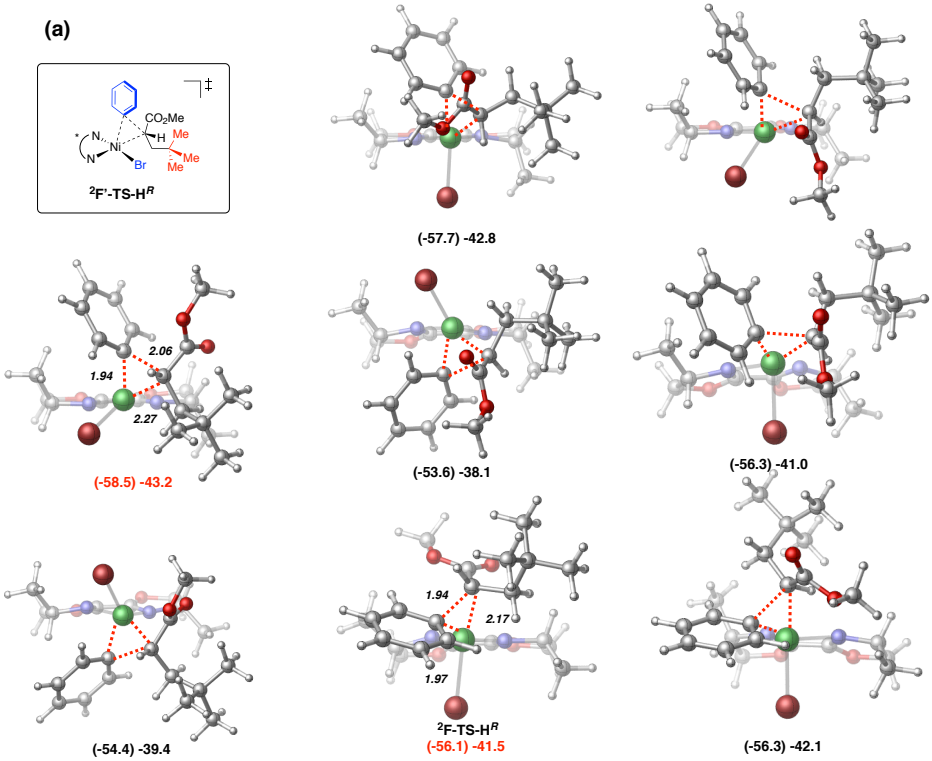
Olefin	50	58	59	60	51	52	53
Barrier	12.7 [a]	12.6	12.5	12.1	11.2	9.9	9.8
ΔG	-5.6	-9.7	-9.0	-8.9	-6.3	-11.9	-12.5
Yield	16%	76%	35%	50%	92%	84%	81%

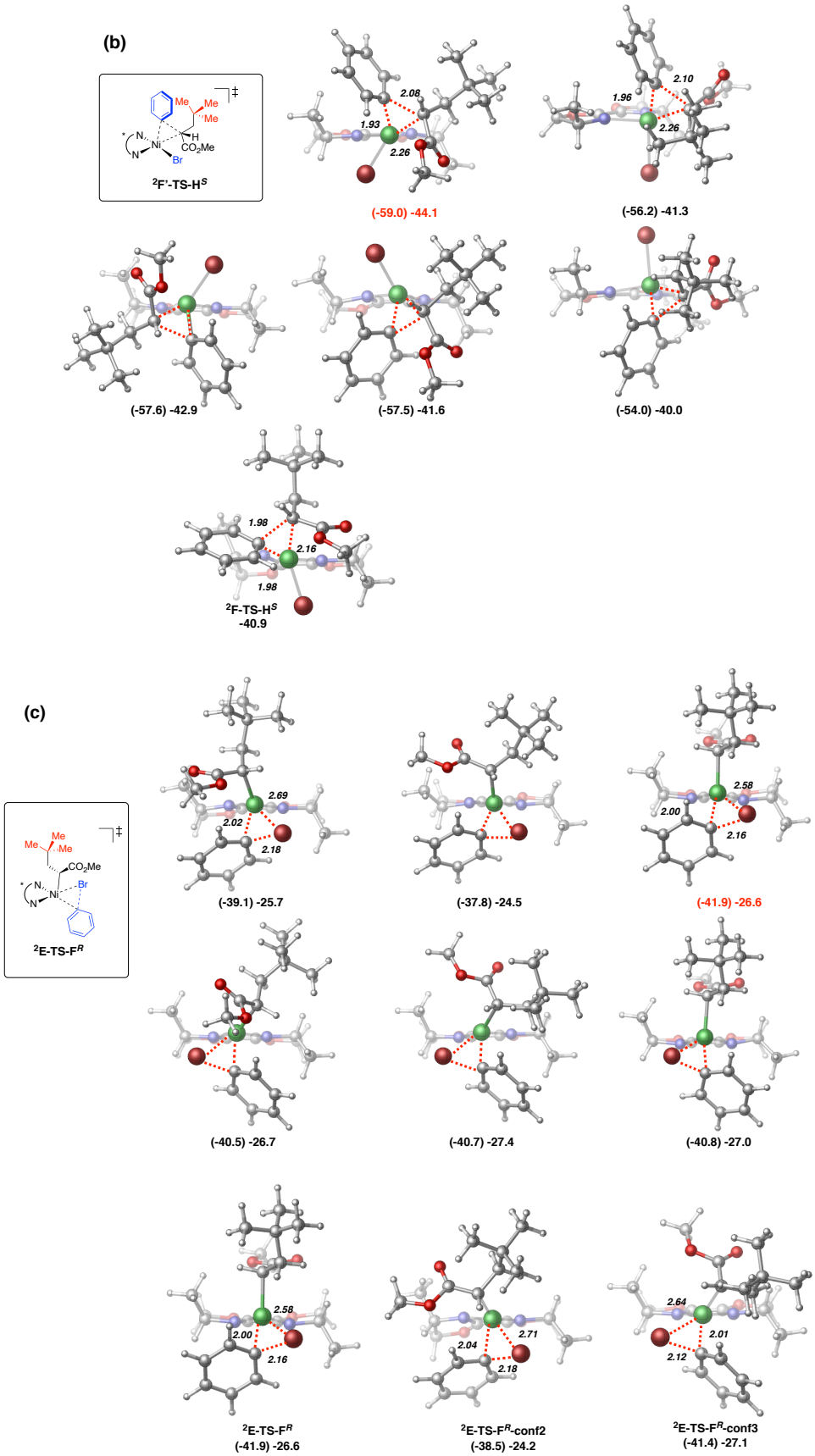
Olefin	57	4	42	49	54	56	55
Barrier	9	8.6	8.6 [b]	8.3	7.8 [c]	7.1	6.9
ΔG	-10.1	-12.3	-12.1	-12.2	-14.2	-11.2	-11
Yield	89%	82%	89%	52%	38%	81%	82%

Figure A3.5 Calculation of Giese addition of *tert*-Bu radical to different olefins. Free energy values given were calculated at the UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) level of method.

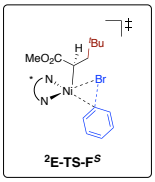
The barrier and the thermodynamic drive of the Giese addition step were calculated between *tert*-butyl radical **A** and a series of different olefins that were tested in experiment as shown in **Figure A3.5** Based on the comparion between the computational results and the experimental yield (**Figure A3.5**), a weak correlation can be found between the calculated barrier and the observed yield. Specifically, olefins found with higher barrier for radical addition (e.g., methyl (*E*)-but-2-enoate, vinyl amines and vinyl ether) generally have lower product yields.

However, the correlation is weak since the selectivity of product (three-component vs two-component) depend on both the barrier for Giese addition and the relative concentration of olefins. Moreover, the calculation of Giese addition only focuses on the applicability of forming α-carbonyl alkyl radical **C**, while possible side reactions (e.g., hydrogen-atom-transfer with solvent THF, β-hydride elimination by Ni catalyst) could occur thus lower the product yield.

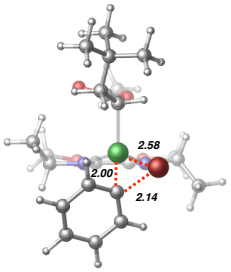



(b)
2F'-TS-H^S
(-59.0) -44.1
(-56.2) -41.3
(-57.6) -42.9
(-57.5) -41.6
(-54.0) -40.0
2F-TS-H^S
-40.9
(c)
2E-TS-F^R
(-39.1) -25.7
(-37.8) -24.5
(-41.9) -26.6
(-40.5) -26.7
(-40.7) -27.4
(-40.8) -27.0
2E-TS-F^R
(-41.9) -26.6
2E-TS-F^R-conf2
(-38.5) -24.2
2E-TS-F^R-conf3
(-41.4) -27.1

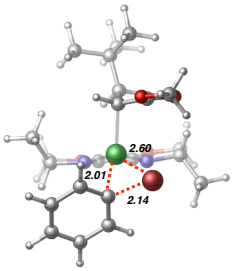
(d)



^{2}E-TS-F^S



^{2}E-TS-F^S
-26.8



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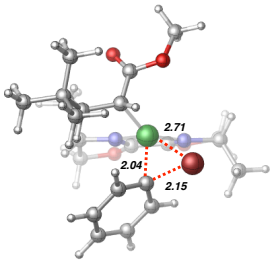
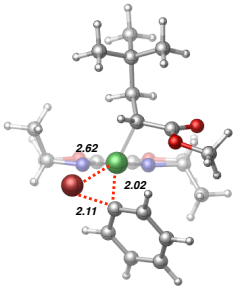
-24.9

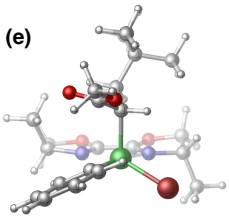


^{2}E-TS-F^S-conf3
-23.1

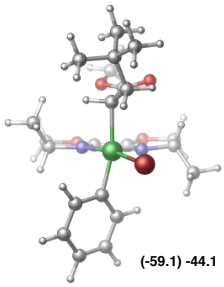


^{2}E-TS-F^S-conf4
-28.1

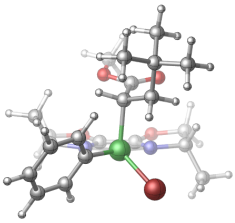
(e)



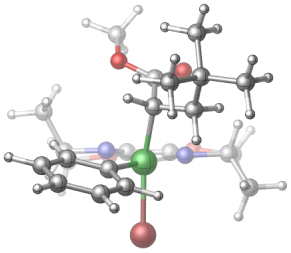
(-57.3) -42.3



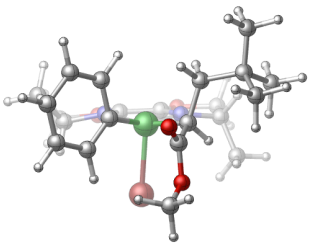
(-59.1) -44.1



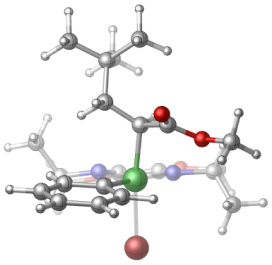
(-66.4) -50.2



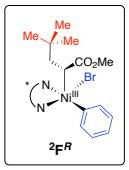
(-68.8) -53.9



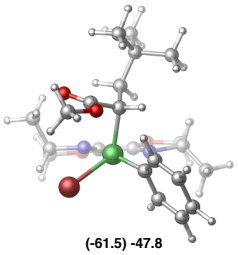
(-65.9) -50.7



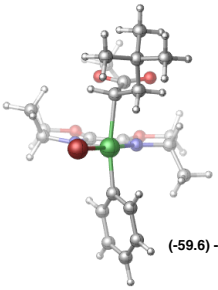
(-67.0) -52.6



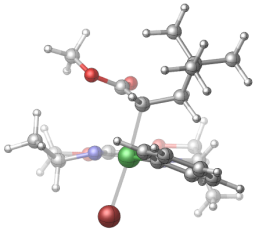
^{2}F^R



(-61.5) -47.8

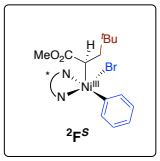


(-59.6) -45.2

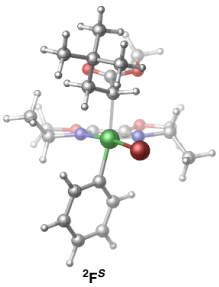


^{2}F^R-conf3
(-64.8) -50.1

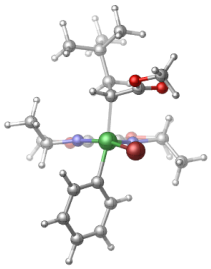
(f)



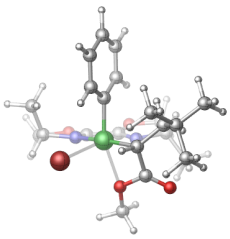
^{2}F^S



^{2}F^S
(-63.1) -47.7



^{2}F^S-conf2
(-57.2) -41.7



^{2}F^S-conf3
(-62.9) -48.8

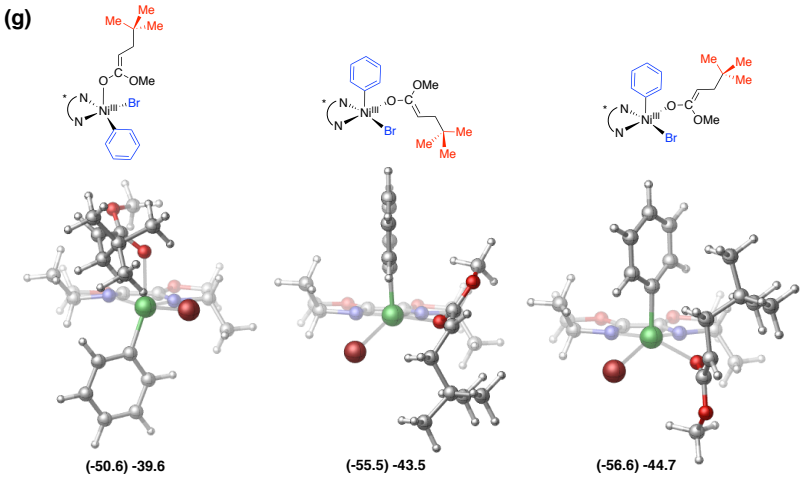


Figure A3.6 Conformational search on key transition states (a) **^{2}F'-TS-H^R** (b) **^{2}F'-TS-H^S** (c) **^{2}E-TS-F^R** (d) **^{2}E-TS-F^S** and intermediates (e) **^{2}F^R** (f) **^{2}F^S** (g) O-coordinated intermediates. Enthalpies (in parenthesis) and free energy values (out of parenthesis) given were calculated at the UB3LYP-D3(BJ)/def2-SVP-CPCM(THF) level of method. Conformations highlighted in red were the lowest-energy conformations of each species.

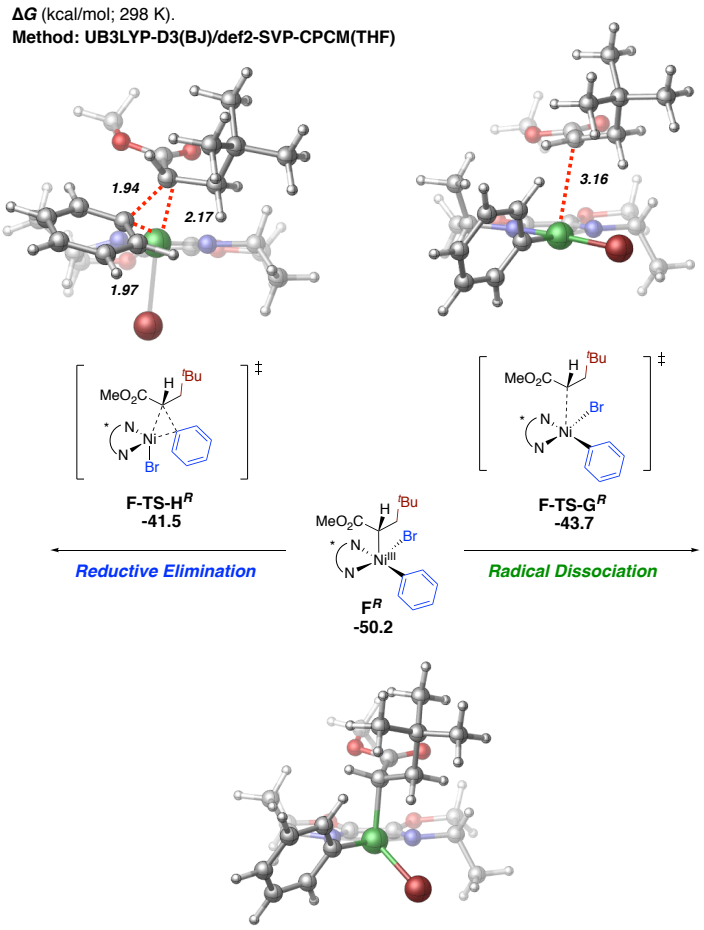


Figure A3.7 Comparison between reductive elimination and radical dissociation pathways from intermediate **F**.

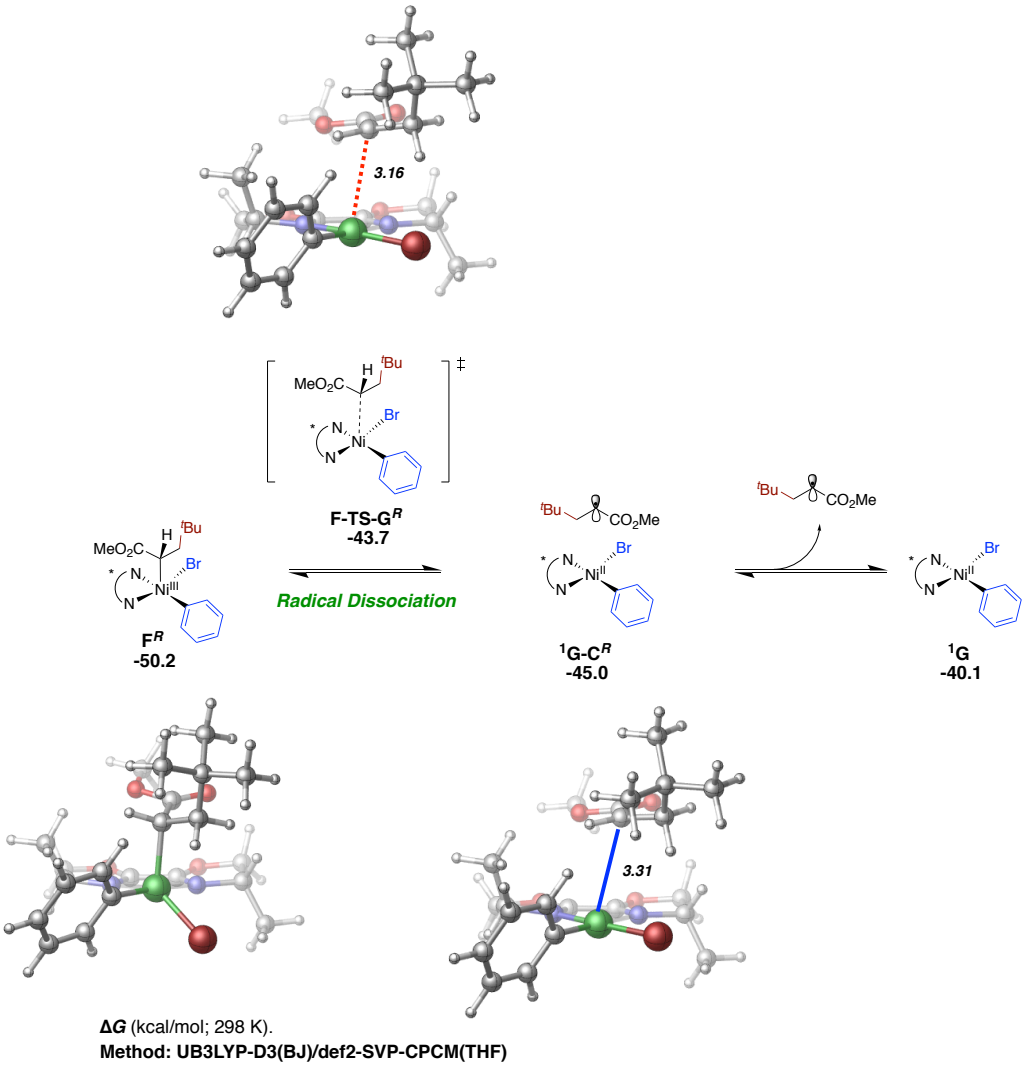


Figure A3.8 Formation of alkyl radical Ni complex resulting from radical dissociation.

The radical addition transition state **F-TS-G** connects to two lower intermediate *complexes* which, as a complex but not as separated structures, are lower in energy than the transition state connecting them. However, decomplexation of the **^{1}G-C** complex to separated **C** and **^{1}G** (as shown in **Figure 4.4**) results in a higher energy.

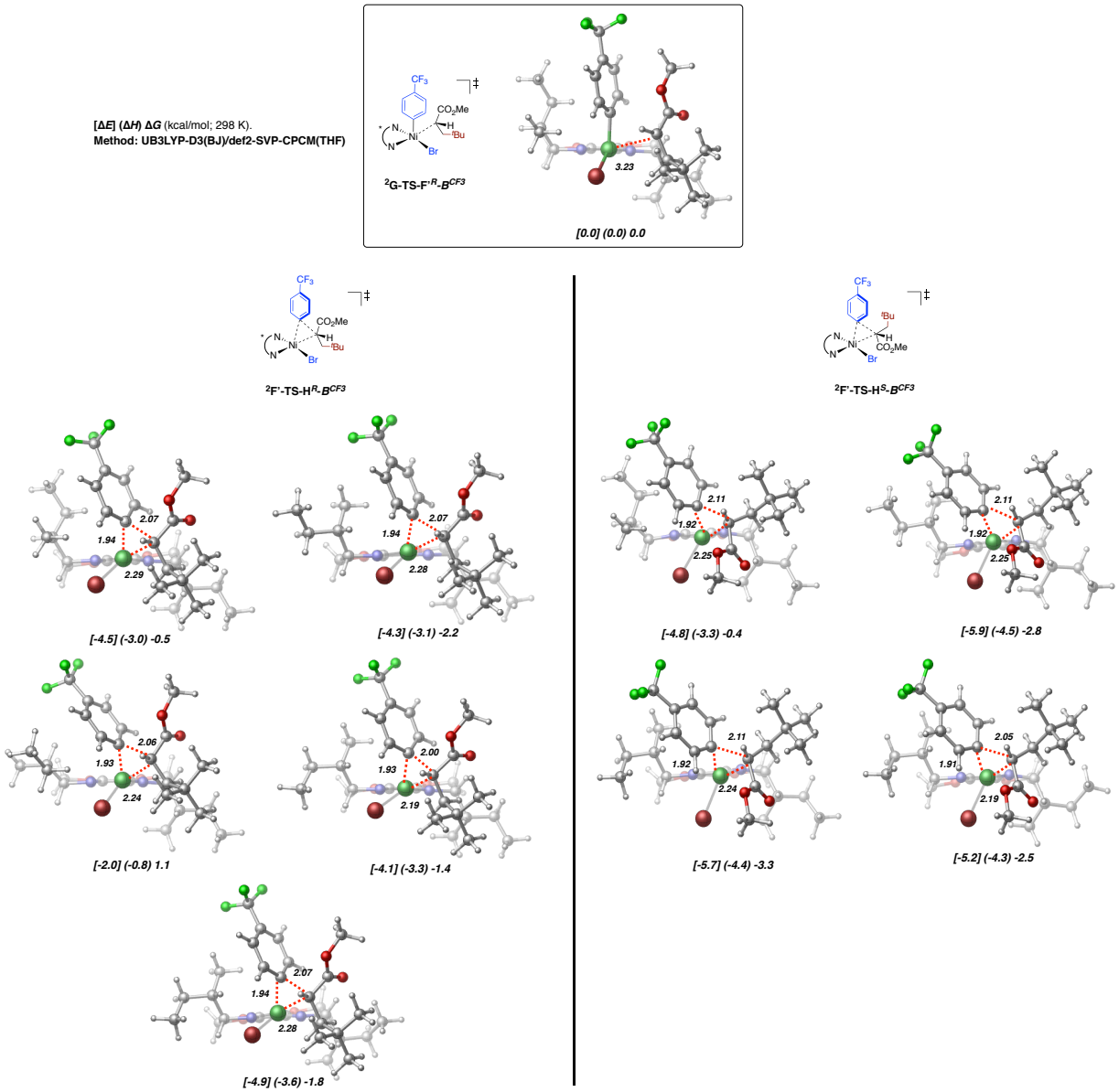


Figure A3.9 Lowest energy diastereomeric reductive elimination transition states with full ligand. All relative energies are with respect to the lowest energy radical addition transition state (inset).

Based on the results obtained with the full ligand on the reductive elimination transition states, they were found all lower in energy than the radical addition (i.e. the lowest-energy conformer of **G-TS-F'** with full ligand). Specifically, the lowest energy reductive elimination step is found to be as much as ~5 kcal/mol lower in energy than the lowest energy radical addition step.

These results suggest that our calculations using the truncated ligand are adequate for exploring the mechanism and, in agreement with experiment, the substituents on the chiral ligand are crucial for inducing enantioselectivity. Moreover, we calculated the predicted enantioselectivity by Boltzmann distribution analysis based on the nine lowest energy conformers of reductive elimination transition states (as shown above) and, contrary to experiment, predicted the opposite stereochemistry. Specifically, the predicted product from the reductive elimination transition states is the *S*-product (calculated ee% = -68.7%). The wrong stereochemistry of product predicted by the analysis on the reductive elimination step, in addition to the much higher energy for the radical addition versus reductive elimination, further supports our finding that radical addition is the stereodetermining step in this reaction system.

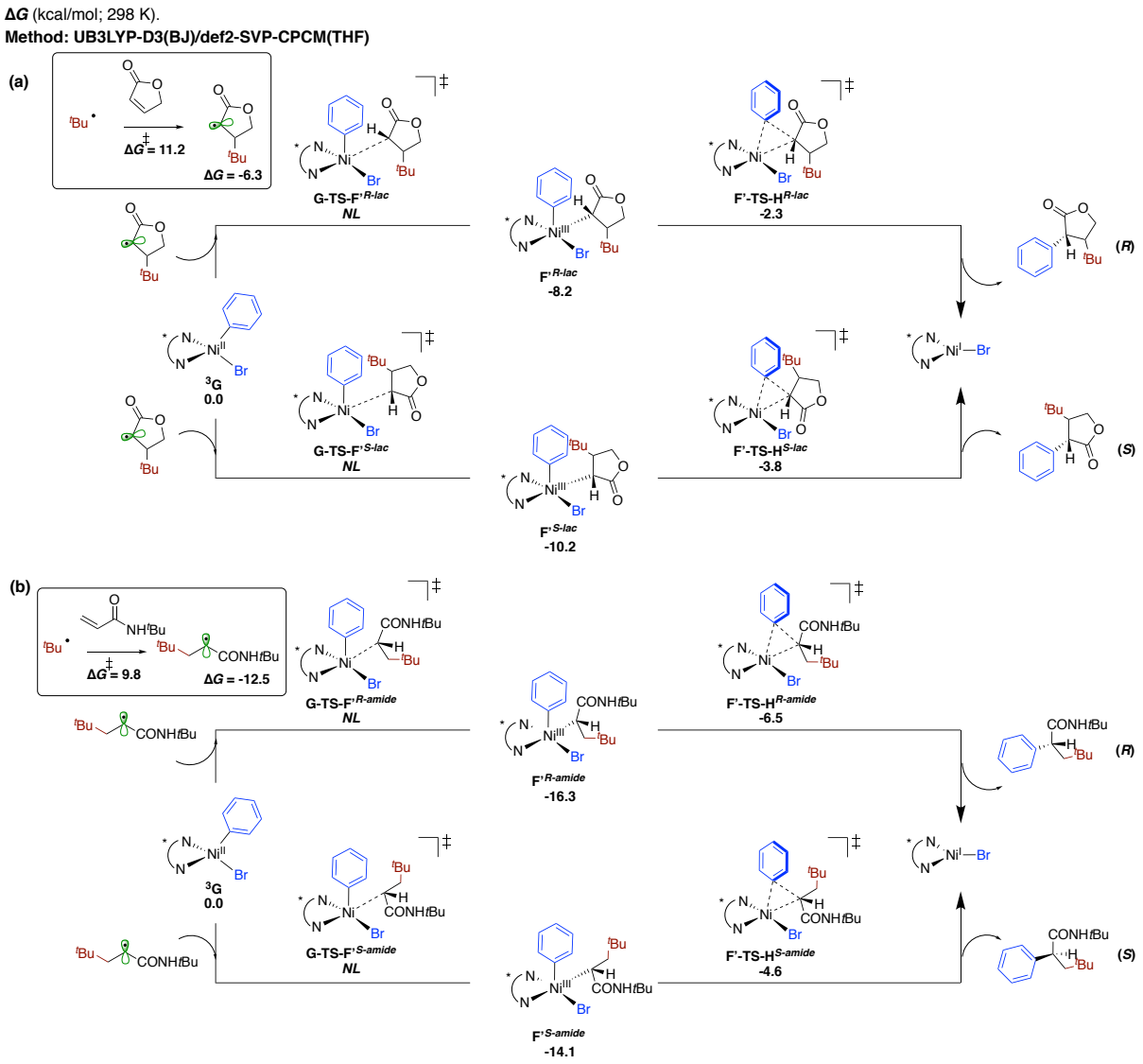


Figure A3.10 Product-forming pathways via radical addition/reductive elimination with internal acrylate and acrylamide as olefin substrates.

We also calculated the radical addition/reductive elimination pathways leading to product formation with internal acrylate **11** and acrylamide since they reveal diminished ee in experiment (15% and 61% ee, respectively, as shown in experiment). The results suggest that, consistent with our model system (methyl acrylate), the formation of Ni(III) intermediate **F'** for both systems is favorable (i.e., downhill in energy by 8-16 kcal/mol), followed by fast reductive elimination (relative barrier of 6-10 kcal/mol) to give the corresponding products. However, given that the

energy for the reductive elimination transition states with respect to the tetrahedral Ni(II) species is lower by 2.3 to 6.5 kcal/mol, these results suggest that the radical addition transition states are likely the stereodetermining step. Unfortunately, all attempts to locate the radical addition transition states failed and formdirectly the Ni(III) intermediates. Presumably, as observed previously for reactions in relatively flat energy surfaces, the low barriers make it very challenging to locate the stationary points corresponding to the radical addition transition states. Overall, the low barriers for the stereodetermining radical addition transition states will imply that achieving enantiocontrol in these substrates will be challenging as observed experimentally. Notably, we observed that in the internal acrylate case, its rigid structure prevents the carbonyl group from staying parallel to phenyl ligand as shown in the transition state of radical addition with methyl acrylate in the manuscript. As for the acrylamide case, the amide group also tends to stay away from the Ph ligand rather than staying parallel thus preventing π-π interactions. Taken together, these results support that noncovalent interactions (in parallel orientation) between acrylate and Ph ligand are important for stereocontrol, and the modification of olefins (by their electronic and steric character) might lead to change in the resulted enantioselectivity.

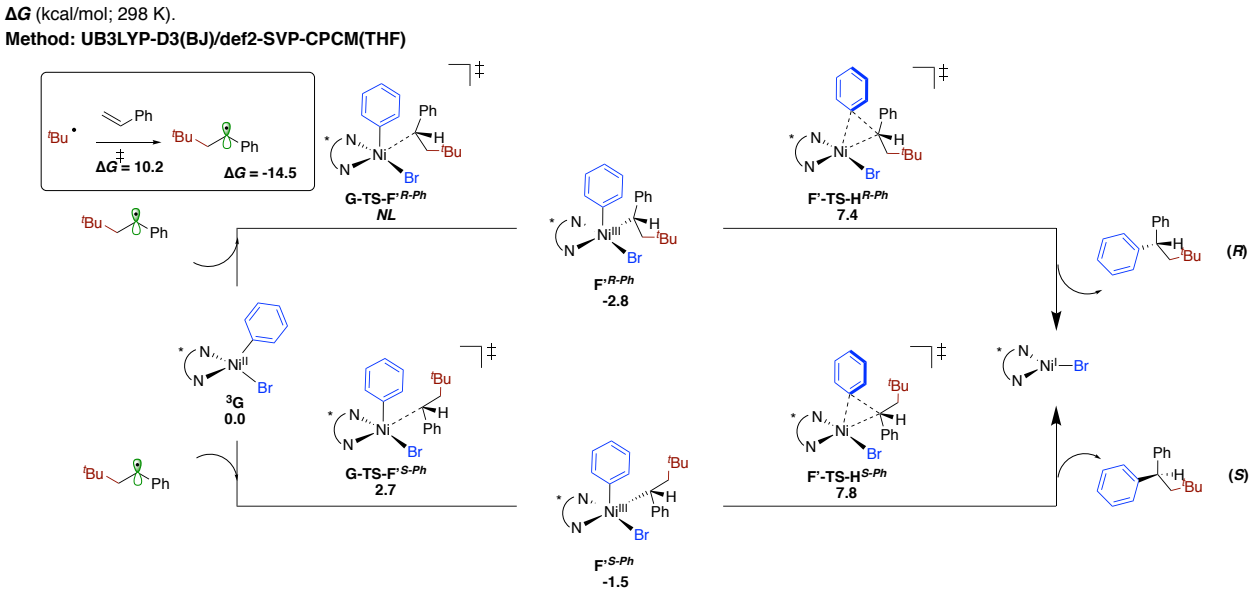


Figure A3.11 Product-forming pathways via radical addition/reductive elimination with styrene as olefin substrate.

We also used computations to gain insights into the observed lower yields and enantioselectivity with styrenyl substrates (as shown before in the experimental part). In particular, we calculated the radical dissociation/reductive elimination pathway with vinylbenzene as a model substrate. Surprisingly, the radical addition transition state was found to be only 2.7 kcal/mol this time (for *S*-pathway, the *R*-pathway cannot be located). Also, it is noticeable that the generated Ni(III) intermediates **F'** in this case were found to be nearly isoenergetic (only 2~3 kcal/mol lower in energy) with the starting tetrahedral Ni(II) species (as comparison, the Ni(III) intermediate in methyl acrylate system is ~10 kcal/mol lower in energy). Moreover, the reductive elimination transition states in this system **F'-TS-H** were found to be ~8 kcal/mol higher than the starting Ni(II) species, while the energy of which was around -1 kcal/mol in the methyl acrylate system. Overall, in contrast to the methyl acrylate system, reductive elimination was found to be *higher in energy* than radical addition in the styrene system, indicating a change in the identity of stereodetermining step. Altogether these suggest that the formation of Ni(III) intermediate in styrene system is

reversible, which might be due to the stability of a secondary benzyl radical formed after Giese addition. Therefore, the formation of product is slower than the acrylate system and is consistent with the observed lower yields of styrenyl substrates in the experiment.

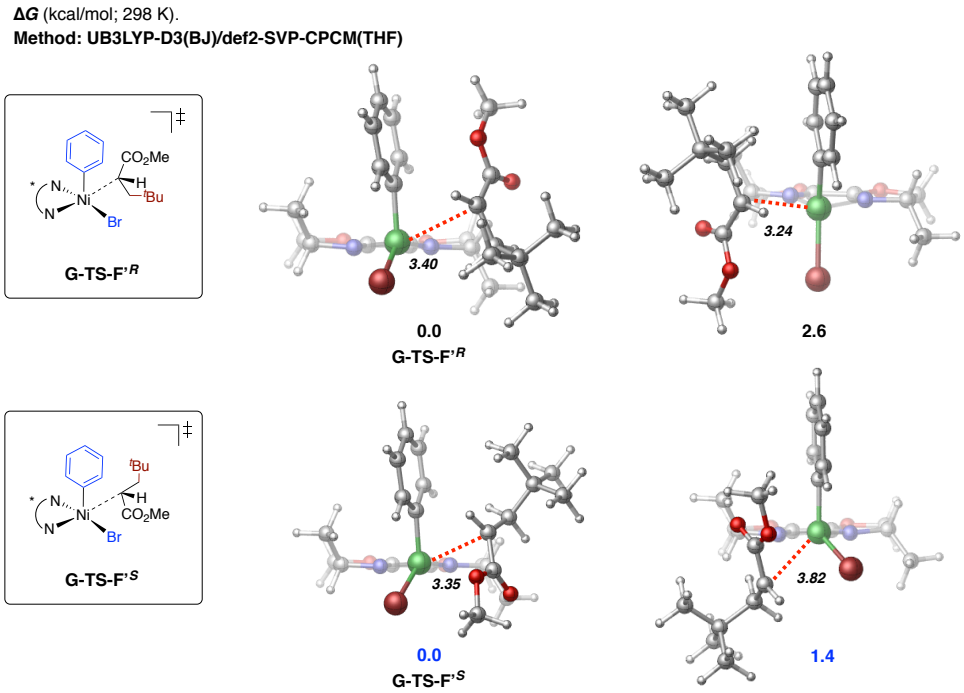


Figure A3.12 Different conformations of radical addition to the tetrahedral Ni species (**G-TS-F'**). Relative free energies were with respect to the lowest-energy radical addition transition states.

A3.3 Coordinates and Energies

Figure 4.3

A

C	-4.78826100	-5.14730900	-2.55233700
C	-6.18086900	-5.46619300	-2.11142900
H	-6.68885300	-6.15630800	-2.82202500
H	-6.19720600	-5.96654300	-1.12853400
H	-6.81119500	-4.56291000	-2.05272000
C	-3.70882600	-6.15188000	-2.30512300
H	-2.70404900	-5.70211900	-2.37447600
H	-3.80907100	-6.62898600	-1.31566800
H	-3.73501100	-6.97558700	-3.05349300
C	-4.59144200	-4.13276600	-3.63281700
H	-4.78837700	-4.56252600	-4.64067500
H	-5.27653500	-3.27539000	-3.52233000
H	-3.55683800	-3.75095300	-3.65565900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)

Zero-point correction= 0.115454 (Hartree/Particle)

Thermal correction to Energy= 0.121830

Thermal correction to Enthalpy= 0.122774

Thermal correction to Gibbs Free Energy= 0.086016
Sum of electronic and zero-point Energies= -157.583185
Sum of electronic and thermal Energies= -157.576809
Sum of electronic and thermal Enthalpies= -157.575865
Sum of electronic and thermal Free Energies= -157.612623
HF=-157.6986389
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-157.877899

B

C	-4.30541400	-3.77861800	-0.90237400
H	-3.34032700	-3.74703000	-1.41607800
C	-4.41007900	-4.35357000	0.30014300
H	-5.35744100	-4.40341600	0.84228500
H	-5.16867100	-3.33018600	-1.39943300
C	-3.22744300	-4.95957300	0.96455900
O	-2.10266100	-4.99445900	0.51220900
O	-3.55935700	-5.47871700	2.15823900
C	-2.50494100	-6.09361700	2.90132800
H	-1.71034300	-5.36587100	3.12371600
H	-2.95683000	-6.45791800	3.83118900
H	-2.06803800	-6.93059900	2.33658700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.094952 (Hartree/Particle)
Thermal correction to Energy= 0.101583
Thermal correction to Enthalpy= 0.102527
Thermal correction to Gibbs Free Energy= 0.064550
Sum of electronic and zero-point Energies= -306.166441
Sum of electronic and thermal Energies= -306.159810
Sum of electronic and thermal Enthalpies= -306.158866
Sum of electronic and thermal Free Energies= -306.196843
HF=-306.2613926
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-306.6188516

B-TS-C

C	-4.63202900	-3.79047800	-1.09273600
H	-3.70695900	-3.53738700	-1.61309100
C	-4.57709000	-4.42648200	0.10212500
H	-5.47327700	-4.63252800	0.69119900
H	-5.55911300	-3.34580000	-1.45596100
C	-4.92896800	-5.51713600	-2.85803700
C	-6.40071800	-5.74816600	-2.71698100
H	-6.73369400	-6.56139200	-3.39582800
H	-6.66512500	-6.05895000	-1.69324300
H	-6.98805100	-4.85314900	-2.97687600
C	-4.01722800	-6.57312100	-2.32030300
H	-2.98094400	-6.21511500	-2.22830400
H	-4.34929100	-6.92653600	-1.33097100
H	-4.00697900	-7.45612900	-2.99303100
C	-4.45830500	-4.71261500	-4.02812200
H	-4.56445100	-5.29350100	-4.96881700
H	-5.04894800	-3.79103600	-4.15798200
H	-3.39455700	-4.44055700	-3.93976600
C	-3.30120700	-4.93624700	0.62071100
O	-2.21178800	-4.81305200	0.08945500
O	-3.46729400	-5.58693900	1.79307300
C	-2.29112200	-6.13205900	2.38710100
H	-1.55906200	-5.34053500	2.60847200
H	-2.61187500	-6.61931800	3.31571900
H	-1.81811700	-6.86686700	1.71787400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.212760 (Hartree/Particle)
Thermal correction to Energy= 0.225980
Thermal correction to Enthalpy= 0.226924
Thermal correction to Gibbs Free Energy= 0.172027
Sum of electronic and zero-point Energies= -463.755009
Sum of electronic and thermal Energies= -463.741789
Sum of electronic and thermal Enthalpies= -463.740845
Sum of electronic and thermal Free Energies= -463.795742
HF=-463.9677686
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-464.5019013

C

C	-4.35990500	-3.97061100	-1.10299800
H	-3.33441400	-3.60649700	-1.26864000
C	-4.44155400	-4.57066200	0.24863300
H	-5.40454100	-4.73603500	0.73668800
H	-5.04462300	-3.10584700	-1.15778300
C	-4.73027400	-4.93266800	-2.28244300
C	-6.19100300	-5.39005000	-2.15531100
H	-6.46988000	-6.03040700	-3.00756200
H	-6.35503700	-5.97132100	-1.23445300
H	-6.87828000	-4.52843300	-2.14149300
C	-3.79873700	-6.15402500	-2.27369900
H	-2.74147400	-5.84944400	-2.31495900
H	-3.93773500	-6.75858400	-1.36350000
H	-4.00469000	-6.80144800	-3.14123500
C	-4.54730800	-4.15435200	-3.59312000
H	-4.79973200	-4.78702400	-4.45931900
H	-5.19742200	-3.26496400	-3.62229700
H	-3.50500400	-3.81719200	-3.71169400
C	-3.25138500	-5.01070900	0.95197400
O	-2.10807800	-4.91694900	0.52848600
O	-3.54188900	-5.55432800	2.15601600
C	-2.43379000	-6.02299900	2.92075200
H	-1.73272700	-5.20318600	3.14038100
H	-2.84978600	-6.42354500	3.85293900
H	-1.88880900	-6.81176600	2.37971700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.217079 (Hartree/Particle)
Thermal correction to Energy= 0.229388
Thermal correction to Enthalpy= 0.230332
Thermal correction to Gibbs Free Energy= 0.178156

Sum of electronic and zero-point Energies= -463.789785
Sum of electronic and thermal Energies= -463.777477
Sum of electronic and thermal Enthalpies= -463.776533
Sum of electronic and thermal Free Energies= -463.828708
HF=-464.0068643
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-464.5374266

Figure A3.1
^{1}D

Ni	-0.94258000	1.43594000	-0.77848100
C	-2.57987200	2.01673500	-1.41495100
C	-2.87097400	0.15643900	-3.56327400
C	-2.62500000	2.46170800	-2.78791900
C	-2.67279200	0.57665500	-1.15206900
C	-2.88348700	-0.30657700	-2.26948800
C	-2.71669000	1.55597000	-3.81761300
H	-2.57180800	3.53364800	-2.99619900
H	-3.04155300	0.23099800	-0.17810600
H	-3.08215900	-1.36483900	-2.07067100
H	-2.69456900	1.91466900	-4.85076900
H	-3.01148800	-0.53147900	-4.40077800
Br	-3.67354500	3.27150700	-0.17422200
C	1.64688300	2.32929300	-0.23793000
C	2.16210900	4.49181200	-0.19075600
C	0.62733900	4.30435500	-0.37050700
N	0.48390900	2.83948000	-0.44611000
H	2.65349400	4.95190600	-1.05845800
H	0.28971400	4.72849300	-1.32901500
C	0.97481400	-1.21602400	-0.43609500
C	2.49442700	-1.22045900	-0.09948100
C	1.73489600	0.86589800	-0.22252300
N	0.63764000	0.21691900	-0.39548000
H	0.39909100	-1.73009000	0.34921400
H	3.11030500	-1.71197800	-0.86461600
H	2.42802300	5.04436000	0.72059300
H	2.72240700	-1.64469700	0.88754100
O	2.68736200	3.13435100	-0.05520000
O	2.86911300	0.19256300	-0.06891400
C	-0.21515100	4.87909100	0.76175300
H	-0.11444200	5.97500800	0.79237200
H	-1.27298800	4.62210200	0.60943000
H	0.11029200	4.46981600	1.73130900
C	0.62171700	-1.80934700	-1.79522400
H	0.83470300	-2.88912100	-1.81123500
H	-0.44541300	-1.65188400	-2.00586200
H	1.20531900	-1.32300100	-2.59267300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.291659 (Hartree/Particle)
Thermal correction to Energy= 0.311891
Thermal correction to Enthalpy= 0.312835
Thermal correction to Gibbs Free Energy= 0.239949
Sum of electronic and zero-point Energies= -4884.933396
Sum of electronic and thermal Energies= -4884.913164
Sum of electronic and thermal Enthalpies= -4884.912219
Sum of electronic and thermal Free Energies= -4884.985105
HF=-4885.2250546
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-4886.6504419

^{3}D

Ni	-1.03209500	0.92430100	-0.59379800
C	-2.57185900	0.47705500	-1.82470700
C	-2.90496400	3.15067900	-2.62571200
C	-3.07430000	1.44026800	-0.89733100
C	-2.25722400	0.86490700	-3.15774300
C	-2.40311800	2.18682300	-3.53375500
C	-3.23712000	2.78129600	-1.33594300
H	-3.53280000	1.11797900	0.04051500
H	-1.90373600	0.11432900	-3.86613100
H	-2.13796000	2.48597000	-4.55035600
H	-3.65449500	3.51326200	-0.64067600
H	-3.03112000	4.18561000	-2.94921400
Br	-2.93937600	-1.41138900	-1.50001500
C	1.52700600	1.94093800	-0.78901900
C	1.98509600	3.69819300	-2.07842100
C	0.45759700	3.61360300	-1.84568700
N	0.31572400	2.29761100	-1.22238000
H	2.26332800	3.36388100	-3.09279600
H	-0.07641000	3.63879700	-2.80858000
C	0.95754900	-1.16691100	0.89283300
C	2.42206200	-0.85964600	1.28675400
C	1.64685600	0.77535500	-0.01726900
N	0.53330500	0.10312500	0.30080600
H	0.36074200	-1.39116300	1.79242100
H	3.11255900	-1.69965000	1.12891300
H	2.41029300	4.69481300	-1.89596000
H	2.50046100	-0.51513800	2.33208600
O	2.54786600	2.77938400	-1.11876200
O	2.81224900	0.22096200	0.41321100
C	-0.07543600	4.72824100	-0.94358100
H	0.01084700	5.71107000	-1.43539800
H	-1.13305300	4.55032400	-0.70412300
H	0.49160700	4.75976500	0.00092700
C	0.82464400	-2.32332000	-0.09988900
H	1.12266200	-3.27925200	0.36109500
H	-0.21646000	-2.40840300	-0.44453900
H	1.46272000	-2.14624600	-0.98098500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.290845 (Hartree/Particle)
Thermal correction to Energy= 0.311013
Thermal correction to Enthalpy= 0.311957
Thermal correction to Gibbs Free Energy= 0.239012
Sum of electronic and zero-point Energies= -4884.928978
Sum of electronic and thermal Energies= -4884.908810
Sum of electronic and thermal Enthalpies= -4884.907866
Sum of electronic and thermal Free Energies= -4884.980811
HF=-4885.2198229

UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-4886.6409439

[1]D-TS-G

Ni	-0.83110500	1.36977800	-0.80861700
C	-2.31714400	1.88978200	-1.66477700
C	-3.18775800	0.30912600	-3.81514000
C	-2.52641600	2.48718600	-2.92669500
C	-2.62024200	0.51017200	-1.45985100
C	-3.05319700	-0.27116700	-2.56455000
C	-2.92457300	1.69026900	-3.99046600
H	-2.32773200	3.55184600	-3.06933900
H	-2.74668900	0.09942100	-0.45083700
H	-3.33382300	-1.31685200	-2.40911800
H	-3.02383600	2.13355500	-4.98541500
H	-3.52516000	-0.28814500	-4.66541700
Br	-3.65196600	3.38731200	0.05896100
C	1.65377000	2.33211700	-0.20371800
C	2.08814500	4.50518200	-0.33262300
C	0.55266800	4.26353500	-0.38253100
N	0.46745700	2.78929600	-0.40782000
H	2.50713400	4.86923800	-1.28055600
H	0.12276900	4.64660400	-1.31988600
C	1.06584600	-1.23488200	-0.27446200
C	2.59302900	-1.19450700	0.02867600
C	1.78807200	0.87093500	-0.13552300
N	0.70802200	0.19326700	-0.29821400
H	0.51735100	-1.71257100	0.55236700
H	3.20536900	-1.66634300	-0.75147000
H	2.40113200	5.16037800	0.49008300
H	2.85705800	-1.60876200	1.01002800
O	2.66201700	3.17917700	-0.08560500
O	2.93019400	0.23155900	0.04897300
C	-0.20972400	4.83624500	0.80606400
H	-0.13568500	5.93489800	0.80163100
H	-1.26966400	4.54753100	0.74630100
H	0.21292200	4.46113100	1.75191900
C	0.69145600	-1.90971700	-1.58862700
H	0.93801000	-2.98164200	-1.55227800
H	-0.38710600	-1.80127300	-1.77349600
H	1.23484700	-1.45065500	-2.42917900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.291693 (Hartree/Particle)
Thermal correction to Energy= 0.311482
Thermal correction to Enthalpy= 0.312426
Thermal correction to Gibbs Free Energy= 0.240116
Sum of electronic and zero-point Energies= -4884.929204
Sum of electronic and thermal Energies= -4884.909415
Sum of electronic and thermal Enthalpies= -4884.908471
Sum of electronic and thermal Free Energies= -4884.980781
HF=-4885.220897
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-4886.6483641

[3]D-TS-G

Ni	-1.01342900	1.23965900	-0.00535300
C	-2.48634200	0.84282400	-1.22759300
C	-2.62962200	2.32564400	-3.58376200
C	-3.10521600	2.11345600	-1.21085400
C	-2.04890700	0.25919400	-2.43733800
C	-2.09612800	1.02326200	-3.59728100
C	-3.13566100	2.85807400	-2.39806200
H	-3.54014900	2.50879600	-0.29151300
H	-1.63121000	-0.74767700	-2.44043000
H	-1.71206300	0.60136500	-4.52932000
H	-3.57674700	3.85767700	-2.38752800
H	-2.66506100	2.90923000	-4.50576300
Br	-2.99577700	-0.40911000	0.34928800
C	1.53125500	2.05298700	-0.63596700
C	1.91597100	4.13293300	-1.34419700
C	0.39054100	3.88459400	-1.28815300
N	0.31771400	2.61025600	-0.57907300
H	2.26675000	4.56153400	-2.29259500
H	-0.00483400	3.75395600	-2.31578900
C	1.00594300	-1.29641000	0.52241800
C	2.55081500	-1.19342500	0.53727400
C	1.68521400	0.73588700	-0.17448900
N	0.61124600	0.09443700	0.29982700
H	0.63938000	-1.64850800	1.50106400
H	3.05779900	-2.02802500	0.03333200
H	2.24504100	4.77827700	-0.50968400
H	2.94398900	-1.09584500	1.56350000
O	2.50905000	2.82792800	-1.18139600
O	2.84265100	0.02086100	-0.18624400
C	-0.39630400	4.99316600	-0.60515100
H	-0.30594000	5.94270000	-1.15680700
H	-1.46214900	4.72521300	-0.55756400
H	-0.03189400	5.14571400	0.42334900
C	0.46633300	-2.21934300	-0.57218300
H	0.77084500	-3.26370300	-0.39502600
H	-0.63242800	-2.17727700	-0.59308900
H	0.84477000	-1.90727700	-1.55905500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.290180 (Hartree/Particle)
Thermal correction to Energy= 0.309933
Thermal correction to Enthalpy= 0.310878
Thermal correction to Gibbs Free Energy= 0.238909
Sum of electronic and zero-point Energies= -4884.923162
Sum of electronic and thermal Energies= -4884.903409
Sum of electronic and thermal Enthalpies= -4884.902464
Sum of electronic and thermal Free Energies= -4884.974432
HF=-4885.213342
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-4886.6344331

[1]G

Ni	-0.60698600	0.52697600	-1.02379800
C	-2.04929000	1.27531300	-1.96942100
C	-4.12342000	2.53188300	-3.44255700
C	-1.83352900	1.74578900	-3.27697500
C	-3.33474400	1.43752800	-1.42323700

C	-4.35777100	2.06539400	-2.14385400
C	-2.85652000	2.36327200	-4.00959500
H	-0.84753500	1.63802100	-3.74138100
H	-3.54684400	1.06436000	-0.41752200
H	-5.34620500	2.18627800	-1.69040200
H	-2.66040400	2.71653100	-5.02644800
H	-4.92234800	3.01867100	-4.00805400
Br	-1.64648100	-1.56773600	-0.88054800
C	1.50965900	2.17738300	-0.39391700
C	1.44705100	4.30712400	-1.00896300
C	0.06975600	3.64041100	-1.27033400
N	0.34584500	2.22391100	-0.94709800
H	1.99715100	4.54807800	-1.92882400
H	-0.20834200	3.70708200	-2.33073400
C	1.76040400	-1.33335400	0.38566200
C	3.03352700	-0.78688700	1.09205900
C	1.93892900	0.86587200	0.09987900
N	1.11252100	-0.09751300	-0.08818300
H	1.08469200	-1.82525300	1.10015700
H	3.96282700	-1.26287900	0.75473100
H	1.39292400	5.19183000	-0.36268600
H	2.97362700	-0.81827500	2.18844600
O	2.22054700	3.28531700	-0.29788400
O	3.09220500	0.62614800	0.70125700
C	-1.06011500	4.19226800	-0.40835300
H	-1.23234300	5.25100100	-0.65564900
H	-1.98608900	3.63191000	-0.59083100
H	-0.80505600	4.11903500	0.66053300
C	2.04796800	-2.27708400	-0.77785200
H	2.53100600	-3.19423100	-0.40706200
H	1.10681800	-2.54509600	-1.27644100
H	2.71801100	-1.79905600	-1.50982800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.294154 (Hartree/Particle)
Thermal correction to Energy= 0.314093
Thermal correction to Enthalpy= 0.315037
Thermal correction to Gibbs Free Energy= 0.243493
Sum of electronic and zero-point Energies= -4884.998406
Sum of electronic and thermal Energies= -4884.978467
Sum of electronic and thermal Enthalpies= -4884.977523
Sum of electronic and thermal Free Energies= -4885.049067
HF=-4885.2925602
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-4886.7158846

^{3}G

Ni	-1.12100400	1.57322200	0.18362300
C	-1.85411200	1.37899100	-1.64337000
C	-2.97596000	1.07046600	-4.24117700
C	-3.24426200	1.26609300	-1.83747800
C	-1.04692200	1.32817200	-2.79462900
C	-1.59026900	1.17451300	-4.07693100
C	-3.80325100	1.11784700	-3.11421200
H	-3.91220600	1.28637600	-0.96962000
H	0.04355200	1.40555500	-2.70847400
H	-0.93172500	1.13572100	-4.95020700
H	-4.88841600	1.03456900	-3.22969500
H	-3.40664400	0.95147700	-5.23911600
Br	-2.56926900	0.84629100	1.96790900
C	1.53734200	2.22908200	-0.50719700
C	2.14213500	4.27073500	-1.14122400
C	0.63779000	4.25109600	-0.75141600
N	0.45037200	2.87150200	-0.27307100
H	2.33548100	4.60695800	-2.16660700
H	0.00219300	4.36756000	-1.64542700
C	0.66632800	-1.18657000	0.32716600
C	2.14234200	-1.35726200	-0.13977200
C	1.54762700	0.78393200	-0.23563300
N	0.45503100	0.26006900	0.18219000
H	0.56060500	-1.43490800	1.39544100
H	2.23641800	-1.94452600	-1.06393600
H	2.75669500	4.84892200	-0.43565700
H	2.80687500	-1.76645600	0.63094300
O	2.56359000	2.87234300	-1.04342900
O	2.59781300	0.00391300	-0.43953000
C	0.23693200	5.28100000	0.29395100
H	0.38933600	6.29947400	-0.09422900
H	-0.82595500	5.16552700	0.55223700
H	0.83619900	5.15960300	1.20941000
C	-0.36131400	-1.97249900	-0.47670000
H	-0.19379800	-3.05362200	-0.35766200
H	-1.37261500	-1.72882400	-0.12100100
H	-0.29819200	-1.71471700	-1.54467700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.292282 (Hartree/Particle)
Thermal correction to Energy= 0.313210
Thermal correction to Enthalpy= 0.314155
Thermal correction to Gibbs Free Energy= 0.236600
Sum of electronic and zero-point Energies= -4884.997373
Sum of electronic and thermal Energies= -4884.976445
Sum of electronic and thermal Enthalpies= -4884.975501
Sum of electronic and thermal Free Energies= -4885.053056
HF=-4885.2896557
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-4886.7104469

^{2}E^R

Ni	-0.71114700	-0.02876000	-0.12036400
C	-1.63492800	1.15436000	-1.56325400
C	-0.22581300	3.48448800	-0.90720300
C	-1.83453100	1.75529800	-0.27967600
C	-0.75123300	1.73546500	-2.51257700
C	-0.03468800	2.86500200	-2.17044500
C	-1.11781000	2.95585300	0.00304800
H	-2.71771600	1.51481800	0.31535700
H	-0.64447700	1.27593500	-3.49657700
H	0.67184800	3.29277800	-2.88524900
H	-1.30756300	3.46546500	0.95063700
Br	-3.03733200	-0.02075900	-2.23501600
C	-3.32849600	0.37064900	3.83990800
H	-2.31771300	0.79276500	3.95357900
H	-3.89523600	1.03027700	3.16141400

H	-3.81699800	0.40284100	4.82792900
C	-3.27863500	-1.06610400	3.29575800
C	-2.62209200	-1.07649900	1.88561300
H	-2.73799500	-2.08559800	1.45738300
H	-3.23473500	-0.41020700	1.25134800
C	-1.14782400	-0.70395300	1.81899100
C	-4.71293900	-1.60038100	3.15928200
H	-4.71283000	-2.64104500	2.79524000
H	-5.24264800	-1.58008100	4.12625900
H	-5.29397900	-0.99452500	2.44403800
H	-0.87088200	0.17185100	2.41708300
C	-0.22566600	-1.79916200	2.00981100
O	-0.41211000	-2.99760700	1.79471500
O	1.02148400	-1.38151000	2.43343500
C	1.99998600	-2.38964300	2.64693100
H	2.30973100	-2.86431200	1.70342000
H	2.86536000	-1.88543700	3.09743200
H	1.62768300	-3.17232700	3.32517900
C	-2.49601600	-1.95611200	4.27299400
H	-2.40798300	-2.98397200	3.88944400
H	-1.47652100	-1.57245200	4.43204300
H	-2.99815800	-1.99309500	5.25415900
H	0.31951300	4.40021100	-0.66793100
C	2.03160900	-0.53817200	-0.27972300
C	3.57029800	0.85285900	0.52447700
C	2.16394900	1.51814900	0.56094800
N	1.29688900	0.49049300	-0.04424300
H	4.27583800	1.35744900	-0.14940100
H	2.13933600	2.40982300	-0.08262000
C	-0.29779600	-3.08942200	-1.33586000
C	0.97595800	-3.92362000	-1.03298700
C	1.38660000	-1.75539600	-0.75806800
N	0.12385800	-1.71697500	-1.00133500
H	-1.09949400	-3.36454100	-0.63637300
H	1.28979500	-4.57434700	-1.85958100
H	4.02361400	0.74608300	1.51976900
H	0.88391600	-4.49557400	-0.10079300
O	3.33327500	-0.48500700	-0.00011100
O	2.02322200	-2.92709800	-0.82381200
C	1.69443400	1.88455400	1.96372900
H	2.37513400	2.62863400	2.40578000
H	0.68522000	2.31556900	1.92674400
H	1.66631900	0.98736400	2.59734200
C	-0.78357300	-3.18286800	-2.77790500
H	-1.10951800	-4.21018300	-3.00279700
H	-1.63012900	-2.50179800	-2.94072500
H	0.02212500	-2.91141100	-3.47847300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511926 (Hartree/Particle)
Thermal correction to Energy= 0.545475
Thermal correction to Enthalpy= 0.546419
Thermal correction to Gibbs Free Energy= 0.445087
Sum of electronic and zero-point Energies= -5348.798887
Sum of electronic and thermal Energies= -5348.765338
Sum of electronic and thermal Enthalpies= -5348.764394
Sum of electronic and thermal Free Energies= -5348.865726
HF=-5349.3108128

UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2465461

^{2}E^S

Ni	-0.1251943	0.4790690	-0.8701145
C	-0.9677233	1.6639030	-2.3678395
C	0.9903267	3.6498950	-2.2907585
C	-0.8792743	2.5005410	-1.2201245
C	-0.1047083	1.8336670	-3.4771635
C	0.8823197	2.8029390	-3.4192155
C	0.1157087	3.5148780	-1.2268645
H	-1.6938783	2.5502870	-0.4971625
H	-0.2162893	1.1905710	-4.3510955
H	1.5736687	2.9180440	-4.2568725
H	0.1641537	4.2062210	-0.3828165
Br	-2.5957433	0.6264980	-2.5905905
H	1.7529787	4.4315690	-2.2731465
C	2.4925557	-0.4455090	-0.9999715
C	4.1873067	0.6697220	-0.0834745
C	2.9442137	1.5930000	-0.2165925
N	1.9174757	0.6819920	-0.7594655
H	5.0760087	1.0422950	-0.6080545
H	3.1225207	2.3739410	-0.9729275
C	-0.1561823	-2.5795860	-2.2064135
C	0.9619507	-3.6099220	-1.8829145
C	1.6802797	-1.5402020	-1.5123575
N	0.4556377	-1.2963570	-1.8228385
H	-1.0340123	-2.7449400	-1.5629915
H	1.2138007	-4.2643320	-2.7281845
H	4.4411497	0.4528010	0.9650185
H	0.7419437	-4.2163830	-0.9936635
O	3.7871917	-0.5844270	-0.7083595
O	2.1305617	-2.7957070	-1.5794175
C	2.5125327	2.2363700	1.0927085
H	3.3285437	2.8589430	1.4918975
H	1.6370787	2.8790880	0.9304365
H	2.2395087	1.4655900	1.8277875
C	-0.5880213	-2.5678130	-3.6695305
H	-1.0499343	-3.5300490	-3.9398785
H	-1.3192453	-1.7664750	-3.8445065
H	0.2797967	-2.4001880	-4.3268765
C	-1.8513053	0.6287670	1.6527995
H	-2.4287003	1.2458140	0.9420385
C	-0.9107263	-0.3025220	0.9100785
H	-1.4101993	-1.1588300	0.4350265
H	-1.2413483	1.3315020	2.2444995
C	-2.8967683	-0.0325210	2.5962515
C	-3.6452373	1.0875190	3.3358645
H	-4.4319883	0.6796580	3.9921985
H	-2.9542513	1.6764320	3.9614195
H	-4.1257383	1.7791420	2.6237515
C	-2.2196493	-0.9529710	3.6228485
H	-1.7226703	-1.8022960	3.1292585
H	-1.4546543	-0.4109980	4.1987215
H	-2.9628673	-1.3626040	4.3273035
C	-3.9048163	-0.8469420	1.7689625
H	-4.6759853	-1.2966760	2.4161975
H	-4.4146493	-0.2095100	1.0273535
H	-3.4087353	-1.6651460	1.2236475
C	0.2676307	-0.7226280	1.6302125
O	0.8273597	-0.1562620	2.5681465

O	0.8101887	-1.8971860	1.1338385
C	1.9821337	-2.3714270	1.7793215
H	1.7942397	-2.5929390	2.8416115
H	2.2764497	-3.2869280	1.2503815
H	2.8032787	-1.6403840	1.7226035

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511268 (Hartree/Particle)
Thermal correction to Energy= 0.545162
Thermal correction to Enthalpy= 0.546107
Thermal correction to Gibbs Free Energy= 0.442933
Sum of electronic and zero-point Energies= -5348.796079
Sum of electronic and thermal Energies= -5348.762184
Sum of electronic and thermal Enthalpies= -5348.761240
Sum of electronic and thermal Free Energies= -5348.864414
HF=-5349.3073465

^{2}E-TS-F^R

Ni	-0.82109500	-0.01116200	-0.03852300
C	-1.31311000	1.30632800	-1.45681600
C	0.09510700	3.65992300	-1.92928800
C	-1.48255800	2.39739600	-0.58261500
C	-0.54776700	1.42024300	-2.63185300
C	0.17420900	2.58917500	-2.84143400
C	-0.73559100	3.56246500	-0.81304600
H	-2.16558700	2.32952500	0.26696100
H	-0.47187200	0.57721100	-3.32013100
H	0.81883700	2.67015300	-3.72061000
H	-0.82731700	4.40236400	-0.11968200
Br	-2.98488000	-0.06199400	-1.44777600
C	-3.25347900	0.11556900	4.18759100
H	-2.22937800	0.51118200	4.27577800
H	-3.85332900	0.85284100	3.62813900
H	-3.67182100	0.04264400	5.20530300
C	-3.26695600	-1.25222700	3.48590400
C	-2.71130600	-1.11194300	2.03947100
H	-2.88703300	-2.06155500	1.50719800
H	-3.34036100	-0.36448200	1.52763900
C	-1.23950600	-0.75326900	1.90343400
C	-4.71749200	-1.75117600	3.39024700
H	-4.76114300	-2.74662300	2.91820100
H	-5.18266600	-1.82864200	4.38716900
H	-5.33224200	-1.06536600	2.78364800
H	-0.92764700	0.09663100	2.52316400
C	-0.31136300	-1.85484100	2.01379800
O	-0.49410700	-3.03676100	1.72152800
O	0.93766900	-1.46046500	2.45940700
C	1.91109400	-2.48236300	2.62850200
H	2.22770800	-2.91076400	1.66536700
H	2.77447300	-2.00600200	3.11176900
H	1.52926400	-3.29663400	3.26270300
C	-2.44111900	-2.25211700	4.30964000
H	-2.38416500	-3.22998300	3.80831500
H	-1.41044300	-1.89343800	4.45467800
H	-2.88840900	-2.39702400	5.30731400
H	0.66475600	4.57365600	-2.11111000
C	1.95651300	-0.44672700	-0.12751300
C	3.40671700	0.90497300	0.88109400
C	2.00240500	1.57312400	0.80682200
N	1.18766400	0.54306500	0.14306700
H	4.19199900	1.46670700	0.35953800
H	2.02235600	2.45747900	0.14990100
C	-0.29999200	-2.94720500	-1.44270900
C	0.98958000	-3.77979200	-1.20397600
C	1.35054900	-1.64010800	-0.71597700
N	0.09471700	-1.60473600	-0.98601500
H	-1.10129500	-3.29450500	-0.77524300
H	1.33504900	-4.32915400	-2.08932500
H	3.72504900	0.69340400	1.91205600
H	0.89947200	-4.45341900	-0.34232000
O	3.24505700	-0.37557700	0.19961300
O	2.00982800	-2.78709200	-0.86725700
C	1.42250100	1.95807300	2.16164400
H	2.06402700	2.70776900	2.64995300
H	0.41889500	2.38859300	2.03565200
H	1.34583600	1.06875400	2.80307500
C	-0.77944200	-2.92054900	-2.88968800
H	-1.08090800	-3.93022900	-3.20850900
H	-1.64262400	-2.24796400	-2.98971900
H	0.02096500	-2.56727400	-3.55902400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511327 (Hartree/Particle)
Thermal correction to Energy= 0.544533
Thermal correction to Enthalpy= 0.545477
Thermal correction to Gibbs Free Energy= 0.444805
Sum of electronic and zero-point Energies= -5348.789724
Sum of electronic and thermal Energies= -5348.756519
Sum of electronic and thermal Enthalpies= -5348.755575
Sum of electronic and thermal Free Energies= -5348.856246
HF=-5349.3010513
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2370475

^{2}E-TS-F^R-conf2

Ni	-0.92244200	0.41923500	-0.17564000
C	0.12300900	2.04683500	-0.82041900
C	2.64991200	2.87904000	0.05620800
C	0.22512300	2.94046000	0.26303800
C	1.27473200	1.68143400	-1.54789100
C	2.53042900	2.06848500	-1.08156600
C	1.49194000	3.31955200	0.71125300
H	-0.66486800	3.26565200	0.79871400
H	1.18416100	1.06183300	-2.43941500
H	3.42412200	1.73962600	-1.61829100
H	1.57108800	3.96564800	1.58960100
Br	-1.64914600	2.20765500	-2.08447000
H	3.63560200	3.18448600	0.41362200
C	1.48649600	-1.16383000	0.28513700
C	3.03468300	-0.51707500	1.73269900
C	1.63334000	-0.03697500	2.18621600
N	0.78795900	-0.38814900	1.02458500
H	3.66151300	0.29681200	1.34030200
H	1.61051700	1.05447000	2.31005800
C	-0.53346300	-1.93175100	-2.63865200

C	0.59992100	-2.99323900	-2.74124000
C	0.89839300	-1.70771200	-0.94905000
N	-0.16741900	-1.17770200	-1.42289000
H	-1.50480500	-2.41557700	-2.44681300
H	1.22186000	-2.87305800	-3.63943900
H	3.58129700	-1.08419100	2.49592700
H	0.24494800	-4.02927700	-2.67278500
O	2.75008100	-1.41833500	0.61669800
O	1.44807800	-2.73667400	-1.58090400
C	1.12583300	-0.73024700	3.44773000
H	1.72953900	-0.41788000	4.31416800
H	0.07266100	-0.47447600	3.62653000
H	1.21085400	-1.82395700	3.34267500
C	-0.65447500	-1.03456400	-3.86271900
H	-1.41368100	-0.25842900	-3.69840300
H	0.30485100	-0.53960400	-4.08030200
H	-0.94198700	-1.63418500	-4.73986000
C	-5.48566900	1.44159000	0.04109800
H	-4.87437000	2.34979800	0.15746500
H	-5.37739700	1.09661500	-1.00066600
H	-6.53996600	1.72478200	0.19654700
C	-5.05835300	0.34627500	1.03127000
C	-3.58104000	-0.06272900	0.76530300
H	-3.35119900	-0.95067500	1.37782200
H	-3.53687800	-0.39669800	-0.28835600
C	-2.51714500	0.99438400	1.04778500
C	-5.94257900	-0.89274600	0.82069200
H	-5.67961500	-1.69093100	1.53437800
H	-7.00985600	-0.65249200	0.95955500
H	-5.81845000	-1.29807600	-0.19746600
H	-2.77638000	1.99025100	0.67136200
C	-2.05505300	1.06145100	2.41516300
O	-2.00422700	0.15184100	3.24098200
O	-1.59835300	2.31698000	2.75275100
C	-0.99654200	2.46252800	4.02847500
H	-0.01731100	1.95851500	4.07360700
H	-0.85345500	3.54005000	4.18544300
H	-1.63362000	2.04794300	4.82396000
C	-5.23549200	0.85895800	2.46849500
H	-4.89344300	0.11266900	3.20171400
H	-4.65721800	1.78024300	2.63727700
H	-6.29516600	1.08618100	2.67265300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.512099 (Hartree/Particle)
Thermal correction to Energy= 0.545488
Thermal correction to Enthalpy= 0.546432
Thermal correction to Gibbs Free Energy= 0.444184
Sum of electronic and zero-point Energies= -5348.784424
Sum of electronic and thermal Energies= -5348.751035
Sum of electronic and thermal Enthalpies= -5348.750091
Sum of electronic and thermal Free Energies= -5348.852339
HF=-5349.2965236

^{2}E-TS-F^R-conf3

Ni	-0.50310800	-0.42670000	0.41019600
C	-1.85932400	-1.32999800	-0.77392900
C	-1.74120300	-3.94870400	-1.75570400
C	-1.12191200	-1.60673400	-1.94583500
C	-2.64291100	-2.33752400	-0.17552700
C	-2.55082500	-3.64351600	-0.65139300
C	-1.03794800	-2.92468400	-2.40009300
H	-0.59745700	-0.80441400	-2.46499900
H	-3.28337200	-2.09618500	0.67200900
H	-3.12271800	-4.43178000	-0.15499900
H	-0.42459800	-3.14732700	-3.27707600
Br	-2.68138000	0.62391200	-0.64689400
C	-3.55399900	-2.06321400	3.83586000
H	-3.68835400	-1.02131000	3.50571300
H	-3.93609700	-2.72218100	3.03821700
H	-4.18522800	-2.21575200	4.72705000
C	-2.07949300	-2.37039400	4.14334000
C	-1.21125800	-2.15072800	2.87378500
H	-0.20101100	-2.53138600	3.08857400
H	-1.62071600	-2.80519300	2.08674900
C	-1.08297400	-0.72334500	2.37854200
C	-1.95363800	-3.84461400	4.55871300
H	-0.91145100	-4.09316800	4.81906700
H	-2.58465700	-4.07204900	5.43410100
H	-2.26248200	-4.51307200	3.73761200
H	-2.01519000	-0.14484200	2.41207600
C	0.02788700	0.02712800	2.92747300
O	1.09555800	-0.40663100	3.35931000
O	-0.17537000	1.39313700	2.86806400
C	0.93070300	2.20400400	3.22551900
H	1.78860400	2.03330000	2.55419300
H	0.59641400	3.24612800	3.13530800
H	1.26180100	2.00716100	4.25729500
C	-1.59690300	-1.47503800	5.29473100
H	-0.52873300	-1.64229500	5.50338600
H	-1.72367800	-0.40913300	5.05034000
H	-2.16621400	-1.67971100	6.21686100
H	-1.67832300	-4.97490600	-2.12356400
C	2.27211100	-0.82001800	-0.11310400
C	3.39205500	-2.58235400	0.64582100
C	1.89650200	-2.66945400	1.05846300
N	1.31005600	-1.49257900	0.39885300
H	4.09077100	-2.59878700	1.49103300
H	1.78041100	-2.49474500	2.13990500
C	0.69146700	2.18450800	-1.37520100
C	2.14427800	2.35456900	-1.90518400
C	1.95259700	0.45761800	-0.75997300
N	0.73345900	0.85774700	-0.73612300
H	-0.03077900	2.14460400	-2.20485300
H	2.63644900	3.26840600	-1.54678000
H	3.67772600	-3.35139400	-0.08767900
H	2.22119400	2.29714200	-2.99935700
O	3.51538900	-1.28212300	-0.01128900
O	2.87050900	1.21291500	-1.35292900
C	1.20095600	-3.95929100	0.65140000
H	1.65351200	-4.81786500	1.17092200
H	0.13510700	-3.91468900	0.91240700
H	1.28097300	-4.11934300	-0.43453400
C	0.25964100	3.25528200	-0.37886700
H	0.21596700	4.23748400	-0.87399600
H	-0.73451700	3.01981300	0.02530700
H	0.97131100	3.31471300	0.45820800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511114 (Hartree/Particle)

Thermal correction to Energy= 0.544656
Thermal correction to Enthalpy= 0.545600
Thermal correction to Gibbs Free Energy= 0.443294
Sum of electronic and zero-point Energies= -5348.789206
Sum of electronic and thermal Energies= -5348.755664
Sum of electronic and thermal Enthalpies= -5348.754720
Sum of electronic and thermal Free Energies= -5348.857026
HF=-5349.3003202

^{2}E-TS-F^S

Ni	-0.82279500	0.03562400	-0.07607000
C	-1.21743900	1.37888900	-1.50377200
C	0.44952100	3.54069200	-2.04417400
C	-1.25988500	2.50746200	-0.66238300
C	-0.45131600	1.37306800	-2.68464100
C	0.40073600	2.44377300	-2.92654400
C	-0.38606600	3.57197200	-0.92790500
H	-1.94205100	2.54539200	0.18869100
H	-0.47793900	0.50976400	-3.35054600
H	1.04613900	2.42547900	-3.80857600
H	-0.37987200	4.43702000	-0.26007200
Br	-3.00526600	0.19646400	-1.43914900
H	1.12112000	4.37662900	-2.25036800
C	1.87846600	-0.65674600	0.04564300
C	3.24967300	0.45104100	1.39060500
C	2.07587800	1.36258400	0.95882300
N	1.19526200	0.41269500	0.25021300
H	4.24487800	0.87910900	1.22543400
H	2.41189300	2.09956700	0.20801300
C	-0.46950400	-2.89001900	-1.55098500
C	0.78137500	-3.80504900	-1.41025500
C	1.22234600	-1.76402000	-0.64336400
N	0.00587300	-1.60005100	-1.02784800
H	-1.27691600	-3.23429700	-0.88512000
H	1.16918900	-4.15298900	-2.37836400
H	3.13940600	0.11494000	2.43280100
H	0.62562700	-4.66355400	-0.74450200
O	3.11567000	-0.73234900	0.54114000
O	1.79755100	-2.95321300	-0.80528100
C	1.38159700	2.08222500	2.10373000
H	2.09517300	2.74514700	2.61764900
H	0.55818100	2.69879700	1.71808200
H	0.97983800	1.34757600	2.81528200
C	-0.99575800	-2.77032700	-2.97577100
H	-1.33562800	-3.75201700	-3.34036300
H	-1.84270000	-2.07132300	-3.01150600
H	-0.20604200	-2.40186000	-3.64925600
C	-2.22658400	0.30628700	2.55302600
H	-2.79843700	0.95482000	1.86556800
C	-1.46926500	-0.75534200	1.76988700
H	-2.10418300	-1.55396000	1.36439700
H	-1.49274900	0.96160100	3.04972100
C	-3.24181800	-0.19520600	3.62090300
C	-3.77677900	1.02951100	4.37954100
H	-4.53713200	0.74044700	5.12409500
H	-2.96320200	1.54997000	4.91144800
H	-4.24092500	1.75156700	3.68706100
C	-2.57386800	-1.15665700	4.61496700
H	-2.23190300	-2.07437700	4.11225700
H	-1.69635300	-0.69215300	5.08910200
H	-3.28296500	-1.45218900	5.40628000
C	-4.41477600	-0.90938400	2.93035000
H	-5.16225000	-1.24642500	3.66760800
H	-4.92127100	-0.23834500	2.21665800
H	-4.07283600	-1.79526700	2.37255000
C	-0.28301700	-1.29541200	2.38802500
O	0.44416400	-0.77967100	3.23742400
O	0.06678100	-2.53138500	1.87337500
C	1.21534400	-3.15148700	2.43558300
H	1.14834700	-3.19683400	3.53292100
H	1.25157100	-4.16734700	2.02062700
H	2.14062900	-2.61912900	2.16524200

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511168 (Hartree/Particle)
Thermal correction to Energy= 0.544389
Thermal correction to Enthalpy= 0.545333
Thermal correction to Gibbs Free Energy= 0.443705
Sum of electronic and zero-point Energies= -5348.789007
Sum of electronic and thermal Energies= -5348.755786
Sum of electronic and thermal Enthalpies= -5348.754841
Sum of electronic and thermal Free Energies= -5348.856469
HF=-5349.3001745
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2363084

^{2}E-TS-F^S-conf2

Ni	-0.81694700	0.17077800	0.07939500
C	-1.30099300	1.58599700	-1.26754800
C	0.24914600	3.84040500	-1.79889600
C	-1.31971800	2.66731800	-0.36362000
C	-0.60828000	1.67059400	-2.49089400
C	0.18552800	2.78524900	-2.73081900
C	-0.50632700	3.77908100	-0.62797700
H	-1.94785900	2.63301700	0.52930000
H	-0.64889400	0.84237400	-3.20016100
H	0.77206900	2.83700000	-3.65184700
H	-0.48670100	4.60840500	0.08365600
Br	-3.07341200	0.38451600	-1.18907400
H	0.87071400	4.71396700	-2.00608300
C	1.88485700	-0.51124000	-0.30615700
C	3.55292300	0.77229700	0.41595300
C	2.20495700	1.54627000	0.48678200
N	1.23100800	0.53951900	0.03722800
H	4.30967800	1.25564600	-0.21422400
H	2.18710700	2.37124800	-0.24327700
C	-0.72142000	-2.84634400	-1.22027700
C	0.53062700	-3.77103500	-1.20207100
C	1.11612500	-1.66867900	-0.75954000
N	-0.15451400	-1.52595400	-0.89631500
H	-1.42034100	-3.09481500	-0.40544500
H	0.72138800	-4.26086000	-2.16720300
H	3.97664100	0.56390900	1.40967100
H	0.50769400	-4.52505800	-0.40391500
O	3.21225000	-0.50963200	-0.19418000

O	1.65212800	-2.87583600	-0.92859600
C	1.85678900	2.08840900	1.86590300
H	2.60571900	2.82873900	2.18647600
H	0.87271800	2.57687300	1.84131300
H	1.82323100	1.27638900	2.60692500
C	-1.46155800	-2.83410500	-2.55246800
H	-1.86589900	-3.83515400	-2.76855900
H	-2.29464000	-2.11917500	-2.51805600
H	-0.78496900	-2.54625800	-3.37293700
C	0.05786900	-1.66351500	2.32329200
H	1.03287000	-1.30706000	1.94911900
C	-1.05354300	-0.68287300	2.00015000
H	-1.07757600	0.20532900	2.64616300
H	-0.14838200	-2.60076800	1.78243400
C	0.27298700	-2.02032600	3.82127700
C	1.32109000	-3.14183900	3.89509900
H	1.55254900	-3.40819900	4.93979800
H	0.96145900	-4.05103500	3.38558300
H	2.26230200	-2.83516000	3.40867800
C	-1.03557100	-2.50486900	4.46411400
H	-1.79087100	-1.70434400	4.48245500
H	-1.46253500	-3.35013500	3.90331700
H	-0.86278900	-2.82906300	5.50388200
C	0.79687600	-0.79571300	4.58767000
H	0.94771100	-1.03060900	5.65430200
H	1.76454600	-0.45966000	4.17923100
H	0.09235500	0.04836500	4.52698200
C	-2.36708200	-1.27390200	1.85945500
O	-2.63813300	-2.41003000	1.46778700
O	-3.38090100	-0.40769900	2.18954100
C	-4.70223100	-0.87570900	1.96990200
H	-4.92938600	-1.75142600	2.59916300
H	-5.37388400	-0.04768300	2.23344300
H	-4.85798700	-1.15762200	0.91739100

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511041 (Hartree/Particle)
Thermal correction to Energy= 0.544433
Thermal correction to Enthalpy= 0.545378
Thermal correction to Gibbs Free Energy= 0.443586
Sum of electronic and zero-point Energies= -5348.786115
Sum of electronic and thermal Energies= -5348.752723
Sum of electronic and thermal Enthalpies= -5348.751778
Sum of electronic and thermal Free Energies= -5348.853570
HF=-5349.297156

^{2}E-TS-F^S-conf3

Ni	-0.88921500	0.32365200	-0.17636200
C	-0.21389300	2.09469200	-0.93191200
C	2.05143300	3.50493700	-0.06878200
C	-0.36091600	3.20496900	-0.07458600
C	1.05444200	1.79192700	-1.47514600
C	2.17976200	2.46980000	-1.00284400
C	0.77338600	3.87674700	0.37533300
H	-1.35209400	3.50344900	0.26228100
H	1.15607600	1.00761800	-2.22331400
H	3.16606700	2.19313000	-1.38456100
H	0.65561200	4.70388700	1.08035900
Br	-1.87664600	1.76554300	-2.25393800
H	2.93503600	4.03837000	0.28781700
C	1.45742200	-1.32267300	0.33562400
C	2.81692700	-0.82838100	2.01126400
C	1.39631200	-0.28933700	2.29085300
N	0.73794700	-0.48179100	0.98039500
H	3.52580600	-0.04436100	1.70586800
H	1.40507000	0.78155500	2.53522900
C	-0.23773000	-1.98838900	-2.80670900
C	0.76857100	-3.17057100	-2.72093300
C	0.98361800	-1.83341700	-0.95923600
N	-0.02969600	-1.28815100	-1.52161800
H	-1.27483200	-2.35570900	-2.83341200
H	1.43938700	-3.23998500	-3.58705900
H	3.24053100	-1.42693300	2.82619700
H	0.28801300	-4.14280200	-2.54455500
O	2.61977600	-1.70812200	0.85734400
O	1.58189600	-2.86424100	-1.54838500
C	0.65445400	-1.09111300	3.36118800
H	1.02605200	-0.82493100	4.36245100
H	-0.42731300	-0.91205100	3.30402200
H	0.81941900	-2.16941300	3.20460200
C	0.00569900	-1.06435800	-3.99585800
H	-0.66427600	-0.19563600	-3.95261800
H	1.04700400	-0.70491200	-4.00128000
H	-0.17654700	-1.60791700	-4.93555600
C	-1.80017500	1.58179600	2.47245800
H	-0.96434100	2.25199400	2.21045200
C	-2.32173100	0.86442400	1.24088700
H	-2.99938500	1.46474900	0.62055100
H	-1.37899100	0.83110700	3.15591000
C	-2.82783700	2.42594000	3.27715500
C	-2.13972900	2.91758000	4.56041800
H	-2.80809000	3.56340700	5.15407100
H	-1.83773900	2.06850200	5.19565000
H	-1.23267300	3.49858900	4.32342800
C	-4.05436400	1.57970000	3.65172600
H	-4.60824500	1.26248300	2.75472600
H	-3.75565000	0.67021800	4.19513300
H	-4.74700700	2.15453300	4.28901300
C	-3.27897400	3.64468100	2.45613700
H	-4.02232000	4.24176300	3.00998700
H	-2.42588900	4.30444700	2.22645400
H	-3.73914400	3.34078900	1.50275600
C	-2.86628100	-0.45923300	1.47284600
O	-2.60029500	-1.23871400	2.38574000
O	-3.73792000	-0.85009500	0.47716700
C	-4.19167400	-2.19228200	0.53322000
H	-4.69468500	-2.41108000	1.48814400
H	-4.89968900	-2.31781500	-0.29698300
H	-3.35754400	-2.90436500	0.41564400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.512125 (Hartree/Particle)
Thermal correction to Energy= 0.545526
Thermal correction to Enthalpy= 0.546471
Thermal correction to Gibbs Free Energy= 0.443511
Sum of electronic and zero-point Energies= -5348.782016
Sum of electronic and thermal Energies= -5348.748615

Sum of electronic and thermal Enthalpies= -5348.747670
Sum of electronic and thermal Free Energies= -5348.850630
HF=-5349.294141

^{2}E-TS-F^S-conf4

Ni	-0.39384000	-0.63620900	0.45910400
C	-1.81117900	-1.32068100	-0.80604600
C	-1.83468200	-3.80669700	-2.07917400
C	-1.26428400	-1.44481000	-2.09920800
C	-2.45823300	-2.40899500	-0.19070400
C	-2.43748300	-3.65268300	-0.82433800
C	-1.25246600	-2.69918700	-2.70982500
H	-0.82705600	-0.57751600	-2.59409700
H	-2.92084200	-2.28111400	0.78681000
H	-2.90197100	-4.50927500	-0.32927600
H	-0.79042200	-2.80860000	-3.69436800
Br	-2.57632200	0.58192700	-0.31380400
H	-1.82906900	-4.78233900	-2.56968400
C	2.29220300	-1.17040800	-0.29679800
C	3.35172700	-3.04462100	0.26612100
C	1.85838900	-3.11523700	0.69550700
N	1.32731500	-1.81759200	0.24511300
H	4.05649900	-3.09943200	1.10596500
H	1.73676700	-3.14377100	1.78835700
C	0.83906600	2.02914600	-1.16306400
C	2.26536100	2.16702900	-1.76601000
C	2.01708700	0.17525000	-0.80931500
N	0.82170700	0.63158000	-0.69645800
H	0.06801300	2.14948700	-1.93895700
H	2.83040800	3.02037500	-1.36882100
H	3.62022600	-3.79554000	-0.49088600
H	2.27279000	2.19603700	-2.86435300
O	3.49956200	-1.72645500	-0.35023700
O	2.95362000	0.94586500	-1.35370400
C	1.08077200	-4.27706500	0.09437000
H	1.50682800	-5.23285300	0.43682300
H	0.03176500	-4.22809100	0.41365400
H	1.11037000	-4.24899400	-1.00565900
C	0.54983900	2.98204400	-0.00691900
H	0.55745600	4.02415100	-0.36127500
H	-0.43703100	2.76479600	0.42527200
H	1.30849200	2.87401300	0.78398800
C	0.61682800	-0.09347800	3.03116700
H	0.96755300	0.70471100	2.35085500
C	-0.67366900	-0.72567300	2.51966000
H	-1.57350000	-0.11971900	2.68217000
H	1.40331600	-0.86519500	3.01546100
C	0.57569500	0.53154500	4.45433700
C	1.99986400	0.97799600	4.82023700
H	2.02657600	1.46754800	5.80803200
H	2.68746900	0.11661700	4.85081300
H	2.39197700	1.69416800	4.07867600
C	0.08222300	-0.49266900	5.48727800
H	-0.95788600	-0.79136000	5.28603900
H	0.69885300	-1.40430100	5.46647300
H	0.12013300	-0.07010200	6.50525100
C	-0.35172400	1.75709700	4.46235200
H	-0.37371200	2.23080300	5.45789100
H	-0.01164100	2.51371100	3.73533800
H	-1.38483100	1.48003900	4.20089700
C	-0.88734900	-2.09898600	2.90117000
O	-0.04253800	-2.96243200	3.14216400
O	-2.22583700	-2.43568600	2.96310300
C	-2.51539300	-3.80559300	3.19248900
H	-2.06572300	-4.16147400	4.13219700
H	-3.60922300	-3.88769300	3.24839600
H	-2.14043500	-4.43996700	2.37257000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.510891 (Hartree/Particle)
Thermal correction to Energy= 0.544513
Thermal correction to Enthalpy= 0.545457
Thermal correction to Gibbs Free Energy= 0.442158
Sum of electronic and zero-point Energies= -5348.789902
Sum of electronic and thermal Energies= -5348.756280
Sum of electronic and thermal Enthalpies= -5348.755336
Sum of electronic and thermal Free Energies= -5348.858635
HF=-5349.3007929

^{2}F^R

Ni	-0.71668400	0.00420100	-0.18905700
C	-1.43494300	1.68778200	-0.76461000
C	-2.17472000	4.13709100	-1.93997800
C	-2.41252500	2.48619600	-0.17292200
C	-0.84479700	2.10809500	-1.96533800
C	-1.20873600	3.32756300	-2.54713700
C	-2.77855200	3.70783100	-0.75601800
H	-2.90497900	2.18102200	0.74688600
H	-0.09504200	1.48902700	-2.46503500
H	-0.73400900	3.64184100	-3.48068400
H	-3.54231700	4.32380000	-0.27329900
Br	-2.40524000	-1.10939800	-1.56719500
C	-3.76753000	1.69956000	3.17604600
H	-2.89631200	2.36776500	3.09253200
H	-4.41698900	1.87185500	2.30283100
H	-4.33103300	2.00254100	4.07329500
C	-3.34734600	0.22467400	3.27700800
C	-2.55793600	-0.21627900	2.00513300
H	-2.44813900	-1.31152500	2.03415700
H	-3.19649100	-0.00504300	1.13475300
C	-1.18057800	0.38904900	1.78868300
C	-4.61174500	-0.64749800	3.34782000
H	-4.35074500	-1.71198900	3.46339000
H	-5.24497600	-0.35871100	4.20260700
H	-5.21418200	-0.54586700	2.43034900
H	-1.13729200	1.47805200	1.86972300
C	-0.12550500	-0.21794200	2.62574800
O	-0.11490500	-1.34821400	3.08582100
O	0.92203900	0.62249100	2.83701600
C	2.00220500	0.11845000	3.62399400
H	2.48645700	-0.73684000	3.13027100
H	2.71702300	0.94422800	3.72179300
H	1.64888200	-0.19977400	4.61534400
C	-2.53010200	0.02821300	4.56331400
H	-2.17140600	-1.00654500	4.65703100
H	-1.65114300	0.69163700	4.58939600
H	-3.14696600	0.26646300	5.44526000
H	-2.45757300	5.09137900	-2.39081000

C	2.10403700	-0.16838400	0.18342900
C	3.46967000	1.58194800	0.10201700
C	2.02388500	2.00612000	-0.29264500
N	1.28724600	0.72673900	-0.22930600
H	4.19761500	1.68191900	-0.71322300
H	1.99403300	2.36346700	-1.33282100
C	0.04887700	-3.12470300	0.62311600
C	1.37460300	-3.54894500	1.31003900
C	1.57757200	-1.51466700	0.44522900
N	0.32915300	-1.72434400	0.24153100
H	-0.77193300	-3.11096700	1.35214100
H	1.79160100	-4.48788300	0.92566800
H	3.84150700	2.09434400	0.99929800
H	1.30089400	-3.57483800	2.40406900
O	3.36329600	0.15830800	0.42441400
O	2.31688700	-2.47551300	0.97294000
C	1.42180200	3.06622000	0.62293400
H	2.03258700	3.98085200	0.57471500
H	0.40006000	3.31126200	0.30611700
H	1.39101100	2.70334700	1.65913800
C	-0.31831100	-3.97679900	-0.58650600
H	-0.51227900	-5.01130000	-0.26344700
H	-1.21606900	-3.57403900	-1.07295600
H	0.50492300	-3.98794300	-1.31833800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.515294 (Hartree/Particle)
Thermal correction to Energy= 0.548283
Thermal correction to Enthalpy= 0.549227
Thermal correction to Gibbs Free Energy= 0.450026
Sum of electronic and zero-point Energies= -5348.828533
Sum of electronic and thermal Energies= -5348.795544
Sum of electronic and thermal Enthalpies= -5348.794600
Sum of electronic and thermal Free Energies= -5348.893801
HF=-5349.3438272
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.279108

^{2}F^R-conf3

Ni	-0.49816600	-0.63607300	-0.29100300
C	-1.91566800	-1.94067700	-0.40476400
C	-3.99759100	-3.81313300	-0.63762600
C	-1.62658900	-3.29630700	-0.58656800
C	-3.24922900	-1.52219400	-0.35287600
C	-4.28684200	-2.45549300	-0.46888800
C	-2.66411600	-4.23026400	-0.69955700
H	-0.59114500	-3.63803700	-0.64013900
H	-3.49505300	-0.46532500	-0.21365400
H	-5.32555600	-2.11738500	-0.41924300
H	-2.42506300	-5.28805800	-0.83963400
Br	-0.50347700	-0.42141700	-2.73792900
C	-2.99514000	-2.52934500	3.22922300
H	-3.39225600	-1.58024200	2.83853900
H	-3.11944800	-3.28680200	2.43925200
H	-3.61843900	-2.82194100	4.09009200
C	-1.52110300	-2.40119100	3.64633900
C	-0.63948000	-2.07836100	2.41007800
H	0.41619600	-2.12025400	2.71611300
H	-0.79320300	-2.88831900	1.68752400
C	-0.88589100	-0.71884100	1.76919700
C	-1.04220800	-3.74770100	4.21209600
H	0.01158100	-3.69051700	4.53072800
H	-1.64459100	-4.04898600	5.08465200
H	-1.12284200	-4.54429800	3.45433700
H	-1.93554100	-0.40828200	1.79178700
C	-0.04621600	0.33768800	2.38551300
O	1.09659600	0.20162000	2.79136200
O	-0.69249600	1.52171100	2.49068000
C	-0.00088100	2.55830200	3.18572400
H	0.97001200	2.77618300	2.71822600
H	-0.64875700	3.44190000	3.14469500
H	0.17626700	2.26873500	4.23262000
C	-1.37881300	-1.31796400	4.72773800
H	-0.32589200	-1.18831700	5.02390700
H	-1.75215800	-0.34300100	4.37735200
H	-1.95616000	-1.58805900	5.62702000
H	-4.80706400	-4.54229000	-0.72213300
C	2.44500800	-0.82987800	0.40187400
C	3.51789300	-2.59788200	1.21137200
C	2.20228900	-3.03167500	0.50601500
N	1.58687600	-1.74243700	0.14215400
H	3.48819000	-2.72599400	2.30203200
H	1.53612600	-3.55280900	1.20837700
C	1.02385800	2.26111500	-0.85150400
C	2.44109000	2.71589700	-0.43700400
C	2.15269100	0.56963100	0.04837600
N	0.95805200	0.91302600	-0.25477700
H	0.96971900	2.10186000	-1.94212500
H	2.43398400	3.35709200	0.45836900
H	4.41686300	-3.07798600	0.80347000
H	3.01627300	3.19553300	-1.23675300
O	3.61172200	-1.16647800	0.94177500
O	3.12022500	1.47009200	-0.07785500
C	2.41660900	-3.89306800	-0.73555400
H	2.85288100	-4.86360300	-0.45433700
H	1.46230000	-4.07635400	-1.24978900
H	3.09629400	-3.39315200	-1.44289200
C	-0.11444800	3.17333300	-0.43480800
H	-0.03593300	4.13810200	-0.95798200
H	-1.07487100	2.71201100	-0.70733000
H	-0.10868300	3.35766200	0.64663400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.515208 (Hartree/Particle)
Thermal correction to Energy= 0.548676
Thermal correction to Enthalpy= 0.549621
Thermal correction to Gibbs Free Energy= 0.448087
Sum of electronic and zero-point Energies= -5348.826463
Sum of electronic and thermal Energies= -5348.792994
Sum of electronic and thermal Enthalpies= -5348.792050
Sum of electronic and thermal Free Energies= -5348.893584
HF=-5349.3416708

^{2}F^S

Ni	-0.3860868	0.4177150	-0.8250254

C	0.0815182	1.7363110	-2.2108364
C	0.8324282	3.8102380	-3.9611274
C	-0.1749638	3.0736850	-1.8805404
C	0.7186892	1.4445190	-3.4198314
C	1.0889792	2.4766910	-4.2937104
C	0.1990592	4.1070650	-2.7495114
H	-0.6774988	3.3260540	-0.9411414
H	0.9354092	0.4110190	-3.6971244
H	1.5823272	2.2333770	-5.2392234
H	-0.0077188	5.1461340	-2.4776964
Br	-2.6162768	0.3840390	-1.6847114
H	1.1232602	4.6140640	-4.6420354
C	2.3001742	-0.1540690	-0.4887834
C	3.6107812	1.2228770	0.6511946
C	2.2034732	1.8541020	0.4851816
N	1.4555222	0.7539470	-0.1502154
H	4.4311912	1.8502010	0.2846346
H	2.2251432	2.6815740	-0.2440184
C	0.1965022	-2.5095570	-2.2361444
C	1.5676582	-3.2420850	-2.2891604
C	1.7829782	-1.2884840	-1.2536494
N	0.5557542	-1.2236020	-1.6198154
H	-0.4808428	-3.0113420	-1.5270544
H	1.9698392	-3.3173580	-3.3098304
H	3.8056732	0.9100540	1.6874796
H	1.5653602	-4.2301530	-1.8145374
O	3.5727422	0.0101470	-0.1670414
O	2.4777582	-2.3850290	-1.5240744
C	1.5821892	2.3323450	1.7860906
H	2.2122692	3.1155640	2.2340846
H	0.5855562	2.7570430	1.6015266
H	1.4857762	1.4911740	2.4859976
C	-0.4905918	-2.3460730	-3.5832574
H	-0.7605008	-3.3325370	-3.9897814
H	-1.4061238	-1.7495240	-3.4656284
H	0.1705932	-1.8414300	-4.3043364
C	-1.5305928	0.4391730	1.7986466
H	-1.9738328	1.2638720	1.2139816
C	-0.9949318	-0.6407160	0.8725766
H	-1.7682178	-1.2929940	0.4586466
H	-0.6879778	0.8679760	2.3578296
C	-2.6111608	-0.0151850	2.8231656
C	-2.9124478	1.1796510	3.7418106
H	-3.6947538	0.9286780	4.4768496
H	-2.0117898	1.4882820	4.2975976
H	-3.2628948	2.0473600	3.1590026
C	-2.0973398	-1.1896780	3.6706546
H	-1.9250938	-2.0858470	3.0544866
H	-1.1483388	-0.9367970	4.1684476
H	-2.8323968	-1.4577130	4.4472366
C	-3.9003748	-0.4293480	2.0977276
H	-4.6778718	-0.7212120	2.8227656
H	-4.2940288	0.3982080	1.4865206
H	-3.7307638	-1.2839900	1.4253076
C	0.1121752	-1.4300720	1.4131026
O	1.0001732	-1.0502830	2.1638236
O	0.1146202	-2.7139450	0.9433806
C	1.1771452	-3.5533320	1.3899126
H	1.2093702	-3.5987930	2.4882816
H	0.9732342	-4.5495800	0.9779556
H	2.1500902	-3.1924100	1.0239436

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)

Zero-point correction= 0.514544 (Hartree/Particle)
Thermal correction to Energy= 0.547766
Thermal correction to Enthalpy= 0.548710
Thermal correction to Gibbs Free Energy= 0.448208
Sum of electronic and zero-point Energies= -5348.823432
Sum of electronic and thermal Energies= -5348.790210
Sum of electronic and thermal Enthalpies= -5348.789266
Sum of electronic and thermal Free Energies= -5348.889768
HF=-5349.3379762

^{2}F^S-conf2

Ni	-0.79578000	0.37783400	0.21147100
C	-0.45334900	1.67917900	-1.23935900
C	0.18379700	3.68020800	-3.11408200
C	-0.44678600	3.02828300	-0.86405100
C	-0.13860200	1.33687100	-2.55681900
C	0.17556900	2.33418900	-3.49125000
C	-0.12862100	4.02552100	-1.79468600
H	-0.70095400	3.32057000	0.15990200
H	-0.13516300	0.29282400	-2.87388000
H	0.41518900	2.05233200	-4.52064600
H	-0.12846600	5.07484500	-1.48622400
Br	-3.10580200	0.77300700	-0.23680600
H	0.43004300	4.45601300	-3.84328300
C	1.86265300	-0.35648900	-0.01660800
C	3.45544500	0.93547600	0.83555600
C	2.07678200	1.63296200	0.98370100
N	1.15991700	0.58642900	0.50521700
H	4.20438800	1.53181000	0.30239300
H	1.98906000	2.47977800	0.28298100
C	-0.71840400	-2.54118100	-1.28303300
C	0.55481300	-3.37077000	-1.61434600
C	1.12478600	-1.44864100	-0.65349300
N	-0.14524200	-1.29519400	-0.75179900
H	-1.29480700	-2.98499000	-0.45509600
H	0.72863300	-3.47248700	-2.69552700
H	3.86106700	0.59591600	1.80022300
H	0.58057700	-4.35775200	-1.13735800
O	3.18174600	-0.26036800	0.03404400
O	1.66672100	-2.58578000	-1.06551900
C	1.73930700	2.10218200	2.38923600
H	2.45199700	2.87538000	2.71294500
H	0.72857900	2.53502800	2.41112700
H	1.77477800	1.26702100	3.10277200
C	-1.64944500	-2.29294100	-2.46053900
H	-2.09386400	-3.24203300	-2.79640800
H	-2.45827600	-1.61375100	-2.15518100
H	-1.10985600	-1.84234400	-3.30788100
C	0.05993600	-1.72801400	2.33070900
H	1.04521200	-1.33139500	2.05030100
C	-1.05076900	-0.74233800	1.99917800
H	-1.09600200	0.10721200	2.69558800
H	-0.09181500	-2.63623500	1.72666600
C	0.19767900	-2.17015000	3.81840800
C	1.29300100	-3.24762500	3.87600400
H	1.47372400	-3.57589900	4.91264600
H	1.00671900	-4.13314600	3.28529400

H	2.24552400	-2.86690900	3.47142300
C	-1.11389500	-2.75866000	4.36196200
H	-1.90647900	-1.99809500	4.41579900
H	-1.47762500	-3.57706000	3.72234100
H	-0.96379300	-3.15692000	5.37881300
C	0.62398700	-0.98010000	4.69170100
H	0.72758000	-1.28512200	5.74569700
H	1.59723200	-0.57937800	4.36381400
H	-0.11171000	-0.16197300	4.65212300
C	-2.36173900	-1.40907600	1.91713500
O	-2.59236400	-2.47015700	1.35311800
O	-3.33730600	-0.74390200	2.57953900
C	-4.65618000	-1.26372500	2.44859400
H	-4.72204000	-2.28251800	2.86025600
H	-5.31174900	-0.58830100	3.01255800
H	-4.95898800	-1.28533900	1.39153000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.514312 (Hartree/Particle)
Thermal correction to Energy= 0.547538
Thermal correction to Enthalpy= 0.548482
Thermal correction to Gibbs Free Energy= 0.448059
Sum of electronic and zero-point Energies= -5348.814053
Sum of electronic and thermal Energies= -5348.780827
Sum of electronic and thermal Enthalpies= -5348.779882
Sum of electronic and thermal Free Energies= -5348.880306
HF=-5349.3283643

$^2F^S$-conf3

Ni	-1.24440900	-0.01888700	-0.11289100
C	-0.25123600	1.60382000	-0.33557000
C	1.24118700	3.96077700	-0.74785400
C	-0.85514000	2.74064900	-0.88651600
C	1.10464500	1.65825300	0.00945700
C	1.84801400	2.82862600	-0.19837500
C	-0.11410600	3.91057000	-1.09059700
H	-1.90933800	2.71085600	-1.16482000
H	1.60818600	0.79816500	0.45106800
H	2.90695600	2.84918700	0.07414800
H	-0.60355900	4.78940500	-1.51992300
Br	-3.22986400	0.34251400	-1.77897800
H	1.81851000	4.87504300	-0.90610700
C	1.12935800	-1.82838900	0.30338900
C	2.44987100	-2.04872200	2.07965800
C	1.10790600	-1.36301800	2.47089000
N	0.38139500	-1.28004000	1.18341900
H	3.33181500	-1.40800000	2.20967400
H	1.27909100	-0.32992500	2.81463800
C	-0.29638700	-1.15013400	-2.97562300
C	0.72309800	-2.27612500	-3.29149100
C	0.73960300	-1.81629600	-1.11666200
N	-0.24167300	-1.08784200	-1.50115900
H	-1.31827300	-1.42875000	-3.26676200
H	1.47654700	-1.99364200	-4.03734400
H	2.60906900	-3.00698600	2.59270400
H	0.25159100	-3.22643900	-3.57701300
O	2.31137200	-2.32548300	0.65423300
O	1.41851900	-2.50166400	-2.02239000
C	0.33350800	-2.12682400	3.53828200
H	0.92524800	-2.16363900	4.46591600
H	-0.62867100	-1.64561800	3.75139700
H	0.14357200	-3.16120200	3.21028100
C	0.05449000	0.20328300	-3.58337200
H	-0.67480300	0.95471200	-3.25566100
H	1.06008100	0.52350400	-3.26999500
H	0.02973100	0.13386000	-4.68184900
C	-1.56072100	1.74640200	2.48149000
H	-0.72249200	2.29523500	2.03085200
C	-2.16431500	0.81011400	1.45213900
H	-2.98695000	1.24257300	0.86778600
H	-1.13393800	1.14708500	3.30219800
C	-2.52887200	2.79940600	3.08444500
C	-1.75879300	3.57208200	4.16722700
H	-2.38701500	4.36002700	4.61360300
H	-1.43343500	2.89914100	4.97740500
H	-0.86061500	4.05317200	3.74642800
C	-3.75744200	2.12865700	3.71737000
H	-4.36006100	1.59673700	2.96474100
H	-3.45917800	1.39495600	4.48150500
H	-4.40708000	2.88187500	4.19253000
C	-2.97978700	3.78310700	1.99223400
H	-3.63873400	4.55827900	2.41601900
H	-2.11469600	4.28265000	1.52817100
H	-3.53901800	3.27642000	1.19011700
C	-2.55133700	-0.52877500	1.96558900
O	-2.68082000	-0.92923200	3.09678800
O	-2.62370300	-1.37045600	0.88104600
C	-2.77114000	-2.77726600	1.09385400
H	-3.64724400	-2.97077800	1.72640900
H	-2.90756200	-3.21895700	0.10044700
H	-1.86956600	-3.18265600	1.57385700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.513722 (Hartree/Particle)
Thermal correction to Energy= 0.547438
Thermal correction to Enthalpy= 0.548382
Thermal correction to Gibbs Free Energy= 0.445882
Sum of electronic and zero-point Energies= -5348.823721
Sum of electronic and thermal Energies= -5348.790005
Sum of electronic and thermal Enthalpies= -5348.789061
Sum of electronic and thermal Free Energies= -5348.891561
HF=-5349.337443

$^2F^S$-conf4

Ni	-1.24440900	-0.01888700	-0.11289100
C	-0.25123600	1.60382000	-0.33557000
C	1.24118700	3.96077700	-0.74785400
C	-0.85514000	2.74064900	-0.88651600
C	1.10464500	1.65825300	0.00945700
C	1.84801400	2.82862600	-0.19837500
C	-0.11410600	3.91057000	-1.09059700
H	-1.90933800	2.71085600	-1.16482000
H	1.60818600	0.79816500	0.45106800
H	2.90695600	2.84918700	0.07414800
H	-0.60355900	4.78940500	-1.51992300
Br	-3.22986400	0.34251400	-1.77897800

H	1.81851000	4.87504300	-0.90610700
C	1.12935800	-1.82838900	0.30338900
C	2.44987100	-2.04872200	2.07965800
C	1.10790600	-1.36301800	2.47089000
N	0.38139500	-1.28004000	1.18341900
H	3.33181500	-1.40800000	2.20967400
H	1.27909100	-0.32992500	2.81463800
C	-0.29638700	-1.15013400	-2.97562300
C	0.72309800	-2.27612500	-3.29149100
C	0.73960300	-1.81629600	-1.11666200
N	-0.24167300	-1.08784200	-1.50115900
H	-1.31827300	-1.42875000	-3.26676200
H	1.47654700	-1.99364200	-4.03734400
H	2.60906900	-3.00698600	2.59270400
H	0.25159100	-3.22643900	-3.57701300
O	2.31137200	-2.32548300	0.65423300
O	1.41851900	-2.50166400	-2.02239000
C	0.33350800	-2.12682400	3.53828200
H	0.92524800	-2.16363900	4.46591600
H	-0.62867100	-1.64561800	3.75139700
H	0.14357200	-3.16120200	3.21028100
C	0.05449000	0.20328300	-3.58337200
H	-0.67480300	0.95471200	-3.25566100
H	1.06008100	0.52350400	-3.26999500
H	0.02973100	0.13386000	-4.68184900
C	-1.56072100	1.74640200	2.48149000
H	-0.72249200	2.29523500	2.03085200
C	-2.16431500	0.81011400	1.45213900
H	-2.98695000	1.24257300	0.86778600
H	-1.13393800	1.14708500	3.30219800
C	-2.52887200	2.79940600	3.08444500
C	-1.75879300	3.57208200	4.16722700
H	-2.38701500	4.36002700	4.61360300
H	-1.43343500	2.89914100	4.97740500
H	-0.86061500	4.05317200	3.74642800
C	-3.75744200	2.12865700	3.71737000
H	-4.36006100	1.59673700	2.96474100
H	-3.45917800	1.39495600	4.48150500
H	-4.40708000	2.88187500	4.19253000
C	-2.97978700	3.78310700	1.99223400
H	-3.63873400	4.55827900	2.41601900
H	-2.11469600	4.28265000	1.52817100
H	-3.53901800	3.27642000	1.19011700
C	-2.55133700	-0.52877500	1.96558900
O	-2.68082000	-0.92923200	3.09678800
O	-2.62370300	-1.37045600	0.88104600
C	-2.77114000	-2.77726600	1.09385400
H	-3.64724400	-2.97077800	1.72640900
H	-2.90756200	-3.21895700	0.10044700
H	-1.86956600	-3.18265600	1.57385700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.513722 (Hartree/Particle)
Thermal correction to Energy= 0.547438
Thermal correction to Enthalpy= 0.548382
Thermal correction to Gibbs Free Energy= 0.445882
Sum of electronic and zero-point Energies= -5348.823721
Sum of electronic and thermal Energies= -5348.790005
Sum of electronic and thermal Enthalpies= -5348.789061
Sum of electronic and thermal Free Energies= -5348.891561
HF=-5349.337443

^{2}F-TS-G^R

Ni	-0.65029000	0.08414400	-0.61920200
C	-1.23302200	1.74718000	-1.27518400
C	-1.95838100	4.31100600	-2.24060100
C	-2.17032100	2.54087000	-0.59256100
C	-0.68008200	2.25938500	-2.46100100
C	-1.03893700	3.52556600	-2.94288100
C	-2.52375200	3.81166200	-1.06182400
H	-2.63631900	2.16809600	0.32156600
H	0.04956600	1.66894000	-3.02484700
H	-0.59458600	3.90013300	-3.86981700
H	-3.24895600	4.41273700	-0.50529000
Br	-2.71524900	-0.90879600	-1.13955500
C	-3.82833100	1.41204000	2.81772400
H	-2.98969800	2.12506300	2.79475700
H	-4.18383600	1.26939100	1.78494200
H	-4.64292100	1.87754400	3.39545200
C	-3.41977100	0.07140000	3.44584900
C	-2.30511300	-0.60971200	2.59294200
H	-2.11235600	-1.61306800	3.00098900
H	-2.69732100	-0.73584500	1.56880100
C	-1.02184200	0.12438000	2.52113100
C	-4.63095700	-0.87239600	3.45915100
H	-4.37185200	-1.84260200	3.91292200
H	-5.46038200	-0.43672500	4.03940700
H	-4.99348100	-1.06283000	2.43615700
H	-0.96080800	1.12097000	2.08197700
C	0.17313300	-0.42142500	3.12565400
O	0.25467100	-1.51504100	3.67117700
O	1.24534300	0.40484200	3.01686000
C	2.45720500	-0.03913000	3.63172800
H	2.81188100	-0.96904700	3.16542800
H	3.18761100	0.76254800	3.47500200
H	2.30433300	-0.21296700	4.70688200
C	-2.91774700	0.29354000	4.88019200
H	-2.59067400	-0.65457300	5.33669100
H	-2.06299900	0.98898000	4.90059600
H	-3.71394600	0.71947000	5.51193500
H	-2.23539200	5.30160500	-2.61046400
C	1.97115800	-0.09741700	0.21540400
C	3.29809300	1.67043400	0.03353500
C	1.83166800	2.07538500	-0.27521500
N	1.13930500	0.76779500	-0.25111100
H	3.95192700	1.68667000	-0.84881700
H	1.74262900	2.50040100	-1.28382300
C	-0.11563600	-3.03007500	0.48351700
C	1.13837800	-3.48169300	1.28438000
C	1.44334000	-1.44117100	0.46505100
N	0.21883000	-1.63666900	0.13536800
H	-1.00745400	-3.01386400	1.12636200
H	1.58349700	-4.41519200	0.91871900
H	3.75208700	2.24927300	0.84717100
H	0.96315100	-3.52676300	2.36583800
O	3.20842300	0.27704500	0.47909100
O	2.11859400	-2.40846500	1.06206000
C	1.22957800	3.03431300	0.74661200
H	1.78818200	3.98275000	0.73625100
H	0.18057000	3.24273000	0.50002700

H	1.28008000	2.59862800	1.75507400
C	-0.39608600	-3.85831900	-0.76565000
H	-0.64244400	-4.89296700	-0.48159700
H	-1.24407500	-3.42591800	-1.31355600
H	0.48522100	-3.87646500	-1.42610400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.513236 (Hartree/Particle)
Thermal correction to Energy= 0.546202
Thermal correction to Enthalpy= 0.547147
Thermal correction to Gibbs Free Energy= 0.446917
Sum of electronic and zero-point Energies= -5348.817156
Sum of electronic and thermal Energies= -5348.784189
Sum of electronic and thermal Enthalpies= -5348.783245
Sum of electronic and thermal Free Energies= -5348.883475
HF=-5349.3303915
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2730662

^{2}G-complex^R

Ni	-0.70885300	0.14705700	-0.57870400
C	-1.24483000	1.78858300	-1.32173600
C	-1.89610100	4.29971600	-2.46436300
C	-2.16732100	2.64953700	-0.70363400
C	-0.66454600	2.20939000	-2.53086100
C	-0.98791700	3.44813800	-3.10117200
C	-2.48431900	3.89422800	-1.26102700
H	-2.64997600	2.34801100	0.22788500
H	0.05941900	1.56706900	-3.04317600
H	-0.52434400	3.74950600	-4.04526600
H	-3.19959700	4.54885800	-0.75420200
Br	-2.82026900	-0.80394300	-0.96925700
C	-3.75426900	1.23963800	2.61779100
H	-2.94278800	1.98338900	2.64672800
H	-3.95454800	0.99398000	1.56344300
H	-4.65387600	1.71782400	3.03745500
C	-3.39782500	-0.02491200	3.41373900
C	-2.17804400	-0.74684800	2.77092400
H	-1.99446100	-1.69522200	3.29785200
H	-2.45966600	-0.99484800	1.72926500
C	-0.91900900	0.02684000	2.72736400
C	-4.58451500	-0.99900500	3.37142500
H	-4.36058600	-1.92088900	3.93231600
H	-5.48321800	-0.54124300	3.81530600
H	-4.82275800	-1.28249200	2.33371700
H	-0.88358500	1.02282400	2.28385000
C	0.30943500	-0.51564500	3.26174800
O	0.43211200	-1.61723100	3.78269100
O	1.36426000	0.32562700	3.10523400
C	2.61634700	-0.11832900	3.63300800
H	2.94917300	-1.03315100	3.12270700
H	3.32800000	0.69439600	3.44974100
H	2.53264100	-0.31888800	4.71113000
C	-3.07585300	0.34142300	4.87009200
H	-2.80788200	-0.55417600	5.45404700
H	-2.22925100	1.04502000	4.92543900
H	-3.94314700	0.81719500	5.35588200
H	-2.14577500	5.26933500	-2.90300400
C	1.91805400	-0.05487300	0.22480200
C	3.23670700	1.71961500	0.05094300
C	1.76402000	2.12619400	-0.21846900
N	1.07964600	0.81491500	-0.22173900
H	3.86903600	1.74652500	-0.84684300
H	1.65283600	2.58424300	-1.21014400
C	-0.17012500	-2.98623800	0.48790000
C	1.10969000	-3.46479000	1.23019700
C	1.39119700	-1.40003200	0.46494500
N	0.15424500	-1.58177900	0.17420700
H	-1.03875700	-2.99360000	1.16171000
H	1.54008500	-4.38632800	0.81930200
H	3.70988500	2.28831900	0.86064600
H	0.97232800	-3.54497000	2.31511900
O	3.15693500	0.32031400	0.48095700
O	2.08356900	-2.38589600	1.00914200
C	1.16967300	3.04017600	0.84834400
H	1.70793900	4.00030900	0.85657900
H	0.11077000	3.23374000	0.63235500
H	1.25358600	2.57358300	1.84101800
C	-0.49536400	-3.77215400	-0.77759400
H	-0.72883600	-4.81669000	-0.52017200
H	-1.36432200	-3.32438100	-1.27830300
H	0.36048200	-3.76478200	-1.47090700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.513178 (Hartree/Particle)
Thermal correction to Energy= 0.547040
Thermal correction to Enthalpy= 0.547984
Thermal correction to Gibbs Free Energy= 0.444939
Sum of electronic and zero-point Energies= -5348.817365
Sum of electronic and thermal Energies= -5348.783502
Sum of electronic and thermal Enthalpies= -5348.782558
Sum of electronic and thermal Free Energies= -5348.885604
HF=-5349.3305428
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2732646

^{2}F-TS-G^S-conf2

Ni	-0.95344700	0.61851600	0.25802000
C	-0.45937400	1.74112700	-1.31151600
C	0.28140900	3.42718600	-3.47486900
C	-1.08273600	2.98466300	-1.51593300
C	0.54239000	1.36770400	-2.22167900
C	0.90991600	2.19076400	-3.29471900
C	-0.71604800	3.82286600	-2.57781100
H	-1.88148300	3.30725900	-0.84136200
H	1.06413600	0.41006800	-2.11438100
H	1.68948900	1.86550800	-3.99038100
H	-1.21688700	4.78715100	-2.70818600
Br	-3.33341600	0.89371900	0.36860800
H	0.56539000	4.07539600	-4.30819900
C	1.62318800	-0.43655700	0.40531000
C	3.31947400	0.75485200	1.20783600
C	1.98928900	1.54306000	1.36600100
N	0.99042100	0.57342900	0.89061700

H	4.08464400	1.28113400	0.62533800
H	1.95974500	2.40046700	0.67298600
C	-1.06048000	-2.41539100	-0.99797500
C	0.16531700	-3.33120800	-1.28386500
C	0.82072500	-1.48088100	-0.23595000
N	-0.43647600	-1.24981200	-0.35543200
H	-1.72869400	-2.86934300	-0.24937800
H	0.37882400	-3.44326700	-2.35649500
H	3.73869800	0.43273300	2.17249400
H	0.09947300	-4.31893500	-0.81164300
O	2.94767600	-0.45228600	0.46832400
O	1.30566900	-2.63062900	-0.68258000
C	1.69312100	2.01834800	2.78053700
H	2.45696200	2.73833500	3.11095100
H	0.71243000	2.51519500	2.81541800
H	1.68106100	1.17137900	3.48319600
C	-1.86104000	-2.00765700	-2.22696700
H	-2.31953500	-2.89245600	-2.69409900
H	-2.65885600	-1.31011700	-1.93346400
H	-1.21528600	-1.50908700	-2.96621600
C	0.05416500	-2.04873200	2.79869200
H	0.96220600	-1.52661400	2.46821400
C	-1.11546100	-1.13872600	2.76491200
H	-1.07472900	-0.15946500	3.24523600
H	-0.12712500	-2.88848500	2.11159800
C	0.38377100	-2.64012500	4.21132000
C	1.53714700	-3.63720400	4.02881100
H	1.83864700	-4.06728600	4.99742600
H	1.24240200	-4.46631300	3.36565100
H	2.41920300	-3.14660300	3.58588400
C	-0.84018400	-3.36461900	4.79098300
H	-1.66570700	-2.66361600	4.99132200
H	-1.21296100	-4.13427300	4.09739600
H	-0.58127700	-3.85620400	5.74237500
C	0.82414400	-1.51505900	5.15977800
H	1.09117700	-1.92383400	6.14739000
H	1.70799000	-0.98779700	4.76460200
H	0.02445300	-0.77353500	5.31081400
C	-2.43667000	-1.69531200	2.49827400
O	-2.64780600	-2.71375900	1.85325200
O	-3.41643700	-0.99511300	3.09436000
C	-4.75152900	-1.42722900	2.83840200
H	-4.89650000	-2.46626700	3.16998400
H	-5.40520600	-0.75310800	3.40453400
H	-4.97366200	-1.35285600	1.76431700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511367
(Hartree/Particle)
Thermal correction to Energy= 0.545241
Thermal correction to Enthalpy= 0.546185
Thermal correction to Gibbs Free Energy= 0.441048
Sum of electronic and zero-point Energies= -5348.803600
Sum of electronic and thermal Energies= -5348.769726
Sum of electronic and thermal Enthalpies= -5348.768782
Sum of electronic and thermal Free Energies= -5348.873919
HF=-5349.3149668

^{2}F-TS-H^R

Ni	-1.36141200	1.24562200	-0.37638400
C	-3.11461200	2.00729900	0.08091300
C	-4.99910900	4.06136700	-0.38938700
C	-3.18896800	3.12798600	0.93047400
C	-4.04774400	1.90396500	-0.96922700
C	-4.96709500	2.92740900	-1.20857600
C	-4.10561600	4.15055300	0.68545700
H	-2.53735500	3.17337100	1.80109900
H	-4.03787300	1.03807900	-1.63369000
H	-5.66218800	2.83663100	-2.04741500
H	-4.13007900	5.01931400	1.34896000
H	-5.72167000	4.85884700	-0.57665800
C	-3.09124700	-0.93581600	0.22285500
H	-2.19009100	-1.56112800	0.20962900
C	-2.77547700	0.33702800	1.00186300
H	-3.64644600	0.65482500	1.57889000
H	-3.32768600	-0.70579100	-0.82759600
C	-4.26514500	-1.77757600	0.78735900
C	-5.58911200	-1.00704700	0.66207900
H	-6.42551900	-1.60731500	1.05457700
H	-5.57065000	-0.06052100	1.22543800
H	-5.80843400	-0.76396800	-0.38954400
C	-4.01024800	-2.14135100	2.25921200
H	-3.04806000	-2.66249000	2.37789400
H	-3.99007100	-1.24876000	2.90457600
H	-4.80908800	-2.79942100	2.63713500
C	-4.35042400	-3.06677500	-0.04447100
H	-5.18250500	-3.70298400	0.29752800
H	-4.51381500	-2.83978100	-1.11060300
H	-3.41982800	-3.65149300	0.03758000
C	-1.67749300	0.18359500	2.01861200
O	-0.90517200	-0.74887300	2.11694700
O	-1.68481600	1.20383800	2.90174600
C	-0.67945900	1.17284100	3.91414700
H	0.32386900	1.19998300	3.46473900
H	-0.84100500	2.06358600	4.53220600
H	-0.76938200	0.26350400	4.52578700
Br	-0.80119300	2.30851600	-2.56719200
C	1.35400700	1.51713100	0.37372700
C	2.26462900	3.46989500	0.90428600
C	0.72502000	3.60586100	0.78049900
N	0.28971000	2.20674000	0.56943000
H	2.82970500	4.14569800	0.25125500
H	0.45231300	4.14146300	-0.14481400
C	0.29117800	-1.67083100	-0.97424600
C	1.82768100	-1.87208600	-0.86202600
C	1.24685800	0.13810800	-0.11864000
N	0.11324700	-0.27861300	-0.53199100
H	-0.23221800	-2.31013000	-0.24449200
H	2.32277900	-1.91724100	-1.84367600
H	2.61381300	3.57625200	1.94264600
H	2.12131600	-2.73901100	-0.25810700
O	2.54047600	2.10283100	0.48444100
O	2.30256500	-0.66932200	-0.18465100
C	0.09288700	4.29931600	1.97576600
H	0.53307900	5.30172200	2.09177900
H	-0.98720600	4.42019600	1.83570400
H	0.27381500	3.73370500	2.90109500
C	-0.28053000	-1.90098000	-2.36537000
H	-0.10613200	-2.94011600	-2.68357000
H	-1.36419300	-1.71535000	-2.36816300
H	0.18728400	-1.22036900	-3.09234400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.513653 (Hartree/Particle)
Thermal correction to Energy= 0.546913
Thermal correction to Enthalpy= 0.547857
Thermal correction to Gibbs Free Energy= 0.446030
Sum of electronic and zero-point Energies= -5348.812342
Sum of electronic and thermal Energies= -5348.779082
Sum of electronic and thermal Enthalpies= -5348.778138
Sum of electronic and thermal Free Energies= -5348.879965
HF=-5349.325995
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2656888

^{2}F-TS-H^S

Ni	-1.59518000	1.00258500	-0.43897600
C	-3.07256300	2.05375900	0.35638700
C	-4.55523600	4.45728300	0.47162600
C	-2.69199900	3.09862100	1.21500400
C	-4.25145100	2.20871900	-0.40029900
C	-4.97108200	3.40265100	-0.35268000
C	-3.41283500	4.29575800	1.25985500
H	-1.82251400	2.97834000	1.85752800
H	-4.58638200	1.39333400	-1.03870800
H	-5.86919000	3.51067400	-0.96678800
H	-3.07851800	5.09957200	1.92116100
H	-5.12468600	5.38899500	0.50667600
Br	-2.32484900	0.68384800	-2.78016300
C	1.31092500	1.73111300	-0.21017300
C	2.08664400	3.80959000	-0.21828600
C	0.69666000	3.74617000	0.46687300
N	0.27602500	2.34784900	0.22104200
H	2.06282400	4.28505500	-1.20937000
H	-0.02257300	4.42200200	-0.01821700
C	0.40935900	-1.73404500	-0.86125900
C	1.96257500	-1.77976200	-0.91179400
C	1.25596700	0.28926800	-0.50632100
N	0.12976100	-0.30344300	-0.61526900
H	0.01815200	-2.28658400	0.00526500
H	2.35181800	-2.05193500	-1.90348500
H	2.86635100	4.27297000	0.39898900
H	2.41311500	-2.42657400	-0.14812000
O	2.43937400	2.40788000	-0.41446700
O	2.38014500	-0.40909400	-0.63601500
C	0.76627900	4.04665100	1.96358600
H	1.10269000	5.08285400	2.12022200
H	-0.21380400	3.93109800	2.44379700
H	1.47862700	3.37006300	2.46115400
C	-0.26356300	-2.26217800	-2.11896000
H	0.00974900	-3.31942000	-2.26364900
H	-1.35233400	-2.18430200	-2.02276300
H	0.04964500	-1.68778800	-3.00319800
C	-1.67132200	0.15551100	2.22174400
H	-1.07029100	1.07652100	2.24927700
C	-2.79638900	0.28424600	1.20131000
H	-3.73433200	0.56752100	1.68339800
H	-0.99130900	-0.63857000	1.88220700
C	-2.12704600	-0.15838200	3.66988100
C	-2.99105200	-1.42928500	3.70141400
H	-3.25079900	-1.69479400	4.73882600
H	-3.93630300	-1.29507700	3.15164400
H	-2.45918600	-2.28068700	3.24979800
C	-2.91603200	1.02521900	4.25199800
H	-2.29982000	1.93823800	4.27441300
H	-3.82050900	1.24758700	3.66386300
H	-3.23842600	0.80810900	5.28299200
C	-0.86252600	-0.38317800	4.51351000
H	-1.12004100	-0.58515800	5.56573000
H	-0.28265400	-1.24060700	4.13525700
H	-0.20865300	0.50397100	4.48903200
C	-3.09927800	-0.96617600	0.42365600
O	-2.39923100	-1.95763600	0.35678300
O	-4.30428700	-0.88514700	-0.16467800
C	-4.65092600	-1.92813800	-1.07759900
H	-4.50604400	-2.91601200	-0.61915300
H	-5.70641600	-1.77378300	-1.33118300
H	-4.03082300	-1.84165900	-1.98268900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.514313 (Hartree/Particle)
Thermal correction to Energy= 0.547464
Thermal correction to Enthalpy= 0.548409
Thermal correction to Gibbs Free Energy= 0.446586
Sum of electronic and zero-point Energies= -5348.811234
Sum of electronic and thermal Energies= -5348.778083
Sum of electronic and thermal Enthalpies= -5348.777139
Sum of electronic and thermal Free Energies= -5348.878961
HF=-5349.3255474

^{2}G-TS-F'^{R}

Ni	-1.44907600	1.16914700	-0.36769400
C	-1.93655600	1.24982600	1.54737300
C	-2.52591200	1.66939600	4.29540900
C	-1.13689500	0.69809000	2.56195300
C	-3.04134700	2.02106700	1.95214600
C	-3.33942900	2.22830000	3.30407500
C	-1.41859400	0.90307900	3.91856700
H	-0.26465300	0.08647300	2.30688600
H	-3.68714300	2.47407100	1.19265300
H	-4.20847800	2.83073900	3.58615600
H	-0.77500600	0.45898100	4.68408500
H	-2.75300400	1.82928000	5.35293300
C	-4.02419000	-1.35321300	-1.06236600
H	-3.40727300	-2.26128000	-1.12525900
C	-4.05582900	-0.88749500	0.34322100
H	-4.58292800	0.02601200	0.61666900
H	-3.55464700	-0.57823100	-1.69312400
C	-5.42353400	-1.64719100	-1.68817000
C	-6.28570300	-0.37502300	-1.68829100
H	-7.23336300	-0.55210000	-2.22208000
H	-6.53732500	-0.05469900	-0.66536800
H	-5.76116300	0.45845300	-2.18194500
C	-6.12565200	-2.75839200	-0.89407400
H	-5.51771000	-3.67756000	-0.87500300
H	-6.30410600	-2.45065200	0.14897600

H	-7.10087600	-3.00473600	-1.34445000
C	-5.19382100	-2.10776000	-3.13490200
H	-6.15082300	-2.34300200	-3.62805200
H	-4.69204700	-1.32288200	-3.72371200
H	-4.56354100	-3.01132700	-3.16801800
C	-3.50821500	-1.68210200	1.42402700
O	-2.79477700	-2.67132900	1.28362000
O	-3.87835300	-1.22803100	2.63633500
C	-3.35729400	-1.92483100	3.76276900
H	-2.25825300	-1.91731000	3.74864700
H	-3.71838600	-1.38852900	4.64762800
H	-3.70867900	-2.96832000	3.77549300
Br	-2.93119000	2.34219200	-1.88181500
C	1.33365200	1.33579200	-0.00228100
C	2.33670500	3.27342900	0.43003400
C	0.84162400	3.51008800	0.06256700
N	0.36187000	2.14583600	-0.20947900
H	3.04244000	3.72846600	-0.27620700
H	0.75569000	4.09057000	-0.86956600
C	-0.15783500	-1.92898500	-0.52342200
C	1.26577700	-2.31286100	-0.03351400
C	1.05700800	-0.10278200	-0.12867600
N	-0.14505500	-0.45850200	-0.40427400
H	-0.93449400	-2.32350300	0.14780000
H	1.81734700	-2.95448400	-0.73245800
H	2.58412500	3.58175800	1.45507400
H	1.27547400	-2.75887600	0.97032300
O	2.51215100	1.82104800	0.35556500
O	1.97892600	-1.03498300	0.05403900
C	0.01458700	4.17924800	1.15341600
H	0.38770000	5.19812700	1.33792400
H	-1.03834700	4.23699500	0.84454200
H	0.06334600	3.60129600	2.08807800
C	-0.45632900	-2.34413500	-1.96099500
H	-0.50001200	-3.44136300	-2.03573000
H	-1.42440200	-1.93699200	-2.28313200
H	0.32281900	-1.97525100	-2.64632000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511376 (Hartree/Particle)
Thermal correction to Energy= 0.545355
Thermal correction to Enthalpy= 0.546300
Thermal correction to Gibbs Free Energy= 0.441225
Sum of electronic and zero-point Energies= -5348.808231
Sum of electronic and thermal Energies= -5348.774252
Sum of electronic and thermal Enthalpies= -5348.773307
Sum of electronic and thermal Free Energies= -5348.878382
HF=-5349.319607
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2635068

^{2}G-TS-F'^{S}

Ni	-1.16710600	1.21767400	-0.93713300
C	-2.23585400	2.11209700	0.46574000
C	-3.71213300	3.56739700	2.41356500
C	-1.76581600	2.26542100	1.78172700
C	-3.46643200	2.71961000	0.15358600
C	-4.20034700	3.43453100	1.10895700
C	-2.48720600	2.98024900	2.74763400
H	-0.81199900	1.81569800	2.07884100
H	-3.86749500	2.62639600	-0.86108700
H	-5.15747800	3.88892800	0.83518000
H	-2.09295100	3.07824200	3.76375600
H	-4.28170900	4.12272600	3.16349900
Br	-2.03350800	1.38336900	-3.19548100
C	1.40820200	2.18266200	-0.29276700
C	2.04126200	4.23752400	-0.85958200
C	0.65008200	3.91088100	-1.47980800
N	0.40595100	2.54222600	-1.00280200
H	2.82295300	4.43632500	-1.60309800
H	0.70730300	3.87473300	-2.57932900
C	0.49638000	-1.13879700	0.84992800
C	1.92544200	-0.98516900	1.44658100
C	1.35603200	0.84775800	0.32344200
N	0.28995300	0.15074200	0.16425900
H	-0.25090700	-1.21461700	1.65347900
H	2.64499000	-1.70669700	1.03576000
H	2.00472000	5.05709300	-0.12852600
H	1.95375400	-1.01494500	2.54299100
O	2.42046900	3.02144400	-0.13414200
O	2.35697600	0.34992300	1.03036100
C	-0.47391100	4.85119700	-1.06460200
H	-0.26997700	5.86923300	-1.42973300
H	-1.42564900	4.50425100	-1.48980600
H	-0.57632900	4.87513600	0.03061000
C	0.33108300	-2.30985100	-0.10965100
H	0.48318700	-3.25893400	0.42747400
H	-0.67876800	-2.31326000	-0.54510400
H	1.07026400	-2.24725900	-0.92373500
C	-3.07004700	-1.13329400	1.35338000
H	-2.39395900	-0.33801900	1.71043500
C	-3.73556600	-0.66173200	0.11815600
H	-4.40265300	0.19844200	0.14596500
H	-2.45744300	-2.01548600	1.11725900
C	-4.03025700	-1.47958900	2.53007900
C	-4.98666400	-2.60404200	2.10652500
H	-5.65003800	-2.88916300	2.93909200
H	-5.62106100	-2.28919500	1.26218700
H	-4.42937700	-3.50168600	1.79245700
C	-4.83059400	-0.23690900	2.95019500
H	-4.16169400	0.60275200	3.19591800
H	-5.50903100	0.10038900	2.15162000
H	-5.44712900	-0.45799600	3.83644800
C	-3.16499400	-1.94952500	3.70858900
H	-3.79203500	-2.21851300	4.57393500
H	-2.56767100	-2.83434500	3.43422500
H	-2.46901100	-1.15644900	4.02734400
C	-3.63911800	-1.38082900	-1.13654100
O	-2.87391600	-2.31091900	-1.36533900
O	-4.51100200	-0.91388400	-2.05323900
C	-4.43773600	-1.49279600	-3.35331600
H	-4.57556900	-2.58350900	-3.30706600
H	-5.24272700	-1.03296000	-3.93926100
H	-3.46483700	-1.26644900	-3.81387900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511018 (Hartree/Particle)
Thermal correction to Energy= 0.545176
Thermal correction to Enthalpy= 0.546120

Thermal correction to Gibbs Free Energy= 0.440427
Sum of electronic and zero-point Energies= -5348.807324
Sum of electronic and thermal Energies= -5348.773166
Sum of electronic and thermal Enthalpies= -5348.772222
Sum of electronic and thermal Free Energies= -5348.877915
HF=-5349.3183414
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2631476

^{2}F'^{R}

Ni	-1.48511000	1.00665900	-0.05685400
C	-1.63243700	1.13354000	1.85697900
C	-1.67467200	1.62047400	4.61557800
C	-0.72152900	0.48489800	2.69366400
C	-2.58251100	2.00523200	2.39717100
C	-2.59861400	2.25109700	3.77480600
C	-0.73830600	0.73576700	4.07280400
H	-0.00567900	-0.23229400	2.28840700
H	-3.30541500	2.49859700	1.74349200
H	-3.33975000	2.93824000	4.19225200
H	-0.01825100	0.23039700	4.72220500
H	-1.69023200	1.81193300	5.69129700
C	-2.82836000	-0.98422100	-1.35054900
H	-2.07249300	-1.77970900	-1.30937700
C	-2.93690700	-0.36636300	0.03602900
H	-3.83769100	0.23429800	0.19021800
H	-2.47354800	-0.23924600	-2.08435900
C	-4.14938100	-1.58280100	-1.91631300
C	-5.19006800	-0.47720100	-2.14929400
H	-6.10160200	-0.89705800	-2.60487600
H	-5.48313700	0.01219900	-1.20811800
H	-4.79600600	0.30398400	-2.81749600
C	-4.71935300	-2.63845500	-0.95529300
H	-3.97649400	-3.42187100	-0.73774300
H	-5.02787200	-2.19058500	0.00178200
H	-5.60663900	-3.12121600	-1.39584600
C	-3.80947300	-2.24877300	-3.25913400
H	-4.71019200	-2.68510100	-3.72060500
H	-3.38627900	-1.51798800	-3.96731800
H	-3.07191600	-3.05686800	-3.12518000
C	-2.75865600	-1.34398100	1.14249200
O	-1.95654900	-2.26090600	1.16162000
O	-3.61009600	-1.12012800	2.16111500
C	-3.43666000	-1.92446800	3.32587400
H	-2.43479500	-1.76865800	3.75258600
H	-4.20268800	-1.59852400	4.03952500
H	-3.56470400	-2.99149900	3.09075500
Br	-2.87324100	2.73162000	-1.31184100
C	1.39060000	1.71692600	-0.11416500
C	2.00455000	3.85614100	-0.04598100
C	0.45323000	3.73999700	-0.06937700
N	0.24438200	2.28348700	-0.11998300
H	2.42379500	4.37130800	-0.91951400
H	0.03277700	4.16276100	-0.99471900
C	0.88005800	-1.87738700	-0.34422000
C	2.35629100	-1.78003500	0.12716600
C	1.48608900	0.24567500	-0.14477200
N	0.44073300	-0.46664200	-0.32924300
H	0.25138200	-2.42926500	0.36721500
H	3.06544500	-2.30903600	-0.52214900
H	2.38925200	4.31437200	0.87570400
H	2.50381600	-2.09105800	1.17108500
O	2.47921200	2.47289900	-0.07910200
O	2.65867100	-0.35192000	0.05163100
C	-0.24463900	4.37055200	1.12784100
H	-0.03509800	5.45093600	1.15565700
H	-1.32886400	4.22177100	1.04618800
H	0.10230600	3.91554300	2.06791500
C	0.73113200	-2.47764900	-1.74032900
H	1.05315100	-3.53022800	-1.73224200
H	-0.31453700	-2.43832300	-2.07289700
H	1.34818500	-1.92904400	-2.46941500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.514885 (Hartree/Particle)
Thermal correction to Energy= 0.548566
Thermal correction to Enthalpy= 0.549510
Thermal correction to Gibbs Free Energy= 0.447077
Sum of electronic and zero-point Energies= -5348.831174
Sum of electronic and thermal Energies= -5348.797494
Sum of electronic and thermal Enthalpies= -5348.796549
Sum of electronic and thermal Free Energies= -5348.898982
HF=-5349.3460592
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2849533

^{2}F'^{S}

Ni	-1.15832800	1.02824200	-0.04287800
C	-1.69719700	1.54618500	1.72867800
C	-2.26808000	2.54651800	4.28319300
C	-0.97276800	1.09321800	2.83330100
C	-2.71372900	2.49053800	1.89759000
C	-2.99618600	2.99114100	3.17436800
C	-1.25620200	1.59703800	4.11028400
H	-0.18121100	0.34926500	2.71346900
H	-3.28347900	2.84120100	1.03370900
H	-3.79229000	3.72988700	3.30086600
H	-0.68076400	1.24377500	4.97031200
H	-2.49178600	2.93543700	5.27951700
Br	-1.94475600	2.57466400	-1.86583900
C	1.75572700	1.50826100	0.28859400
C	2.52108200	3.59800700	0.29276800
C	0.98976500	3.58502600	0.02413500
N	0.66694000	2.15027100	0.09876700
H	3.11228000	4.04434500	-0.51623700
H	0.75890800	3.91060800	-1.00219200
C	0.96165300	-2.03802800	0.28180400
C	2.46587000	-2.04135700	0.67365100
C	1.73613500	0.03662700	0.37416800
N	0.63404100	-0.59903400	0.25121500
H	0.35346300	-2.51796800	1.06209200
H	3.09802800	-2.62330200	-0.00945600
H	2.78352800	4.07098100	1.24995800
H	2.64792500	-2.35754600	1.71007700

O	2.89141300	2.18609800	0.38738600
O	2.86442100	-0.63983200	0.56730400
C	0.16859000	4.41089100	1.00343200
H	0.47167800	5.46771200	0.94723100
H	-0.89688000	4.33503100	0.75232800
H	0.31030300	4.05248500	2.03426200
C	0.66374500	-2.67841200	-1.07104700
H	0.83850600	-3.76433700	-1.02353900
H	-0.37870700	-2.48708800	-1.36175100
H	1.31935100	-2.25300500	-1.84765600
C	-2.41984000	-1.43655300	0.97220900
H	-1.74900200	-1.16555000	1.79833700
C	-2.75548100	-0.21126000	0.13147700
H	-3.58767300	0.37127100	0.53119700
H	-1.86901000	-2.14826800	0.34147500
C	-3.63775300	-2.16993800	1.59499900
C	-3.10249000	-3.42098900	2.30996900
H	-3.91902300	-3.97950100	2.79589800
H	-2.60393700	-4.09971800	1.59869400
H	-2.36941800	-3.14888900	3.08707900
C	-4.63827900	-2.59593900	0.50884300
H	-5.08805800	-1.72667700	0.00619000
H	-4.14692100	-3.21293900	-0.26080000
H	-5.45805400	-3.18845700	0.94659800
C	-4.33498000	-1.26380600	2.62273400
H	-5.16791900	-1.79648000	3.10969100
H	-3.63012900	-0.94120400	3.40601100
H	-4.74907600	-0.35773600	2.15458500
C	-3.02192300	-0.53623400	-1.30044400
O	-2.33697200	-1.26314200	-2.00007100
O	-4.13934200	0.05480600	-1.75692700
C	-4.40284200	-0.06888700	-3.15319900
H	-4.44827300	-1.12557100	-3.45430400
H	-5.36947800	0.41865500	-3.32754400
H	-3.61518400	0.43981900	-3.72908100

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.514932 (Hartree/Particle)
Thermal correction to Energy= 0.548672
Thermal correction to Enthalpy= 0.549616
Thermal correction to Gibbs Free Energy= 0.446374
Sum of electronic and zero-point Energies= -5348.826695
Sum of electronic and thermal Energies= -5348.792955
Sum of electronic and thermal Enthalpies= -5348.792011
Sum of electronic and thermal Free Energies= -5348.895254
HF=-5349.3416273
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2810774

^{2}F'-TS-H^R

Ni	-1.35061000	1.10235700	-0.28688000
C	-1.90565700	0.92023100	1.56509100
C	-1.63770400	1.91075400	4.18887100
C	-0.92834100	0.39468600	2.43067700
C	-2.79021800	1.89920600	2.05240400
C	-2.64490400	2.39875600	3.34785600
C	-0.78404000	0.90368800	3.72406200
H	-0.28393600	-0.41842200	2.09696600
H	-3.56858600	2.29331000	1.39670800
H	-3.32533500	3.17755200	3.70225900
H	-0.00254100	0.50211000	4.37456200
H	-1.52886600	2.30073100	5.20350100
C	-2.75675300	-0.96251600	-1.06634100
H	-1.99510000	-1.74941400	-1.02438000
C	-2.93097200	-0.39521600	0.35085800
H	-3.86815200	0.15135400	0.46510200
H	-2.40072700	-0.20634500	-1.78800500
C	-4.05553500	-1.55843900	-1.68511500
C	-5.10984200	-0.46212100	-1.90176900
H	-5.99111200	-0.87607300	-2.41783700
H	-5.45705200	-0.03379300	-0.94883200
H	-4.70482400	0.36488900	-2.50411600
C	-4.63687300	-2.67001100	-0.79670800
H	-3.88881000	-3.45184700	-0.59332700
H	-4.98998300	-2.27856800	0.16946000
H	-5.49966000	-3.14270100	-1.29300500
C	-3.66237500	-2.15502300	-3.04685600
H	-4.54132600	-2.57973200	-3.55784900
H	-3.22691700	-1.38562300	-3.70478300
H	-2.91870500	-2.95973200	-2.92765300
C	-2.80650100	-1.46659800	1.38088800
O	-1.98884300	-2.36752700	1.35917900
O	-3.70163000	-1.32776200	2.37230800
C	-3.57949600	-2.23033500	3.47167200
H	-2.60013300	-2.10892700	3.95847900
H	-4.38325300	-1.97135300	4.17071200
H	-3.68565400	-3.27284200	3.13778900
Br	-2.81648600	2.72935200	-1.51829100
C	1.47453000	1.72501800	-0.06622400
C	2.12259700	3.82627900	0.27860900
C	0.58978200	3.76692200	0.01544100
N	0.35369500	2.32909700	-0.18977800
H	2.67898000	4.40569600	-0.46904900
H	0.32782300	4.28398600	-0.92110600
C	0.79903100	-1.81411200	-0.53277400
C	2.26212600	-1.82683100	-0.01247100
C	1.51209200	0.25763900	-0.18017100
N	0.43521300	-0.38535800	-0.43611500
H	0.12680100	-2.37937700	0.12874600
H	2.96316700	-2.35294400	-0.67283100
H	2.37257000	4.18477700	1.28710500
H	2.35728900	-2.21059500	1.01310500
O	2.56764900	2.43634000	0.18434800
O	2.64260800	-0.41585600	0.01291100
C	-0.27355800	4.31182600	1.14543000
H	-0.05563300	5.37876700	1.30712900
H	-1.33432100	4.19976900	0.88514800
H	-0.08577800	3.76257200	2.08060300
C	0.66192900	-2.31229000	-1.97014100
H	0.91903500	-3.38123800	-2.02401000
H	-0.36715700	-2.18525700	-2.33207000
H	1.33559500	-1.75608400	-2.64074500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.514921 (Hartree/Particle)
Thermal correction to Energy= 0.547925
Thermal correction to Enthalpy= 0.548869
Thermal correction to Gibbs Free Energy= 0.448088

Sum of electronic and zero-point Energies= -5348.815868
Sum of electronic and thermal Energies= -5348.782863
Sum of electronic and thermal Enthalpies= -5348.781919
Sum of electronic and thermal Free Energies= -5348.882700
HF=-5349.3307884
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2703752

^{2}F'-TS-H^S

Ni	-1.00974200	0.95255300	-0.16249500
C	-2.05186800	1.41737600	1.39617200
C	-2.48245700	3.12470100	3.58755600
C	-1.42638300	1.16233300	2.62403200
C	-2.93020200	2.50991500	1.28190800
C	-3.13294900	3.36120400	2.36870500
C	-1.63000400	2.02357900	3.70922800
H	-0.75254400	0.31000500	2.73427200
H	-3.44224000	2.68703800	0.33433800
H	-3.80743800	4.21516100	2.26437400
H	-1.11455800	1.82860400	4.65340700
H	-2.64693900	3.79041800	4.43792700
Br	-1.49108600	2.37337200	-2.16167900
C	1.80937100	1.40412500	0.49132600
C	2.60362800	3.46802700	0.71137100
C	1.12703600	3.50329100	0.22647100
N	0.76176900	2.07832900	0.21328100
H	3.31002000	3.96452000	0.03499200
H	1.05662000	3.85511700	-0.81552100
C	0.87924900	-2.08729200	0.14732100
C	2.38018100	-2.19122600	0.53447100
C	1.73132700	-0.06559900	0.47373500
N	0.60425800	-0.63969300	0.26986700
H	0.25769500	-2.62777300	0.87428400
H	2.99522500	-2.69830500	-0.22054500
H	2.72481000	3.86244500	1.73110800
H	2.54791900	-2.64897300	1.51884200
O	2.94454800	2.04584000	0.74906600
O	2.82619700	-0.80330800	0.61346600
C	0.18961600	4.32870600	1.09401500
H	0.51330200	5.38078500	1.10641200
H	-0.83030300	4.27710600	0.69245900
H	0.17179300	3.94762000	2.12598900
C	0.55454500	-2.56728600	-1.26397000
H	0.71604800	-3.65351800	-1.34216800
H	-0.49171200	-2.33825500	-1.51244000
H	1.20273000	-2.06321600	-1.99835000
C	-2.32884900	-1.54345800	1.08644000
H	-1.58795400	-1.33308100	1.86911200
C	-2.81630900	-0.26070100	0.44228500
H	-3.71702700	0.12053400	0.91958000
H	-1.81922900	-2.13842600	0.31916200
C	-3.44562800	-2.41278400	1.72120600
C	-2.79361700	-3.71916200	2.20143700
H	-3.53359400	-4.37652700	2.68587400
H	-2.34982000	-4.27230300	1.35766800
H	-1.99250000	-3.51635900	2.93110400
C	-4.53515300	-2.74098100	0.68722500
H	-5.06201300	-1.83574100	0.34699400
H	-4.10396900	-3.23142400	-0.19948500
H	-5.28925900	-3.41761300	1.12050500
C	-4.06838100	-1.68866500	2.92558600
H	-4.83781700	-2.31727300	3.40201800
H	-3.30369800	-1.45267300	3.68297400
H	-4.55115300	-0.74313600	2.63263400
C	-3.12846200	-0.39266900	-1.01378700
O	-2.59858800	-1.16483200	-1.79455000
O	-4.15517900	0.40347400	-1.36213400
C	-4.51991800	0.41151000	-2.74312700
H	-4.78335100	-0.60131600	-3.08131100
H	-5.38800700	1.07668800	-2.82397800
H	-3.68705500	0.79984800	-3.34597800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.514798 (Hartree/Particle)
Thermal correction to Energy= 0.547859
Thermal correction to Enthalpy= 0.548803
Thermal correction to Gibbs Free Energy= 0.447538
Sum of electronic and zero-point Energies= -5348.816789
Sum of electronic and thermal Energies= -5348.783728
Sum of electronic and thermal Enthalpies= -5348.782784
Sum of electronic and thermal Free Energies= -5348.884048
HF=-5349.3315868
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5351.2701106

^{2}H

Ni	-0.49278500	0.48606900	-0.92633700
Br	-2.70170700	0.22916600	-1.64157700
C	1.58555800	2.23323300	-0.33883000
C	1.42044200	4.42446900	-0.70405400
C	0.17113100	3.68833700	-1.27100500
N	0.43723900	2.28506000	-0.93050900
H	1.99623000	4.96791500	-1.46413600
H	0.13666500	3.77347400	-2.37022700
C	1.80699400	-1.28082200	0.42871900
C	3.22778800	-0.79995200	0.83706800
C	2.01981600	0.92136100	0.10482000
N	1.18074700	-0.05165800	-0.08345700
H	1.23658900	-1.60388600	1.31594300
H	4.01249700	-1.19152200	0.17197200
H	1.17587700	5.10269500	0.12666400
H	3.48740400	-1.02064900	1.88003700
O	2.27134500	3.36366700	-0.17215700
O	3.19446800	0.64849700	0.67750700
C	-1.16308600	4.14641200	-0.69499600
H	-1.38215300	5.18316800	-0.99319400
H	-1.96647300	3.49160000	-1.06332500
H	-1.14864300	4.09050000	0.40491100
C	1.78026900	-2.38957000	-0.61364300
H	2.21978900	-3.31510600	-0.21140700
H	0.74081700	-2.59529800	-0.91033000
H	2.34463400	-2.09098100	-1.51083300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)

Zero-point correction= 0.201468 (Hartree/Particle)
Thermal correction to Energy= 0.216791
Thermal correction to Enthalpy= 0.217736
Thermal correction to Gibbs Free Energy= 0.154564
Sum of electronic and zero-point Energies= -4653.582635
Sum of electronic and thermal Energies= -4653.567311
Sum of electronic and thermal Enthalpies= -4653.566367
Sum of electronic and thermal Free Energies= -4653.629539
HF=-4653.7841028
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-4654.9693954

Ph-C^{R}

C	-2.06322000	0.75924400	1.40145300
C	-1.20219200	2.28742700	3.60407900
C	-0.87209400	0.43773300	2.07124800
C	-2.81642200	1.85302100	1.85059000
C	-2.39013000	2.61363900	2.94341800
C	-0.44554900	1.19617200	3.16438100
H	-0.28314700	-0.41892100	1.73799500
H	-3.74583200	2.11199900	1.33666900
H	-2.98985700	3.46291800	3.27989700
H	0.48290000	0.93218700	3.67678400
H	-0.86795600	2.87971500	4.45921300
C	-1.60285600	0.23179800	-1.03371500
H	-0.67866100	-0.35095500	-0.89136000
C	-2.51854700	-0.02834300	0.17859900
H	-3.54509800	0.28572700	-0.04857200
H	-1.31145400	1.29385300	-1.01530500
C	-2.19717300	-0.07872800	-2.42900000
C	-3.35495800	0.88441700	-2.74212600
H	-3.74869700	0.70068700	-3.75464000
H	-4.19307900	0.76390600	-2.03788600
H	-3.02103000	1.93364800	-2.69400800
C	-2.69990100	-1.52919400	-2.52464000
H	-1.90717600	-2.24645900	-2.26405800
H	-3.55585000	-1.71073200	-1.85594900
H	-3.03803600	-1.74912400	-3.54995200
C	-1.07884100	0.13306700	-3.46354200
H	-1.45081000	-0.04026600	-4.48617800
H	-0.68469000	1.16127400	-3.41659800
H	-0.23982800	-0.55890800	-3.28560400
C	-2.56802200	-1.50467500	0.53818500
O	-1.61606500	-2.25326800	0.54268100
O	-3.80230500	-1.88577000	0.89516200
C	-3.95884400	-3.24914300	1.30279600
H	-3.32061300	-3.46916500	2.17085100
H	-5.01588200	-3.36943000	1.56621800
H	-3.69041300	-3.92966600	0.48155500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.312154 (Hartree/Particle)
Thermal correction to Energy= 0.328961
Thermal correction to Enthalpy= 0.329906
Thermal correction to Gibbs Free Energy= 0.266965
Sum of electronic and zero-point Energies= -695.263265
Sum of electronic and thermal Energies= -695.246457
Sum of electronic and thermal Enthalpies= -695.245513
Sum of electronic and thermal Free Energies= -695.308454
HF=-695.5754188
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-696.3521062

Ph-C^{S}

C	-1.62431900	0.30806800	1.47854800
C	-0.97130800	1.62015400	3.88275400
C	-0.57706300	1.23900000	1.52293900
C	-2.34077900	0.03958800	2.65557800
C	-2.01626100	0.69085200	3.84829100
C	-0.25194400	1.89228800	2.71546100
H	-0.01216700	1.45524500	0.61239200
H	-3.15043500	-0.69241500	2.63609500
H	-2.58207200	0.46977900	4.75671900
H	0.56743700	2.61514600	2.73178300
H	-0.71794600	2.12862900	4.81604900
C	-3.34687600	0.15666300	-0.37390900
H	-3.41083100	1.23283700	-0.14821900
C	-1.99587700	-0.35884100	0.15939000
H	-1.19578000	-0.13400900	-0.55706100
H	-4.14795200	-0.33410200	0.20176300
C	-3.61070500	-0.03283900	-1.88750600
C	-5.04911000	0.43504900	-2.16660100
H	-5.28731100	0.35631100	-3.23956600
H	-5.77832200	-0.17669300	-1.61120300
H	-5.19001600	1.48573100	-1.86493100
C	-3.47183800	-1.50511300	-2.31028000
H	-2.43710600	-1.86616800	-2.20182700
H	-4.12396300	-2.15782000	-1.71068500
H	-3.74714300	-1.62552400	-3.37032700
C	-2.63766600	0.82863500	-2.71044400
H	-2.85385600	0.73636200	-3.78687900
H	-2.72396100	1.89304200	-2.43787300
H	-1.58982300	0.52498300	-2.55954300
C	-2.00977200	-1.86560300	0.36138600
O	-2.93279200	-2.49831600	0.82438600
O	-0.84640500	-2.42377900	-0.00083100
C	-0.72561200	-3.83686400	0.19401700
H	-1.48292400	-4.37315100	-0.39627100
H	0.28136000	-4.10656700	-0.14433600
H	-0.85397900	-4.09334900	1.25564900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.312144 (Hartree/Particle)
Thermal correction to Energy= 0.328948
Thermal correction to Enthalpy= 0.329892
Thermal correction to Gibbs Free Energy= 0.266992
Sum of electronic and zero-point Energies= -695.263283
Sum of electronic and thermal Energies= -695.246479
Sum of electronic and thermal Enthalpies= -695.245535

Sum of electronic and thermal Free Energies= -695.308435
HF=-695.575427
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-696.35212

Figure 4.5
G-TS-F^{A}

Ni	-1.15616200	1.05293400	-0.19875700
C	-1.51097400	0.96460900	1.74897900
C	-2.07618600	0.93597800	4.54135300
C	-0.59172800	0.45465200	2.68470500
C	-2.72082400	1.46922200	2.26352400
C	-3.00658700	1.45633000	3.63478500
C	-0.86239100	0.43507000	4.06000500
H	0.37014400	0.05296500	2.34826300
H	-3.46478000	1.88238800	1.57554700
H	-3.95906100	1.85446700	3.99841700
H	-0.12402200	0.02709600	4.75733000
H	-2.29439800	0.92264700	5.61270700
C	-3.43727700	-1.83511700	-0.04045300
Br	-2.91022500	2.07480700	-1.53231700
C	1.50013700	2.00032300	-0.11338500
C	1.94530000	4.16658600	0.12170900
C	0.41493300	3.94705000	-0.06938200
N	0.32163400	2.48830100	-0.22574600
H	2.41124400	4.75201600	-0.68080200
H	0.06493500	4.40962600	-1.00561900
C	0.96442300	-1.58168800	-0.30487500
C	2.50197500	-1.50914500	-0.07407800
C	1.63425600	0.53693300	-0.16314300
N	0.56812000	-0.16267300	-0.31172800
H	0.46242000	-2.06466700	0.54724000
H	3.08440100	-1.93739000	-0.90111100
H	2.20121600	4.60201900	1.09734400
H	2.82809800	-1.94867500	0.87704200
O	2.52254900	2.82019000	0.07776300
O	2.79801500	-0.07752700	-0.02168400
C	-0.45172800	4.42998200	1.08686100
H	-0.37202100	5.52289900	1.18964900
H	-1.50173300	4.16517600	0.90046500
H	-0.13966500	3.95670800	2.02996100
C	0.55690000	-2.27673100	-1.59711200
H	0.84616500	-3.33814700	-1.56554000
H	-0.53038600	-2.21730500	-1.73444200
H	1.04605300	-1.80374700	-2.46269900
C	-2.47611500	-2.50339200	0.88983000
H	-1.85655800	-3.25483400	0.37455100
H	-1.79213600	-1.77438500	1.36842200
H	-2.99970300	-3.01094000	1.72246900
C	-3.28788900	-1.93493500	-1.52496200
H	-2.74424100	-1.06435500	-1.94712400
H	-2.74409200	-2.84439100	-1.82886200
H	-4.27115500	-1.94191900	-2.02992600
C	-4.54307700	-0.98876600	0.50386100
H	-5.53876700	-1.41825900	0.26535700
H	-4.47778000	-0.87411000	1.59583800
H	-4.52796700	0.02385700	0.06050700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.408906 (Hartree/Particle)
Thermal correction to Energy= 0.437403
Thermal correction to Enthalpy= 0.438347
Thermal correction to Gibbs Free Energy= 0.344341
Sum of electronic and zero-point Energies= -5042.591832
Sum of electronic and thermal Energies= -5042.563335
Sum of electronic and thermal Enthalpies= -5042.562391
Sum of electronic and thermal Free Energies= -5042.656397
HF=-5043.0007384
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5044.5965129

F^{A}

Ni	-1.42218100	0.94115600	0.25189900
C	-1.51284000	1.13629900	2.15457700
C	-1.43360600	1.77136000	4.89878800
C	-0.48622900	0.64297700	2.96985100
C	-2.50142700	1.94710800	2.72589400
C	-2.46326100	2.26352300	4.08956700
C	-0.44443000	0.95932500	4.33428500
H	0.29177800	0.00096700	2.54890800
H	-3.30378200	2.34566300	2.10044400
H	-3.24135100	2.90042400	4.52010400
H	0.36515200	0.56794100	4.95710500
H	-1.40365400	2.01690600	5.96339600
C	-2.68024200	-0.63234200	0.42132900
Br	-2.94264800	2.53403300	-1.04161900
C	1.35274400	1.94919300	-0.11867300
C	1.69928400	4.14771900	-0.17228500
C	0.18445900	3.84058200	-0.00447800
N	0.15233500	2.36677600	0.00688300
H	1.94381600	4.68455500	-1.09784700
H	-0.39483700	4.16945400	-0.88022800
C	1.35530800	-1.68840900	-0.07009300
C	2.87058600	-1.35077900	-0.17074600
C	1.64608600	0.50609800	-0.12892800
N	0.70715600	-0.35926500	-0.07537100
H	1.13110700	-2.16371900	0.89881800
H	3.32571400	-1.69730700	-1.10980900
H	2.12879500	4.67918900	0.68858000
H	3.46352400	-1.70909500	0.68035700
O	2.33558900	2.83464000	-0.24033700
O	2.91495100	0.10390400	-0.16744400
C	-0.44065400	4.42966400	1.25227800
H	-0.36553800	5.52782900	1.22665000
H	-1.49910900	4.14733700	1.30796600
H	0.06839900	4.05888300	2.15494000
C	0.85303400	-2.58524500	-1.19486000
H	1.40537300	-3.53747300	-1.18935500
H	-0.21515700	-2.80868600	-1.07312100
H	1.00138100	-2.10042400	-2.17213100
C	-2.10469400	-1.74216800	1.28983100
H	-2.67937100	-2.67301200	1.11963200
H	-1.05513900	-1.96027800	1.05711100
H	-2.17018600	-1.49825400	2.35834800
C	-2.62928300	-0.99731900	-1.06510500
H	-1.60154600	-1.03048200	-1.46205200
H	-3.04813000	-2.01309500	-1.20301500

H	-3.21058000	-0.29572900	-1.67711800
C	-4.08777000	-0.27351700	0.86122700
H	-4.75514000	-1.13849900	0.67870300
H	-4.13119000	-0.04519000	1.93518900
H	-4.48282000	0.58541200	0.30216300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.414327 (Hartree/Particle)
Thermal correction to Energy= 0.441187
Thermal correction to Enthalpy= 0.442131
Thermal correction to Gibbs Free Energy= 0.355667
Sum of electronic and zero-point Energies= -5042.614342
Sum of electronic and thermal Energies= -5042.587482
Sum of electronic and thermal Enthalpies= -5042.586538
Sum of electronic and thermal Free Energies= -5042.673002
HF=-5043.0286691
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5044.6207074

F-TS-H[A]

Ni	-1.33009000	1.13461500	0.19667200
C	-1.69468100	0.97095200	2.06970700
C	-1.18499200	2.07612500	4.62744100
C	-0.60988000	0.52531800	2.85054600
C	-2.53882100	1.95715600	2.61468300
C	-2.28242900	2.50682800	3.87345900
C	-0.34937600	1.08212100	4.10600800
H	0.05486000	-0.25063600	2.47068000
H	-3.38051600	2.32655400	2.02886700
H	-2.94400700	3.28510200	4.26392000
H	0.51253200	0.73182700	4.68074100
H	-0.98632600	2.50569800	5.61230000
C	-2.69347600	-0.51910400	0.94696700
Br	-3.03559400	2.65797900	-0.94020800
C	1.39311900	2.02523600	-0.20364700
C	1.76198100	4.21933200	-0.29181200
C	0.24491300	3.93168200	-0.10886200
N	0.19258800	2.45903400	-0.11523600
H	2.00682300	4.71081600	-1.24262500
H	-0.34157400	4.28725900	-0.96902700
C	1.27916700	-1.60087700	-0.02278100
C	2.79992000	-1.32455000	-0.19778500
C	1.64790400	0.57793400	-0.17432400
N	0.67881400	-0.25035100	-0.06486100
H	1.07901400	-2.02228900	0.97653800
H	3.19655000	-1.70768700	-1.14939800
H	2.19864500	4.78697800	0.54138000
H	3.41733500	-1.69020500	0.63235900
O	2.38911600	2.89938000	-0.30271000
O	2.90031800	0.12681400	-0.22827400
C	-0.35856700	4.49341900	1.17195800
H	-0.28251000	5.59176900	1.17423600
H	-1.41642700	4.20878600	1.23582000
H	0.16409000	4.09911500	2.05713300
C	0.70094800	-2.53409200	-1.07922400
H	1.22649300	-3.50103200	-1.05297100
H	-0.36598300	-2.72104100	-0.89860200
H	0.81634100	-2.10022900	-2.08443300
C	-2.15180000	-1.71798700	1.71228300
H	-2.74573000	-2.60949100	1.44086900
H	-1.10647000	-1.93382400	1.45521500
H	-2.21786300	-1.58534600	2.80026400
C	-2.67547600	-0.84185600	-0.56327200
H	-1.66485400	-0.92344300	-0.99090700
H	-3.14976200	-1.83288700	-0.69971300
H	-3.24554600	-0.11134100	-1.15003400
C	-4.12241500	-0.19650600	1.35144600
H	-4.77643200	-1.02962100	1.03443500
H	-4.23173200	-0.07706000	2.43804100
H	-4.47905500	0.71543100	0.85229700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.414825 (Hartree/Particle)
Thermal correction to Energy= 0.440631
Thermal correction to Enthalpy= 0.441575
Thermal correction to Gibbs Free Energy= 0.357673
Sum of electronic and zero-point Energies= -5042.599705
Sum of electronic and thermal Energies= -5042.573898
Sum of electronic and thermal Enthalpies= -5042.572954
Sum of electronic and thermal Free Energies= -5042.656856
HF=-5043.0145295
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5044.6073643

Ph-*t*Bu

C	-2.65049300	0.95100600	-1.34603200
C	-2.42329700	0.45341500	-4.12915400
C	-2.99956600	1.92953600	-2.29606700
C	-2.18509900	-0.28185000	-1.82899800
C	-2.07214700	-0.52924300	-3.20259600
C	-2.88940700	1.68882700	-3.66636900
H	-3.36609900	2.90271100	-1.96228600
H	-1.90225100	-1.07217300	-1.13408500
H	-1.70605400	-1.50038300	-3.54562700
H	-3.16918200	2.47065000	-4.37713500
H	-2.33561800	0.26117800	-5.20118800
C	-2.78736800	1.26039300	0.15323200
C	-2.36648000	0.07288900	1.03254300
H	-2.48216300	0.33938600	2.09439900
H	-2.98691400	-0.81641500	0.84246700
H	-1.31290200	-0.20240500	0.87099300
C	-4.25879100	1.60136900	0.47098200
H	-4.60694600	2.47716100	-0.09668900
H	-4.91861700	0.75428400	0.22548200
H	-4.37615200	1.82770400	1.54307500
C	-1.89256400	2.46723000	0.50708100
H	-1.97889700	2.70651300	1.57932600
H	-0.83546700	2.24775400	0.28904000
H	-2.17580800	3.36570700	-0.06121100

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.212333 (Hartree/Particle)
Thermal correction to Energy= 0.222060
Thermal correction to Enthalpy= 0.223005

Thermal correction to Gibbs Free Energy= 0.177939
Sum of electronic and zero-point Energies= -389.058242
Sum of electronic and thermal Energies= -389.048515
Sum of electronic and thermal Enthalpies= -389.047571
Sum of electronic and thermal Free Energies= -389.092637
HF=-389.2705756
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-389.6985297

Figure A4.3
^{2}G-TS-F'^{R}-B^{CF3}

Ni	-1.47212800	1.12405500	-0.23789000
C	-2.00755400	1.04105800	1.66180700
C	-2.52250000	1.35329100	4.42749500
C	-1.26667700	0.33930100	2.62921500
C	-3.03441800	1.87965400	2.12629600
C	-3.29556500	2.04284300	3.48880800
C	-1.50765000	0.49060100	3.99420300
H	-0.46404100	-0.33781000	2.32603400
H	-3.64587100	2.43324400	1.40760900
H	-4.09064600	2.71117900	3.82432300
H	-0.90539500	-0.05564000	4.72447500
C	-3.95110400	-1.33196300	-1.18780800
H	-3.32299100	-2.23208700	-1.23006600
C	-3.99915400	-0.84420700	0.21022500
H	-4.50204100	0.09063200	0.45460900
H	-3.49930300	-0.56005000	-1.83268100
C	-5.34712000	-1.67858300	-1.80073200
C	-6.22371500	-0.41921500	-1.87438400
H	-7.17717200	-0.64234300	-2.37983300
H	-6.46247000	-0.03199100	-0.87170300
H	-5.71676300	0.38395700	-2.43214400
C	-6.03978100	-2.75276500	-0.94906600
H	-5.41155300	-3.65349800	-0.85780300
H	-6.24922600	-2.38369300	0.06788100
H	-6.99918200	-3.05043300	-1.40218200
C	-5.10511900	-2.21883200	-3.21740200
H	-6.05870600	-2.47285600	-3.70772000
H	-4.58900300	-1.47303900	-3.84331600
H	-4.48430900	-3.12888000	-3.19275800
C	-3.61276100	-1.70129500	1.31678400
O	-2.94629900	-2.72624100	1.21324800
O	-4.07964000	-1.25982200	2.50021100
C	-3.72720800	-2.01793000	3.65427200
H	-2.64573900	-2.20916100	3.67782300
H	-4.01384500	-1.41235800	4.52111700
H	-4.26050800	-2.98166000	3.66339000
Br	-2.92927600	2.33676000	-1.73291500
C	1.33532100	1.34374200	0.07952700
C	2.42661700	3.27186900	0.24381200
C	0.89908900	3.52937500	0.10629000
N	0.35264300	2.16171600	-0.02680300
H	3.00833000	3.64274300	-0.60961900
H	0.68503500	4.06163900	-0.83303900
C	-0.15228600	-1.92230800	-0.43388100
C	1.26556600	-2.30556400	0.06820400
C	1.05792800	-0.09654500	-0.03088200
N	-0.14346800	-0.45747200	-0.29660500
H	-0.93376500	-2.32942500	0.22355600
H	1.82490700	-2.96668800	-0.60370900
H	2.85622300	3.65629500	1.17768800
H	1.26401500	-2.72589700	1.08284600
O	2.55758400	1.81539300	0.26182400
O	1.98390700	-1.02718000	0.13229100
C	0.27356400	4.33385500	1.26476500
H	0.89320100	5.24748400	1.34272100
C	-0.48056700	-2.32279900	-1.88735300
H	-1.41790600	-1.79488400	-2.12370700
C	-1.15089200	4.76001600	0.90255900
H	-1.58347300	5.40888200	1.67716300
H	-1.16493400	5.31606000	-0.04772600
H	-1.80401800	3.88580000	0.78463000
C	0.35959900	3.57658700	2.59977100
H	1.40411800	3.26434300	2.77497200
H	-0.22461400	2.65147000	2.51632200
C	-0.12598700	4.36341200	3.81606200
H	-1.19281800	4.61967800	3.73207300
H	-0.01345700	3.76508600	4.73352100
H	0.43839700	5.30200200	3.94817700
C	0.57716900	-1.85126700	-2.88752200
H	0.76387100	-0.77058800	-2.79079300
H	1.53543500	-2.38038300	-2.75800600
H	0.24382700	-2.02835000	-3.91988700
C	-0.76842800	-3.83082900	-1.95486900
H	-1.51086800	-4.07043100	-1.17477600
H	0.14569500	-4.39282300	-1.68941500
C	-1.28688800	-4.31061300	-3.30960800
H	-0.53466400	-4.19457300	-4.10490100
H	-1.56324000	-5.37564400	-3.26956900
H	-2.18221100	-3.74312000	-3.61225400
C	-2.77021000	1.49999800	5.89718000
F	-3.22415900	0.34885100	6.45275000
F	-3.67604900	2.45049600	6.18505600
F	-1.64025000	1.81449500	6.57125700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.686644 (Hartree/Particle)
Thermal correction to Energy= 0.732063
Thermal correction to Enthalpy= 0.733007
Thermal correction to Gibbs Free Energy= 0.602778
Sum of electronic and zero-point Energies= -5921.185894
Sum of electronic and thermal Energies= -5921.140475
Sum of electronic and thermal Enthalpies= -5921.139531
Sum of electronic and thermal Free Energies= -5921.269760
HF=-5921.8725379
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.4763259
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.6820834
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.9199479

M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.8922488

^{2}G-TS-F'^{R}-B^{CF3}-conf2

Ni	-1.37140200	1.13521400	-0.26359900
C	-1.91200700	1.10204200	1.64075600
C	-2.59755500	1.27747100	4.38727500
C	-1.21929100	0.36988100	2.62159400
C	-2.95656600	1.93268400	2.08694700
C	-3.30628200	2.02146600	3.43625900
C	-1.54402300	0.45294600	3.97659600
H	-0.39487500	-0.28957300	2.33666800
H	-3.51946800	2.52518000	1.35938100
H	-4.12524900	2.67056400	3.75391000
H	-0.98410500	-0.12439000	4.71569600
C	-4.00280000	-1.17973500	-1.12999300
H	-3.35643900	-2.05883600	-1.25740900
C	-4.08622000	-0.85287500	0.31123200
H	-4.61145200	0.03879600	0.65309100
H	-3.54004600	-0.33078900	-1.66396500
C	-5.37059600	-1.46186200	-1.82665600
C	-6.27738200	-0.22459800	-1.74187200
H	-7.20534000	-0.38625500	-2.31376300
H	-6.56354200	-0.00202500	-0.70214100
H	-5.77123700	0.66468400	-2.15008600
C	-6.05439700	-2.66420300	-1.15947800
H	-5.40997600	-3.55750800	-1.19669200
H	-6.28204000	-2.45695500	-0.10135000
H	-7.00217400	-2.90652600	-1.66691800
C	-5.07767200	-1.78263100	-3.29944100
H	-6.00897800	-2.00185500	-3.84606800
H	-4.58180400	-0.93390400	-3.79747200
H	-4.41739600	-2.66053800	-3.38949300
C	-3.58785000	-1.75629400	1.32879000
O	-2.89640900	-2.74825400	1.11851000
O	-3.97780300	-1.39588800	2.56722200
C	-3.53165700	-2.21390600	3.64471200
H	-2.43882200	-2.32749600	3.62068200
H	-3.83139000	-1.69751100	4.56276000
H	-3.99393100	-3.21224200	3.59283400
Br	-2.80664300	2.47638000	-1.68218000
C	1.42462800	1.39778900	-0.01835600
C	2.39569900	3.39454700	0.12273700
C	0.85403700	3.55465000	-0.02862100
N	0.40608200	2.16336000	-0.15869400
H	2.95896600	3.77720100	-0.73749500
H	0.60836500	4.07591700	-0.96654700
C	-0.02089700	-1.91112700	-0.32899400
C	1.43218400	-2.25576200	0.10031300
C	1.18293600	-0.05352600	-0.06952100
N	-0.02222200	-0.44298000	-0.27616500
H	-0.75500300	-2.28303200	0.39984500
H	1.96681200	-2.91795300	-0.59085700
H	2.80261500	3.81963000	1.04832400
H	1.49689600	-2.65744800	1.12011400
O	2.61337900	1.94359600	0.17504300
O	2.12831800	-0.96272700	0.10126500
C	0.11803200	4.27227100	1.11979000
H	-0.95312400	4.10632300	0.91082500
C	-0.45155700	-2.39903000	-1.72685200
H	-1.40661800	-1.88481500	-1.92053300
C	0.43081300	3.66758900	2.48988500
H	-0.26659500	4.04718200	3.24985900
H	0.32151100	2.57487400	2.47965500
H	1.45092300	3.91823300	2.82474800
C	0.38626300	5.78377100	1.05074900
H	0.16770400	6.13123900	0.02614500
H	1.46367200	5.97208700	1.21353600
C	-0.43023300	6.60858700	2.04453200
H	-0.16512500	6.37647900	3.08739400
H	-0.26261200	7.68622000	1.89298000
H	-1.50913300	6.41565500	1.92387300
C	0.52684000	-1.98503200	-2.82786900
H	0.72087900	-0.90149200	-2.80193200
H	1.49225700	-2.51030900	-2.74265500
H	0.11716700	-2.21535900	-3.82159900
C	-0.73976700	-3.90752300	-1.68350000
H	-1.42437600	-4.09332400	-0.83949100
H	0.19344800	-4.45454500	-1.45476500
C	-1.35744700	-4.46469400	-2.96514100
H	-0.67191200	-4.38951400	-3.82326800
H	-1.62049500	-5.52706400	-2.84490300
H	-2.27977000	-3.91983300	-3.22690000
C	-3.00652000	1.30109800	5.82838100
F	-3.63542400	2.44108800	6.17108900
F	-1.95779200	1.15796300	6.66339300
F	-3.86505800	0.29133800	6.13042400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.685697 (Hartree/Particle)
Thermal correction to Energy= 0.731497
Thermal correction to Enthalpy= 0.732441
Thermal correction to Gibbs Free Energy= 0.599217
Sum of electronic and zero-point Energies= -5921.185124
Sum of electronic and thermal Energies= -5921.139323
Sum of electronic and thermal Enthalpies= -5921.138379
Sum of electronic and thermal Free Energies= -5921.271604
HF=-5921.8708206
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.4766396
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.6828092
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.9181946
M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.8916641

^{2}G-TS-F'^{R}-B^{CF3}-conf3

Ni	-1.48322600	1.09496900	-0.24003000
C	-1.99438200	1.19064300	1.66749100
C	-2.67173600	1.52498900	4.39660400
C	-1.19080300	0.66294000	2.69136100
C	-3.14182100	1.90352800	2.05591200
C	-3.48756800	2.06973200	3.39767600
C	-1.51411900	0.82332400	4.04074100

H	-0.28364400	0.10118300	2.44849700
H	-3.78872900	2.34415800	1.29137500
H	-4.38676700	2.62592500	3.67158500
H	-0.87237800	0.40151200	4.81727700
C	-3.92504900	-1.44404800	-1.09849900
H	-3.28313200	-2.33431100	-1.13744200
C	-3.92236600	-0.90485900	0.28042300
H	-4.43553700	0.02780400	0.51044200
H	-3.51581100	-0.68534000	-1.78593000
C	-5.33885500	-1.83753300	-1.63797200
C	-6.23866900	-0.59597300	-1.72890900
H	-7.21014100	-0.85629300	-2.17923300
H	-6.43826600	-0.16590100	-0.73515200
H	-5.77107700	0.18741800	-2.34590700
C	-5.97813200	-2.88447200	-0.71369600
H	-5.32906400	-3.76844100	-0.60595900
H	-6.15755900	-2.47357900	0.29291300
H	-6.94736500	-3.21991700	-1.11669400
C	-5.14422700	-2.43497400	-3.03892200
H	-6.11264800	-2.72005100	-3.48071100
H	-4.66185300	-1.71083500	-3.71515300
H	-4.51115200	-3.33585400	-2.99986800
C	-3.47960800	-1.71403200	1.40284400
O	-2.80466600	-2.73448600	1.31095700
O	-3.90507600	-1.23561200	2.58559100
C	-3.48935400	-1.94295500	3.75105300
H	-2.39399300	-2.03080600	3.77916200
H	-3.83596100	-1.35232700	4.60538900
H	-3.92894900	-2.95223600	3.77216100
Br	-2.93623300	2.14763600	-1.86197500
C	1.31677400	1.22773800	0.14230700
C	2.38952700	3.08726200	0.69266500
C	0.94155600	3.42149900	0.23614300
N	0.36783000	2.07936200	-0.00091300
H	3.17178500	3.60236000	0.12371500
H	0.94996800	3.94873300	-0.73369600
C	-0.22031700	-1.97765400	-0.55127200
C	1.18932700	-2.40855300	-0.07244400
C	1.01152700	-0.19792400	-0.03741100
N	-0.20206300	-0.52824000	-0.28905200
H	-1.00589500	-2.43694400	0.06415300
H	1.73499500	-3.05239400	-0.77159100
H	2.54369300	3.24931200	1.76877500
H	1.18015500	-2.86824700	0.92530300
O	2.52934800	1.65278500	0.45716800
O	1.92979900	-1.14697500	0.04151600
C	0.14387000	4.27095200	1.23951900
H	0.02589600	3.66035300	2.15324900
C	-0.53029500	-2.24298700	-2.04048100
H	-1.46326300	-1.69352000	-2.24235200
C	0.92612600	5.54380200	1.58543300
H	0.37444700	6.15385200	2.31411700
H	1.91074500	5.32910800	2.02754600
H	1.08525900	6.15942300	0.68411300
C	-1.25169000	4.59472600	0.68920100
H	-1.71804500	3.66582000	0.33837200
H	-1.13907100	5.23164100	-0.20706400
C	-2.18700600	5.26571900	1.69205500
H	-1.83657100	6.26634400	1.98981600
H	-3.19391000	5.38346200	1.26187400
H	-2.28816200	4.65499500	2.60307800
C	0.54129700	-1.68628500	-2.98073300
H	0.71563400	-0.61484500	-2.79835600
H	1.50203900	-2.21603900	-2.87465000
H	0.22796100	-1.78476400	-4.02965100
C	-0.81688000	-3.73807100	-2.25157100
H	-1.55973000	-4.05543400	-1.49971100
H	0.09688500	-4.32262200	-2.03979000
C	-1.33437200	-4.08569500	-3.64655000
H	-0.58078100	-3.89559000	-4.42608200
H	-1.61206700	-5.14933200	-3.70853700
H	-2.22845700	-3.49049800	-3.89371000
C	-3.07651100	1.62670500	5.83551400
F	-3.77601700	2.74757600	6.09765600
F	-2.02027600	1.61137800	6.67187300
F	-3.87118200	0.59110400	6.21506300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.686586 (Hartree/Particle)
Thermal correction to Energy= 0.731971
Thermal correction to Enthalpy= 0.732915
Thermal correction to Gibbs Free Energy= 0.602164
Sum of electronic and zero-point Energies= -5921.184703
Sum of electronic and thermal Energies= -5921.139319
Sum of electronic and thermal Enthalpies= -5921.138375
Sum of electronic and thermal Free Energies= -5921.269125
HF=-5921.8712896
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.4753011
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.68136
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.9172952
M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.8903189

^{2}G-TS-F'^{R}-B^{CF3}-conf4

Ni	-1.42605100	1.07321800	-0.32155700
C	-2.02634100	1.11140900	1.56965200
C	-2.77010500	1.40904900	4.29265900
C	-1.36005100	0.41907800	2.59733300
C	-3.08188900	1.95831400	1.95766900
C	-3.45879400	2.10856700	3.29468400
C	-1.71302400	0.56241400	3.94012100
H	-0.53164000	-0.25422300	2.35968900
H	-3.62818700	2.51872300	1.19315300
H	-4.28214800	2.77319500	3.56562400
H	-1.16926400	0.01880100	4.71574200
C	-4.15968700	-1.18006400	-0.76948400
H	-3.43677500	-1.99641700	-0.89599900
C	-4.34734800	-0.92546300	0.67498200
H	-4.98378800	-0.11086600	1.02126800
H	-3.73253200	-0.27598000	-1.24058500
C	-5.45376800	-1.51605600	-1.57099100
C	-6.44767900	-0.34737600	-1.48791600
H	-7.32499600	-0.53992900	-2.12624500

H	-6.81292800	-0.19603100	-0.46029300
H	-5.97944600	0.59210200	-1.82333000
C	-6.09442500	-2.79572600	-1.01432900
H	-5.39072300	-3.64263500	-1.05744700
H	-6.39739100	-2.66364500	0.03691900
H	-6.99146000	-3.06890400	-1.59333200
C	-5.04326000	-1.73146100	-3.03540400
H	-5.91993900	-1.97344100	-3.65754500
H	-4.57039100	-0.82590900	-3.44848700
H	-4.32312700	-2.56038400	-3.12860800
C	-3.74111100	-1.75933400	1.69054200
O	-2.94787400	-2.67290000	1.48429500
O	-4.15398800	-1.42928800	2.93115100
C	-3.62023700	-2.19239600	4.00896100
H	-2.52345900	-2.22911000	3.95474900
H	-3.93320600	-1.68285800	4.92636700
H	-4.01068400	-3.22219300	3.98632100
Br	-2.80594200	2.39664700	-1.80087900
C	1.36388200	1.13550600	0.04099200
C	2.47655600	3.05748200	0.19295500
C	0.96220900	3.32864100	-0.04720000
N	0.41367800	1.97200000	-0.15924400
H	3.11350200	3.38080000	-0.63976200
H	0.80875700	3.82152900	-1.01759400
C	-0.27026000	-2.06969600	-0.40274600
C	1.12599300	-2.50878200	0.11610300
C	1.02260500	-0.29510900	-0.01982200
N	-0.19489800	-0.60431700	-0.28378600
H	-1.07185600	-2.42692000	0.25808800
H	1.66059400	-3.20389300	-0.54183600
H	2.86312200	3.46917700	1.13323000
H	1.09708500	-2.91484100	1.13613700
O	2.58078600	1.59573100	0.27924000
O	1.90244800	-1.26471200	0.16855600
C	0.22561600	4.14311700	1.03435300
H	-0.84413200	4.03470800	0.78421300
C	-0.58973300	-2.47355500	-1.86095200
H	-1.55061900	-1.98571100	-2.09767300
C	0.43888200	3.58569500	2.44237100
H	-0.24606500	4.07719700	3.14971400
H	0.23368900	2.50801700	2.48862500
H	1.46470100	3.76533700	2.80333700
C	0.58208900	5.63686100	0.96121600
H	1.66463500	5.76505700	1.14648900
H	0.07768000	6.13681300	1.80495100
C	0.18915500	6.33436400	-0.34119600
H	-0.87818400	6.17696700	-0.56789200
H	0.36272400	7.41946400	-0.27319900
H	0.76783500	5.96877300	-1.20444300
C	0.45301900	-1.94959400	-2.85186700
H	0.56200000	-0.85656300	-2.78591200
H	1.44362600	-2.40462700	-2.68749800
H	0.15165200	-2.19004100	-3.88248900
C	-0.78118500	-3.99535800	-1.98841200
H	0.10451800	-4.50953400	-1.57318000
H	-0.78604900	-4.24686200	-3.06211400
C	-2.05403500	-4.54332000	-1.34227100
H	-2.94883000	-4.15084000	-1.85118800
H	-2.08834200	-5.64150300	-1.41601000
H	-2.14253900	-4.26996500	-0.28093400
C	-3.20112300	1.51030100	5.72418800
F	-4.09486000	0.54291200	6.05910500
F	-3.80061700	2.68357500	6.00249700
F	-2.17008100	1.37635200	6.58230000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.685713 (Hartree/Particle)
Thermal correction to Energy= 0.731517
Thermal correction to Enthalpy= 0.732461
Thermal correction to Gibbs Free Energy= 0.599268
Sum of electronic and zero-point Energies= -5921.184889
Sum of electronic and thermal Energies= -5921.139085
Sum of electronic and thermal Enthalpies= -5921.138141
Sum of electronic and thermal Free Energies= -5921.271334
HF=-5921.8706021
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.4759634
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.6825104
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.9185719
M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.8913846

^{2}G-TS-F'^{R}-B^{CF3}-conf5

Ni	-1.37364500	1.13174500	-0.26327400
C	-1.91525500	1.09805300	1.64096100
C	-2.60811500	1.26306600	4.38654500
C	-1.21778700	0.37097500	2.62235100
C	-2.96772200	1.91915000	2.08651000
C	-3.32102600	2.00258700	3.43518900
C	-1.54621100	0.44890100	3.97687000
H	-0.38677800	-0.28048500	2.33826500
H	-3.53385300	2.50829800	1.35879200
H	-4.14636700	2.64394000	3.75211300
H	-0.98274500	-0.12468000	4.71619900
C	-4.00721500	-1.17484600	-1.13838400
H	-3.35951400	-2.05241200	-1.26958400
C	-4.09420000	-0.85717400	0.30475300
H	-4.62300800	0.03055900	0.65139100
H	-3.54334700	-0.32232600	-1.66604000
C	-5.37259800	-1.45343500	-1.84077200
C	-6.27909900	-0.21613900	-1.75369100
H	-7.20562100	-0.37513900	-2.32863700
H	-6.56790600	0.00268600	-0.71389400
H	-5.77148200	0.67443800	-2.15728400
C	-6.05895000	-2.65841800	-1.18101200
H	-5.41456100	-3.55168400	-1.21982000
H	-6.29010300	-2.45559400	-0.12278900
H	-7.00502300	-2.89839500	-1.69271500
C	-5.07471500	-1.76807900	-3.31390300
H	-6.00420600	-1.98462200	-3.86467000
H	-4.57683000	-0.91743700	-3.80663500
H	-4.41437400	-2.64583100	-3.40532700
C	-3.59000100	-1.76270200	1.31755900
O	-2.89637400	-2.75184900	1.10157200

O	-3.97696300	-1.40763500	2.55845600
C	-3.52447100	-2.22778700	3.63167400
H	-2.43092900	-2.33424600	3.60593300
H	-3.82631100	-1.71737500	4.55235700
H	-3.98046500	-3.22877300	3.57580700
Br	-2.80231100	2.49791300	-1.67032500
C	1.42168700	1.40698200	-0.03231800
C	2.37831700	3.41376800	0.07649100
C	0.83475800	3.55907300	-0.06646000
N	0.39645200	2.16342700	-0.16980800
H	2.93230300	3.79181800	-0.79184200
H	0.57963500	4.05317400	-1.01431700
C	-0.00850200	-1.91143800	-0.31188000
C	1.44867500	-2.24612200	0.11173800
C	1.18751500	-0.04610600	-0.07111400
N	-0.01646000	-0.44300800	-0.27148200
H	-0.73664300	-2.28042400	0.42432100
H	1.98337700	-2.90858100	-0.57917200
H	2.78841700	3.85265500	0.99434300
H	1.52077900	-2.64281400	1.13296900
O	2.60820500	1.96480000	0.14275700
O	2.13788700	-0.94941600	0.10317500
C	0.09873900	4.28644500	1.07602700
H	-0.97151500	4.10572100	0.87561300
C	-0.44626300	-2.41306700	-1.70253200
H	-1.40393800	-1.90305800	-1.89427500
C	0.42371500	3.70527300	2.45278300
H	-0.24185800	4.14246700	3.21236700
H	0.27534800	2.61728500	2.47940200
H	1.45905900	3.92796900	2.75863300
C	0.33945700	5.80396900	1.03189500
H	1.41541300	6.01039600	1.18117100
H	-0.16897900	6.24277700	1.90667000
C	-0.15460200	6.50055400	-0.23636600
H	-1.21151900	6.25786800	-0.43499600
H	-0.07172600	7.59431800	-0.14157100
H	0.42410300	6.20926300	-1.12739100
C	0.52398100	-2.00586800	-2.81323600
H	0.71641900	-0.92184100	-2.79694600
H	1.49083800	-2.52886700	-2.73031600
H	0.10819100	-2.24465800	-3.80242600
C	-0.73057000	-3.92175300	-1.64482300
H	-1.40848700	-4.10176400	-0.79433700
H	0.20567400	-4.46498900	-1.41937200
C	-1.35743200	-4.48992600	-2.91720300
H	-0.67922600	-4.41976900	-3.78157800
H	-1.61726800	-5.55190700	-2.78689500
H	-2.28312400	-3.94897400	-3.17539900
C	-3.02110000	1.28038900	5.82661700
F	-3.65769200	2.41573300	6.17060700
F	-1.97391600	1.14116500	6.66416700
F	-3.87460900	0.26484900	6.12357400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.685742 (Hartree/Particle)
Thermal correction to Energy= 0.731525
Thermal correction to Enthalpy= 0.732469
Thermal correction to Gibbs Free Energy= 0.599763
Sum of electronic and zero-point Energies= -5921.185051
Sum of electronic and thermal Energies= -5921.139268
Sum of electronic and thermal Enthalpies= -5921.138324
Sum of electronic and thermal Free Energies= -5921.271030
HF=-5921.8707934
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.4764462
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.6826683
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.918112
M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.891514

^{2}G-TS-F'^{S}-*B*^{CF3}

Ni	-1.23489900	1.32346600	-0.74674200
C	-2.25460700	2.08095700	0.77538100
C	-3.71012200	3.25270900	2.91616200
C	-1.74028200	2.12263300	2.08499000
C	-3.52435100	2.65811900	0.58054100
C	-4.24999200	3.23641100	1.62531200
C	-2.44688200	2.69433500	3.14534300
H	-0.75379200	1.70095000	2.29740900
H	-3.97674400	2.65776100	-0.41675900
H	-5.23461900	3.67119500	1.44100300
H	-2.01961900	2.70902200	4.15050500
Br	-1.20830300	0.50719300	-3.03117100
C	1.39036900	2.31171900	-0.33883500
C	2.09984600	4.25090900	-1.16298400
C	0.61377600	4.01030200	-1.55239200
N	0.31876000	2.71661700	-0.91269800
H	2.77157500	4.31247300	-2.02774100
H	0.52480900	3.85907500	-2.63979200
C	0.51020400	-0.96917300	0.92244500
C	1.96027100	-0.81465200	1.46378000
C	1.36460700	0.99864300	0.32270900
N	0.27068500	0.33233100	0.28535800
H	-0.19968700	-1.08134200	1.75460200
H	2.65598100	-1.58698700	1.11421000
H	2.24956900	5.12590400	-0.51680500
H	2.00869200	-0.74243400	2.55778600
O	2.47847000	3.06420100	-0.39481100
O	2.41818500	0.46859200	0.92217600
C	-0.37160700	5.12009200	-1.13916500
H	0.04870300	6.05634500	-1.55213200
C	0.26773900	-2.11577200	-0.07694900
H	-0.75395000	-1.95943800	-0.45728500
C	-3.09444500	-1.23741700	1.39809600
H	-2.46027200	-0.44080600	1.81954600
C	-3.63656000	-0.77520000	0.10113400
H	-4.20724900	0.15036900	0.03912300
H	-2.46722200	-2.12426500	1.22886300
C	-4.16729700	-1.58586500	2.47779400
C	-5.07925700	-2.70751400	1.95976300
H	-5.80739400	-3.00570400	2.73129600
H	-5.64491500	-2.38333200	1.07137200
H	-4.49430900	-3.59815400	1.67925600
C	-5.00278500	-0.34411800	2.82311800

H	-4.36850900	0.48515400	3.16969500
H	-5.57582900	0.01522100	1.95470300
H	-5.72370400	-0.57634700	3.62358800
C	-3.41782600	-2.06118800	3.73074600
H	-4.12492400	-2.32852100	4.53254300
H	-2.80099000	-2.94808300	3.51195200
H	-2.75222300	-1.27112100	4.11480800
C	-3.58512300	-1.60381900	-1.08951000
O	-3.00247800	-2.67688100	-1.17845700
O	-4.27559700	-1.06209300	-2.11285300
C	-4.22510000	-1.76465100	-3.35258100
H	-4.60721700	-2.79024300	-3.23842500
H	-4.85528800	-1.20044300	-4.05046900
H	-3.19098900	-1.80119200	-3.72505600
C	1.21799600	-2.05615000	-1.27439100
H	0.94230500	-2.81260900	-2.02284200
H	1.15909400	-1.07841000	-1.77451900
H	2.26457500	-2.24733600	-0.98423700
C	0.28636300	-3.46645200	0.65591600
H	-0.35181800	-3.38371100	1.55347800
H	1.30664100	-3.67529400	1.02755200
C	-0.20880300	-4.63520400	-0.19570900
H	0.45783900	-4.83136200	-1.04993800
H	-0.26226200	-5.56077700	0.39878600
H	-1.21269200	-4.41816100	-0.59174400
C	-1.73144000	4.87833400	-1.80033300
H	-2.42409600	5.71056000	-1.61163400
H	-1.62685600	4.76813200	-2.89073100
H	-2.19466500	3.96205800	-1.40863700
C	-0.46403400	5.26165200	0.38883200
H	0.54995400	5.39803100	0.80279800
H	-0.84149400	4.31711000	0.80775300
C	-1.34671800	6.41374100	0.86641000
H	-2.40220700	6.25669200	0.59652500
H	-1.30198400	6.50890500	1.96251300
H	-1.02800900	7.37621900	0.43192400
C	-4.51411700	3.78047100	4.06574500
F	-5.23257500	2.80223900	4.66979100
F	-5.40025100	4.72155000	3.68708700
F	-3.74049800	4.32559800	5.02587800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.686304 (Hartree/Particle)
Thermal correction to Energy= 0.731871
Thermal correction to Enthalpy= 0.732815
Thermal correction to Gibbs Free Energy= 0.601058
Sum of electronic and zero-point Energies= -5921.185076
Sum of electronic and thermal Energies= -5921.139509
Sum of electronic and thermal Enthalpies= -5921.138565
Sum of electronic and thermal Free Energies= -5921.270322
HF=-5921.8713796
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.4771618
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.6840862
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.9212352
M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.8937697

^{2}G-TS-F'^{S}-*B*^{CF3}-conf2

Ni	-1.10822300	1.25417000	-0.79901600
C	-2.22918700	2.11502800	0.57950300
C	-3.84554200	3.41900800	2.51146200
C	-1.86131900	2.16275000	1.93670400
C	-3.42418900	2.76535200	0.22095300
C	-4.23065000	3.40712000	1.16568900
C	-2.64974000	2.80023900	2.89666600
H	-0.93288100	1.68704200	2.26679800
H	-3.74871900	2.76071700	-0.82475500
H	-5.15986800	3.89361700	0.86157700
H	-2.34191200	2.81509600	3.94474100
Br	-1.79372500	1.05652000	-3.10566200
C	1.49389100	2.24489600	-0.28788400
C	2.16680600	4.20526000	-1.09585900
C	0.69179100	3.92699800	-1.51197300
N	0.44574300	2.60328400	-0.93044800
H	2.86021700	4.24060600	-1.94512000
H	0.60732300	3.82954600	-2.60531800
C	0.57168000	-1.02936600	0.95535900
C	2.03376500	-0.91363600	1.47445400
C	1.45211900	0.93508100	0.38300700
N	0.34602300	0.28640700	0.34429200
H	-0.12581400	-1.14650400	1.79759600
H	2.71304100	-1.68059600	1.08223600
H	2.29551900	5.10211300	-0.47746800
H	2.10484600	-0.88321100	2.56890900
O	2.54338700	3.04962700	-0.27273100
O	2.49939900	0.38303500	0.97047400
C	-0.35986600	4.95077800	-1.04322100
H	-1.33145200	4.49198800	-1.29677900
C	0.28620900	-2.14721700	-0.06491800
H	-0.75592600	-1.99122200	-0.38601700
C	-3.06255700	-1.17717500	1.39825200
H	-2.41803600	-0.37690700	1.79631400
C	-3.64187600	-0.72581700	0.11352300
H	-4.23553600	0.18603500	0.06540800
H	-2.43654500	-2.06333800	1.22022700
C	-4.10739600	-1.51913700	2.50670800
C	-5.00656600	-2.66979000	2.03151700
H	-5.72054700	-2.95873400	2.81962200
H	-5.58774300	-2.37971700	1.14132200
H	-4.40978900	-3.55838200	1.76926900
C	-4.96215800	-0.28673000	2.83980200
H	-4.33806500	0.56887300	3.13752200
H	-5.57289700	0.02985400	1.98040800
H	-5.65099700	-0.50999900	3.67040200
C	-3.32522700	-1.95129700	3.75530500
H	-4.01132600	-2.22079900	4.57441000
H	-2.68994400	-2.82659900	3.54229200
H	-2.67311100	-1.13775300	4.11260400
C	-3.58921600	-1.54421500	-1.08320100
O	-2.91938000	-2.56166200	-1.21598300
O	-4.38165000	-1.06262900	-2.06032300
C	-4.32431500	-1.73734400	-3.31429400

H	-4.58797800	-2.79970800	-3.20224700
H	-5.04675700	-1.23316400	-3.96718700
H	-3.31401400	-1.65717200	-3.74207400
C	1.16824600	-2.03982700	-1.31075400
H	0.88347900	-2.79911800	-2.05265100
H	1.05120200	-1.05807600	-1.79455200
H	2.23643800	-2.18913100	-1.08075100
C	0.35012200	-3.52066900	0.62106700
H	-0.23662800	-3.46798400	1.55534400
H	1.38984100	-3.73933700	0.92701400
C	-0.19155500	-4.66267000	-0.23897700
H	0.43160700	-4.83597800	-1.13018900
H	-0.21990000	-5.60506100	0.33009600
H	-1.21217800	-4.43184200	-0.58108700
C	-0.32802000	5.17629300	0.46958600
H	-1.21259400	5.74084400	0.79675100
H	-0.34064700	4.22297500	1.01506400
H	0.56131700	5.74918500	0.78013500
C	-0.22279500	6.24980400	-1.85281700
H	-0.21659000	5.99370800	-2.92646900
H	0.76068500	6.70971000	-1.64326400
C	-1.32804800	7.27081000	-1.58698100
H	-1.30421300	7.64219500	-0.55098800
H	-1.22726000	8.14207500	-2.25260200
H	-2.32316800	6.82853000	-1.75985900
C	-4.74609300	4.00817100	3.55462900
F	-5.56928200	4.95048300	3.05673900
F	-4.05755100	4.57562900	4.56601100
F	-5.54157500	3.06811800	4.12226700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.685422 (Hartree/Particle)
Thermal correction to Energy= 0.731471
Thermal correction to Enthalpy= 0.732415
Thermal correction to Gibbs Free Energy= 0.597969
Sum of electronic and zero-point Energies= -5921.183404
Sum of electronic and thermal Energies= -5921.137356
Sum of electronic and thermal Enthalpies= -5921.136412
Sum of electronic and thermal Free Energies= -5921.270857
HF=-5921.8688265
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.4759019
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.682429
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.9192238
M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.892584

^{2}G-TS-F'^{S}-B^{CF3}-conf3

Ni	-1.18601500	1.31387500	-0.73781600
C	-2.19160100	2.13060400	0.76227900
C	-3.68810700	3.29703200	2.87579100
C	-1.67564200	2.22531300	2.06770100
C	-3.47831700	2.66339200	0.55268900
C	-4.22531000	3.23603200	1.58495100
C	-2.40341200	2.79506900	3.11574700
H	-0.67746500	1.83661200	2.29051900
H	-3.92682100	2.62922400	-0.44550900
H	-5.22458500	3.63138500	1.39074100
H	-1.97776200	2.84744700	4.12030500
Br	-1.33032500	0.58948300	-3.04125000
C	1.42849500	2.27528500	-0.23556100
C	2.07198000	4.32776400	-0.76663300
C	0.69768100	4.01442500	-1.41644100
N	0.38294300	2.69039400	-0.84984300
H	2.84444300	4.64941100	-1.47364300
H	0.80337800	3.88044400	-2.50773600
C	0.50825800	-1.04441500	0.88568600
C	1.95880200	-0.92889300	1.43607000
C	1.38760800	0.93517700	0.36641600
N	0.28891000	0.27979500	0.28901200
H	-0.20505000	-1.17129600	1.71244000
H	2.64859900	-1.68796000	1.04744700
H	1.99462000	5.05101600	0.05850500
H	2.00692200	-0.91377300	2.53221200
O	2.49645300	3.05638700	-0.18079600
O	2.42827400	0.37624000	0.96110500
C	-0.39560200	5.06139500	-1.16120200
H	-0.58070600	5.07230400	-0.07146000
C	0.25227800	-2.15617000	-0.14859700
H	-0.77452500	-1.98806800	-0.50941100
C	-3.06473500	-1.18763600	1.41428200
H	-2.42616500	-0.38468600	1.81713700
C	-3.63304300	-0.73922700	0.12382100
H	-4.19852800	0.18951300	0.06204500
H	-2.43799200	-2.07397300	1.24035400
C	-4.11588400	-1.53320700	2.51641600
C	-5.03512800	-2.65961800	2.02220800
H	-5.74605100	-2.95630600	2.81017700
H	-5.62036100	-2.34090100	1.14460700
H	-4.45379000	-3.54992200	1.73332000
C	-4.94659900	-0.29124900	2.87120800
H	-4.30697200	0.53989400	3.20257300
H	-5.53517900	0.06410800	2.01155600
H	-5.65283100	-0.52027000	3.68554500
C	-3.34089900	-2.00025200	3.75689200
H	-4.03158500	-2.26383200	4.57408700
H	-2.72723000	-2.88757700	3.53098400
H	-2.66902000	-1.20702800	4.12310900
C	-3.61098600	-1.58162500	-1.05777600
O	-3.02807100	-2.65447000	-1.14914000
O	-4.32667000	-1.05214700	-2.06978700
C	-4.29586400	-1.76226100	-3.30575200
H	-4.66846200	-2.78970600	-3.17795800
H	-4.94308800	-1.20665200	-3.99482900
H	-3.26889100	-1.79445200	-3.69815800
C	1.18683700	-2.05520900	-1.35559200
H	0.90942900	-2.79371300	-2.12107300
H	1.11339300	-1.06420800	-1.82710600
H	2.23905400	-2.24302900	-1.08399000
C	0.27952100	-3.53020400	0.53904800
H	-0.34990500	-3.47745100	1.44507600
H	1.30361600	-3.74994800	0.89346900
C	-0.22225300	-4.67176500	-0.34493700
H	0.43639900	-4.83933300	-1.21134000

H	-0.26836400	-5.61595900	0.22015900
H	-1.23043200	-4.44450600	-0.72377600
C	0.08978500	6.44786600	-1.59915700
H	-0.68038600	7.20954600	-1.41370400
H	0.99385000	6.76561900	-1.05759600
H	0.31883600	6.45645900	-2.67794200
C	-1.69869600	4.66027600	-1.86918200
H	-1.91090500	3.60607100	-1.64187400
H	-1.53845000	4.70691100	-2.96118100
C	-2.91282800	5.49843000	-1.47796000
H	-2.79709400	6.55658100	-1.75973700
H	-3.82125800	5.12272900	-1.97393000
H	-3.08721200	5.45279500	-0.39117500
C	-4.51717700	3.81241700	4.01319800
F	-5.22366000	2.82193600	4.61184900
F	-5.41848700	4.73287600	3.61893400
F	-3.76850000	4.37761500	4.98112900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.685601
(Hartree/Particle)
Thermal correction to Energy= 0.731508
Thermal correction to Enthalpy= 0.732452
Thermal correction to Gibbs Free Energy= 0.598530
Sum of electronic and zero-point Energies= -5921.184769
Sum of electronic and thermal Energies= -5921.138863
Sum of electronic and thermal Enthalpies= -5921.137919
Sum of electronic and thermal Free Energies= -5921.271841
HF=-5921.8703707
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.4759366
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.6829721
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.9198895
M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.8931311

^{2}G-TS-F'^{S}-B^{CF3}-conf4

Ni	-1.15097800	1.23714000	-0.81694600
C	-2.24427300	2.10895100	0.58030300
C	-3.78385300	3.47091100	2.53525800
C	-1.84608300	2.15847500	1.92884400
C	-3.42805900	2.78912000	0.24127400
C	-4.19686800	3.45886100	1.19766600
C	-2.59692600	2.82372200	2.90018300
H	-0.92397500	1.66155900	2.24489800
H	-3.77125700	2.78627300	-0.79802600
H	-5.11867700	3.96821000	0.90869800
H	-2.26562600	2.83925900	3.94105600
Br	-1.94299500	1.37048500	-3.09803800
C	1.44392400	2.20070700	-0.23882600
C	2.14947200	4.14985400	-1.04928400
C	0.68919300	3.86886400	-1.51126500
N	0.41712800	2.55818500	-0.91372600
H	2.87071800	4.17536100	-1.87554800
H	0.64472500	3.73757000	-2.60156400
C	0.52997000	-1.10866900	0.91400500
C	1.92745200	-0.93495400	1.57119000
C	1.38178000	0.88866400	0.42533800
N	0.29386200	0.21556200	0.31806300
H	-0.23579800	-1.28572700	1.67980800
H	2.66268200	-1.69424400	1.27828200
H	2.25949100	5.05330100	-0.43675900
H	1.88513100	-0.86646600	2.66609000
O	2.49673100	3.00168300	-0.20187600
O	2.40549600	0.35701800	1.07149200
C	-0.37589800	4.90432000	-1.10295800
H	-1.33758600	4.43280100	-1.36864800
C	0.42431400	-2.20508600	-0.16757100
H	-0.60404900	-2.13748500	-0.55759600
C	-3.12808000	-1.08764400	1.54548200
H	-2.51180900	-0.27298800	1.95797300
C	-3.65438300	-0.66713400	0.22852900
H	-4.27283800	0.22452400	0.13907800
H	-2.48353200	-1.96620400	1.41122000
C	-4.21658600	-1.42355600	2.61243000
C	-5.08294800	-2.59123000	2.11795800
H	-5.82983000	-2.87310300	2.87766400
H	-5.62494500	-2.32347700	1.19655700
H	-4.46644300	-3.47848400	1.90058700
C	-5.09676700	-0.19505600	2.88882500
H	-4.49494500	0.67091400	3.20280900
H	-5.67104800	0.10337500	1.99827000
H	-5.82050300	-0.41359500	3.69058600
C	-3.48579100	-1.82873700	3.90072100
H	-4.20475100	-2.09002400	4.69390100
H	-2.83590400	-2.70238100	3.73022200
H	-2.85560900	-1.00428800	4.27200900
C	-3.52951800	-1.50227000	-0.95039900
O	-2.83830200	-2.51165400	-1.03580900
O	-4.27271100	-1.04294400	-1.97623900
C	-4.12938300	-1.72166200	-3.22070600
H	-4.36202200	-2.79183300	-3.11538700
H	-4.83325600	-1.24466500	-3.91298500
H	-3.10251300	-1.60805600	-3.59885000
C	1.38875000	-1.96108600	-1.33115400
H	1.25872000	-2.73853100	-2.09907500
H	1.20233800	-0.98889900	-1.81211000
H	2.44423100	-1.99092200	-1.01261100
C	0.59813000	-3.61173600	0.42954300
H	1.59706200	-3.70114000	0.89475500
H	0.60191800	-4.32632200	-0.41041800
C	-0.48568100	-4.02689800	1.42507500
H	-1.48186600	-3.94961700	0.96305700
H	-0.33980000	-5.06793100	1.75267800
H	-0.48609600	-3.40001700	2.33111800
C	-0.38719500	5.18021400	0.40115400
H	-1.26443600	5.78991400	0.66563000
H	-0.44955600	4.25077800	0.98311800
H	0.50719400	5.73814800	0.72339600
C	-0.24466000	6.20355500	-1.91398300
H	0.72729400	6.68061900	-1.68948100
H	-1.01001100	6.90338300	-1.53866400
C	-0.40927400	6.04291800	-3.42560800
H	-1.34172900	5.50702400	-3.66800600
H	-0.44492400	7.02435400	-3.92329100

H	0.42201000	5.48065500	-3.87999900
C	-4.64508600	4.09444800	3.59145900
F	-5.44955100	5.05746200	3.10273800
F	-3.91961800	4.64810200	4.58448700
F	-5.45732400	3.18328800	4.18271200

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.685518 (Hartree/Particle)
Thermal correction to Energy= 0.731517
Thermal correction to Enthalpy= 0.732461
Thermal correction to Gibbs Free Energy= 0.597970
Sum of electronic and zero-point Energies= -5921.183405
Sum of electronic and thermal Energies= -5921.137406
Sum of electronic and thermal Enthalpies= -5921.136461
Sum of electronic and thermal Free Energies= -5921.270953
HF=-5921.8689228
UB3LYP-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5924.475699
PBE0-D3(BJ)/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5921.682036
M06-D3/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.9186702
M06/def2-TZVPP-CPCM(THF)//UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
HF=-5922.8915719

Figure A3.5

B[50]

C	-4.34827600	-3.68665100	-0.81733300
H	-3.33791200	-3.45612600	-1.17650200
C	-4.44825500	-4.42846400	0.29658200
H	-5.41657000	-4.70410300	0.72255200
C	-3.24236300	-4.91076300	1.00381100
O	-2.09126400	-4.70242500	0.67704800
O	-3.57514600	-5.63311400	2.09032000
C	-2.49364600	-6.15718100	2.86121000
H	-1.85682400	-5.34527900	3.24334000
H	-2.94776600	-6.70607300	3.69458500
H	-1.87313900	-6.83360600	2.25438200
C	-5.49370100	-3.15002500	-1.60704000
H	-5.43736900	-2.04942100	-1.66950400
H	-5.45077700	-3.51694300	-2.64721200
H	-6.46486700	-3.42980200	-1.17364700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.122756 (Hartree/Particle)
Thermal correction to Energy= 0.130927
Thermal correction to Enthalpy= 0.131871
Thermal correction to Gibbs Free Energy= 0.090117
Sum of electronic and zero-point Energies= -345.436736
Sum of electronic and thermal Energies= -345.428565
Sum of electronic and thermal Enthalpies= -345.427621
Sum of electronic and thermal Free Energies= -345.469375
HF=-345.5594917

B-TS-C[50]

C	-4.92439700	-3.85569000	-1.07695700
H	-4.06866700	-3.42791400	-1.60709600
C	-4.64324200	-4.54726400	0.07562600
H	-5.44124000	-4.91169700	0.72709300
C	-4.93703300	-5.50119400	-2.75232900
C	-4.66605500	-4.64972700	-3.95653300
H	-4.66531300	-5.27876900	-4.87042400
H	-5.43588000	-3.87703500	-4.10667900
H	-3.68018600	-4.16210400	-3.90157100
C	-6.31707800	-6.07228500	-2.61899000
H	-6.50775100	-6.43158200	-1.59514200
H	-7.10128800	-5.35234900	-2.89401400
H	-6.42758300	-6.94554900	-3.29381900
C	-3.81970400	-6.40244600	-2.32087200
H	-3.68477600	-7.20979500	-3.06870600
H	-2.86580100	-5.86421400	-2.23237700
H	-4.03635800	-6.88572200	-1.35594000
C	-3.27293000	-4.87051100	0.45333200
O	-2.25895700	-4.52050300	-0.13063200
O	-3.23023500	-5.63164100	1.57463100
C	-1.93454500	-5.99684900	2.04018200
H	-1.33319400	-5.10540600	2.27605400
H	-2.08886400	-6.59659500	2.94554400
H	-1.39598600	-6.58790500	1.28346900
C	-6.26331700	-3.21948600	-1.31399900
H	-6.49090900	-3.09426400	-2.38154500
H	-7.07585600	-3.79288300	-0.84390000
H	-6.26842300	-2.20911600	-0.86787000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.241505 (Hartree/Particle)
Thermal correction to Energy= 0.255741
Thermal correction to Enthalpy= 0.256685
Thermal correction to Gibbs Free Energy= 0.200453
Sum of electronic and zero-point Energies= -503.020692
Sum of electronic and thermal Energies= -503.006457
Sum of electronic and thermal Enthalpies= -503.005513
Sum of electronic and thermal Free Energies= -503.061744
HF=-503.2621976

C[50]

C	-4.43293900	-3.93831800	-1.10111700
H	-3.39259700	-3.61571300	-1.26766700
C	-4.46469400	-4.61815800	0.22256100
H	-5.41705100	-4.86440400	0.69891200
C	-4.76175000	-4.92767200	-2.28700700
C	-6.22758800	-5.38658800	-2.24931700
H	-6.41609300	-6.11526800	-3.05397600
H	-6.47567200	-5.87586700	-1.29423900
H	-6.92452000	-4.54744200	-2.39439200
C	-3.84389600	-6.15768900	-2.17727500
H	-2.78493700	-5.86172100	-2.12123900
H	-4.07274100	-6.75378800	-1.27970100

H	-3.97314000	-6.81207800	-3.05397600
C	-4.47727400	-4.22502600	-3.62388000
H	-4.63845600	-4.92318100	-4.46099000
H	-5.13572100	-3.35897600	-3.78686800
H	-3.43340400	-3.87511000	-3.67254600
C	-3.25161100	-4.99319100	0.92193100
O	-2.11340600	-4.79071800	0.52280200
O	-3.51283900	-5.61535500	2.09492800
C	-2.38058700	-6.03015600	2.85526400
H	-1.75233100	-5.16808900	3.12732800
H	-2.77501100	-6.50956900	3.75919200
H	-1.76515700	-6.74362300	2.28599900
C	-5.33080900	-2.68897300	-1.06068800
H	-6.37558600	-2.94648100	-0.82888100
H	-4.98001300	-1.99355000	-0.28322200
H	-5.31586000	-2.15162800	-2.01972400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.244993 (Hartree/Particle)
Thermal correction to Energy= 0.258787
Thermal correction to Enthalpy= 0.259731
Thermal correction to Gibbs Free Energy= 0.204260
Sum of electronic and zero-point Energies= -503.050147
Sum of electronic and thermal Energies= -503.036353
Sum of electronic and thermal Enthalpies= -503.035409
Sum of electronic and thermal Free Energies= -503.090880
HF=-503.29514

B[58]

C	-4.56510400	-3.66964800	-1.10279300
H	-3.62457200	-3.45078800	-1.61688200
C	-4.62587700	-4.49517300	-0.05017700
H	-5.56158400	-4.71771200	0.46751400
H	-5.47304900	-3.19162900	-1.47306200
C	-3.62401800	-5.99537000	1.58386300
O	-4.65236500	-6.25741500	2.17841000
N	-3.53267600	-5.15895300	0.50609200
H	-2.63433300	-6.42049300	1.86527400
H	-2.61401000	-5.01927600	0.09489000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.079410 (Hartree/Particle)
Thermal correction to Energy= 0.084676
Thermal correction to Enthalpy= 0.085620
Thermal correction to Gibbs Free Energy= 0.051284
Sum of electronic and zero-point Energies= -247.050052
Sum of electronic and thermal Energies= -247.044786
Sum of electronic and thermal Enthalpies= -247.043842
Sum of electronic and thermal Free Energies= -247.078178
HF=-247.1294622

B-TS-C[58]

C	-4.32743700	-3.65733800	-0.81107300
H	-3.31350100	-3.56434100	-1.20793800
C	-4.56358900	-4.30864900	0.36039700
H	-5.53749300	-4.31009800	0.85114800
H	-5.06883200	-2.94717200	-1.17720700
C	-4.80728100	-5.08751500	-2.62239100
C	-6.21999700	-5.47972000	-2.31280700
H	-6.60637000	-6.20221600	-3.06203100
H	-6.29534600	-5.96621600	-1.32642400
H	-6.89829900	-4.61096900	-2.32178100
C	-3.76431400	-6.14548400	-2.41931800
H	-2.74307500	-5.73828900	-2.50245300
H	-3.86612400	-6.63024700	-1.43503700
H	-3.85491500	-6.94587300	-3.18385700
C	-4.59644100	-4.13792400	-3.76292400
H	-4.75659400	-4.64428400	-4.73851800
H	-5.29909500	-3.28940000	-3.72517700
H	-3.56918200	-3.73726300	-3.77843500
C	-3.88515900	-5.86673800	2.10797100
O	-4.95967500	-5.90615700	2.68379500
N	-3.62559500	-5.12623700	0.99133900
H	-2.99349500	-6.44223400	2.44422200
H	-2.68865500	-5.17904900	0.60194800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.197108 (Hartree/Particle)
Thermal correction to Energy= 0.208899
Thermal correction to Enthalpy= 0.209843
Thermal correction to Gibbs Free Energy= 0.158297
Sum of electronic and zero-point Energies= -404.631839
Sum of electronic and thermal Energies= -404.620048
Sum of electronic and thermal Enthalpies= -404.619104
Sum of electronic and thermal Free Energies= -404.670649
HF=-404.8289466

C[58]

C	-4.46605500	-3.94501000	-1.13898700
H	-3.42591300	-3.58328400	-1.24044900
C	-4.66823000	-4.50891700	0.22108600
H	-5.63929900	-4.57210000	0.70950300
H	-5.11592000	-3.06049700	-1.25351400
C	-4.75883500	-4.90143500	-2.34220700
C	-6.21971700	-5.37192700	-2.29083700
H	-6.45084600	-6.01923000	-3.15215200
H	-6.42239600	-5.94635600	-1.37327300
H	-6.91363900	-4.51564200	-2.31542100
C	-3.82135600	-6.11712400	-2.29260900
H	-2.76356300	-5.80605000	-2.31982300
H	-3.97847900	-6.71103000	-1.37910700
H	-3.99741800	-6.77825200	-3.15647700
C	-4.51446200	-4.11756500	-3.63988000
H	-4.70817300	-4.74873700	-4.52220200
H	-5.17463600	-3.23717000	-3.70238900
H	-3.47220600	-3.76356900	-3.70011200
C	-3.76369000	-5.80125400	2.07822700
O	-4.81031500	-5.90087200	2.70213100
N	-3.64138500	-5.15101700	0.87940400
H	-2.79795800	-6.23041100	2.42440800
H	-2.71597300	-5.13596400	0.45813100

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)

Zero-point correction= 0.201266 (Hartree/Particle)
Thermal correction to Energy= 0.212301
Thermal correction to Enthalpy= 0.213245
Thermal correction to Gibbs Free Energy= 0.164072
Sum of electronic and zero-point Energies= -404.669107
Sum of electronic and thermal Energies= -404.658072
Sum of electronic and thermal Enthalpies= -404.657128
Sum of electronic and thermal Free Energies= -404.706301
HF=-404.8703729

B[59]

C	-4.52789300	-3.63234200	-1.06233200
H	-3.56237700	-3.33616500	-1.48308800
C	-4.62783900	-4.51556800	-0.05974000
H	-5.58874300	-4.81527400	0.36441800
H	-5.42803300	-3.18382400	-1.48492000
C	-3.69874300	-6.05977900	1.58049200
O	-4.79262100	-6.36331100	2.03095400
N	-3.55302000	-5.14973900	0.55655900
H	-2.61627900	-4.93719000	0.22821000
C	-2.40441500	-6.67286300	2.07176900
H	-2.13120500	-7.51777700	1.41813800
H	-1.57172100	-5.95424700	2.06327500
H	-2.55467100	-7.05744300	3.08811400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.106762 (Hartree/Particle)
Thermal correction to Energy= 0.113702
Thermal correction to Enthalpy= 0.114646
Thermal correction to Gibbs Free Energy= 0.075705
Sum of electronic and zero-point Energies= -286.322374
Sum of electronic and thermal Energies= -286.315435
Sum of electronic and thermal Enthalpies= -286.314491
Sum of electronic and thermal Free Energies= -286.353432
HF=-286.4291365

B-TS-C[59]

C	-4.34367600	-3.64402200	-0.81366500
H	-3.34484200	-3.49997000	-1.23334700
C	-4.52378300	-4.34489500	0.33981400
H	-5.48179300	-4.39974100	0.85779200
H	-5.11796900	-2.94601700	-1.13234300
C	-4.81682400	-5.03201200	-2.65307600
C	-6.20862300	-5.48143700	-2.32634900
H	-6.58695300	-6.19597200	-3.08733700
H	-6.24611400	-5.99691100	-1.35249600
H	-6.91592400	-4.63653000	-2.29635900
C	-3.73609500	-6.06119000	-2.50577600
H	-2.73053800	-5.61826000	-2.59819300
H	-3.79957900	-6.57783400	-1.53454000
H	-3.81765900	-6.84117100	-3.29222500
C	-4.66356300	-4.04448600	-3.77053200
H	-4.83059600	-4.52717700	-4.75702500
H	-5.39155000	-3.22042000	-3.69166200
H	-3.65026200	-3.61011900	-3.79754100
C	-3.75932200	-5.95886100	2.00120300
O	-4.84501900	-6.01736700	2.56509300
N	-3.54356100	-5.15398100	0.91013700
H	-2.62153900	-5.15516100	0.48706300
C	-2.56672100	-6.77754600	2.44888800
H	-2.39786300	-6.60235500	3.52187700
H	-2.80556700	-7.84579200	2.32747500
H	-1.64450100	-6.55324700	1.89529400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.224357 (Hartree/Particle)
Thermal correction to Energy= 0.237918
Thermal correction to Enthalpy= 0.238862
Thermal correction to Gibbs Free Energy= 0.182202
Sum of electronic and zero-point Energies= -443.904042
Sum of electronic and thermal Energies= -443.890481
Sum of electronic and thermal Enthalpies= -443.889537
Sum of electronic and thermal Free Energies= -443.946197
HF=-444.1283986

C[59]

C	-4.46771400	-3.95188000	-1.12904500
H	-3.43147300	-3.57726800	-1.22723500
C	-4.64780300	-4.58149000	0.20537700
H	-5.61032700	-4.67423900	0.70539100
H	-5.12525200	-3.06798400	-1.19320900
C	-4.76845800	-4.85145300	-2.37369400
C	-6.22403800	-5.33823200	-2.32528500
H	-6.46159100	-5.94612100	-3.21322600
H	-6.40816700	-5.95716900	-1.43310900
H	-6.92604200	-4.48856400	-2.29935600
C	-3.81969000	-6.05923300	-2.39684600
H	-2.76517100	-5.73697300	-2.42405100
H	-3.95781800	-6.69785800	-1.51101800
H	-4.00242300	-6.67935400	-3.28933600
C	-4.54957300	-4.00350200	-3.63515800
H	-4.74962100	-4.59289500	-4.54462300
H	-5.21859700	-3.12759700	-3.64595800
H	-3.51157400	-3.63657100	-3.69210200
C	-3.72998400	-5.99992200	1.96426700
O	-4.79891900	-6.09903400	2.55882800
N	-3.61368300	-5.27166300	0.80220400
H	-2.70008400	-5.23021300	0.36133600
C	-2.45785900	-6.65922000	2.45123200
H	-2.21974900	-6.28076600	3.45777600
H	-2.63073300	-7.74248900	2.54602600
H	-1.59409500	-6.49078400	1.79298300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.228809 (Hartree/Particle)
Thermal correction to Energy= 0.241492
Thermal correction to Enthalpy= 0.242436
Thermal correction to Gibbs Free Energy= 0.189114
Sum of electronic and zero-point Energies= -443.940733

Sum of electronic and thermal Energies= -443.928050
Sum of electronic and thermal Enthalpies= -443.927106
Sum of electronic and thermal Free Energies= -443.980428
HF=-444.1695418

B^{60}

C	-4.36664600	-3.66755900	-0.97464600
H	-3.35698800	-3.44825700	-1.32996100
C	-4.58701300	-4.54986900	-0.00200400
H	-5.56793300	-4.81331900	0.39712600
H	-5.21043300	-3.14841500	-1.43106300
C	-3.78686300	-6.11110100	1.57736200
O	-4.90209600	-6.35832500	1.97433700
O	-3.53423200	-5.21406100	0.58526800
C	-2.54034500	-6.73138600	2.09525700
C	-1.27217000	-6.40073000	1.58986800
C	-2.65704300	-7.67868600	3.12566400
C	-0.13406800	-7.01502500	2.11379100
H	-1.18559700	-5.66517700	0.79034700
C	-1.51720300	-8.28964800	3.64585900
H	-3.65006900	-7.92308500	3.50587200
C	-0.25468400	-7.95820400	3.14023500
H	0.85169100	-6.75753700	1.72035700
H	-1.61061500	-9.02597000	4.44701700
H	0.63871400	-8.43709600	3.54787500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.147935 (Hartree/Particle)
Thermal correction to Energy= 0.157453
Thermal correction to Enthalpy= 0.158398
Thermal correction to Gibbs Free Energy= 0.112107
Sum of electronic and zero-point Energies= -497.741879
Sum of electronic and thermal Energies= -497.732360
Sum of electronic and thermal Enthalpies= -497.731416
Sum of electronic and thermal Free Energies= -497.777707
HF=-497.889814

B-TS-C^{60}

C	-4.45743200	-3.66406000	-0.88835300
H	-3.43620300	-3.41024200	-1.17702200
C	-4.68797500	-4.44286600	0.19598200
H	-5.66306100	-4.65157900	0.63494800
H	-5.26382800	-3.02700300	-1.25190700
C	-3.87553800	-6.03514300	1.74119900
O	-4.97720800	-6.22249000	2.21125900
O	-3.63863700	-5.15107700	0.74261800
C	-2.63638900	-6.73426300	2.16892400
C	-1.39264100	-6.49544500	1.56031100
C	-2.73307400	-7.66743200	3.21420400
C	-0.26092800	-7.18549800	1.99628600
H	-1.32128600	-5.77148900	0.74866400
C	-1.59937200	-8.35374800	3.64724300
H	-3.70689300	-7.84116200	3.67462500
C	-0.36187600	-8.11364100	3.03871700
H	0.70487400	-6.99922200	1.52136500
H	-1.67831100	-9.07830200	4.46073800
H	0.52648600	-8.65179400	3.37769700
C	-4.56766900	-4.98674200	-2.81961900
C	-5.92357800	-5.60744600	-2.67097700
H	-6.12932800	-6.31027100	-3.50493700
H	-6.00185600	-6.18464600	-1.73523400
H	-6.72508300	-4.85108800	-2.67973400
C	-3.39334000	-5.89200000	-2.59421400
H	-2.44424200	-5.33307200	-2.55552200
H	-3.49510900	-6.46355900	-1.65846200
H	-3.30188800	-6.62922100	-3.41925100
C	-4.41420500	-3.92497700	-3.86667900
H	-4.41053200	-4.37085000	-4.88366800
H	-5.24239500	-3.19832200	-3.83953300
H	-3.46471500	-3.37541200	-3.75736900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.265540 (Hartree/Particle)
Thermal correction to Energy= 0.281653
Thermal correction to Enthalpy= 0.282598
Thermal correction to Gibbs Free Energy= 0.218988
Sum of electronic and zero-point Energies= -655.324443
Sum of electronic and thermal Energies= -655.308330
Sum of electronic and thermal Enthalpies= -655.307386
Sum of electronic and thermal Free Energies= -655.370995
HF=-655.5899832

C^{60}

C	-4.50443900	-3.93111100	-1.22426500
H	-3.51528500	-3.44155600	-1.17569800
C	-4.76746400	-4.61858700	0.05908300
H	-5.74795600	-4.83061200	0.48411400
H	-5.25612400	-3.13262900	-1.34146100
C	-3.90671500	-6.09696800	1.68930300
O	-4.99167400	-6.24210900	2.20993600
O	-3.71509700	-5.29313300	0.60880500
C	-2.64849000	-6.75197900	2.12264500
C	-1.42839300	-6.55131900	1.45421000
C	-2.69941800	-7.60361900	3.23889400
C	-0.27568200	-7.19728600	1.90183100
H	-1.39161300	-5.89152200	0.58741800
C	-1.54459500	-8.24649000	3.68247600
H	-3.65476400	-7.74917600	3.74553100
C	-0.33117200	-8.04420700	3.01464800
H	0.67127000	-7.04034900	1.38062900
H	-1.58827000	-8.90757600	4.55083200
H	0.57374100	-8.54821400	3.36216600
C	-4.54212600	-4.81725900	-2.51484700
C	-5.91776800	-5.48685400	-2.64788600
H	-5.97236900	-6.08164100	-3.57387500
H	-6.11764100	-6.16307500	-1.80161200
H	-6.72452800	-4.73625800	-2.68017800
C	-3.44521600	-5.89143300	-2.45840200
H	-2.44819400	-5.43598900	-2.34223700
H	-3.59774600	-6.58357700	-1.61722200
H	-3.44010700	-6.48374000	-3.38781900
C	-4.29656700	-3.89803500	-3.72038700
H	-4.31045400	-4.47352100	-4.66007400

H	-5.07141400	-3.11730800	-3.79022500
H	-3.31746000	-3.39743300	-3.64503300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.269610 (Hartree/Particle)
Thermal correction to Energy= 0.285013
Thermal correction to Enthalpy= 0.285957
Thermal correction to Gibbs Free Energy= 0.224987
Sum of electronic and zero-point Energies= -655.359960
Sum of electronic and thermal Energies= -655.344557
Sum of electronic and thermal Enthalpies= -655.343612
Sum of electronic and thermal Free Energies= -655.404582
HF=-655.6295692

B[51]

C	-4.51175100	-4.51608300	0.21109900
C	-4.65991600	-3.78978400	-1.08934600
C	-5.90782500	-3.31224300	-1.17938200
C	-6.64509400	-3.69523500	0.04844300
O	-5.78574500	-4.40415300	0.84262600
H	-4.26206600	-5.58240300	0.07424900
H	-3.85177500	-3.69175000	-1.81528500
H	-6.36393500	-2.73737000	-1.98323100
O	-7.78330200	-3.47210200	0.37510000
H	-3.73935100	-4.06858200	0.86016800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.074597 (Hartree/Particle)
Thermal correction to Energy= 0.079227
Thermal correction to Enthalpy= 0.080171
Thermal correction to Gibbs Free Energy= 0.046664
Sum of electronic and zero-point Energies= -304.987496
Sum of electronic and thermal Energies= -304.982865
Sum of electronic and thermal Enthalpies= -304.981921
Sum of electronic and thermal Free Energies= -305.015428
HF=-305.0620923

B-TS-C[51]

C	-4.81645600	-5.25637100	-2.50313800
C	-6.19565000	-5.77927000	-2.24311200
H	-6.46800500	-6.52614000	-3.01595000
H	-6.27713600	-6.28594000	-1.26924200
H	-6.94910500	-4.97796900	-2.28981600
C	-3.66905100	-6.17733800	-2.21964000
H	-2.70149100	-5.65073900	-2.23650400
H	-3.77419500	-6.69643000	-1.25423700
H	-3.61864400	-6.96589100	-2.99789200
C	-4.66148800	-4.33884600	-3.67813700
H	-4.73427200	-4.91772300	-4.62081700
H	-5.45213500	-3.57383600	-3.70602400
H	-3.68095400	-3.83669600	-3.68463900
C	-4.84757800	-4.50578300	0.46282800
C	-4.56489200	-3.68917200	-0.77099600
C	-5.60685800	-2.81570400	-0.92292300
C	-6.66588800	-3.17369200	0.02038500
O	-6.19888500	-4.20169300	0.80776800
H	-4.74891300	-5.59274200	0.32949600
H	-3.55662600	-3.56268100	-1.16349000
H	-5.71380600	-2.01203500	-1.64808600
O	-7.77716000	-2.71987500	0.17369100
H	-4.18256100	-4.20791000	1.29325100

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.192859 (Hartree/Particle)
Thermal correction to Energy= 0.203874
Thermal correction to Enthalpy= 0.204819
Thermal correction to Gibbs Free Energy= 0.155672
Sum of electronic and zero-point Energies= -462.573087
Sum of electronic and thermal Energies= -462.562071
Sum of electronic and thermal Enthalpies= -462.561127
Sum of electronic and thermal Free Energies= -462.610274
HF=-462.7659456

C[51]

C	-4.80134400	-5.04512400	-2.25515300
C	-6.17280700	-5.73635200	-2.21509600
H	-6.25317800	-6.46662800	-3.03544500
H	-6.33473600	-6.28092100	-1.27206800
H	-6.99164300	-5.00909400	-2.33226900
C	-3.67978200	-6.08840000	-2.13923100
H	-2.68794100	-5.60932300	-2.16638200
H	-3.75029700	-6.67263400	-1.20901400
H	-3.73553000	-6.79922700	-2.97865300
C	-4.64336300	-4.29055500	-3.58426800
H	-4.66342900	-4.99837900	-4.42777200
H	-5.45503300	-3.56406000	-3.74093400
H	-3.68526600	-3.74756800	-3.62262500
C	-4.85985800	-4.62181800	0.34211700
C	-4.66272400	-4.01685200	-1.07027200
C	-5.69363900	-2.95081000	-1.06503200
C	-6.60020600	-3.13183700	0.05427100
O	-6.13909000	-4.16867300	0.81523700
H	-4.86608400	-5.71864100	0.35764400
H	-3.65236600	-3.58078900	-1.16332700
H	-5.82913700	-2.16486200	-1.80553400
O	-7.61778400	-2.53413300	0.33559000
H	-4.08651300	-4.26779600	1.04099100

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.196634 (Hartree/Particle)
Thermal correction to Energy= 0.207049
Thermal correction to Enthalpy= 0.207994
Thermal correction to Gibbs Free Energy= 0.160647
Sum of electronic and zero-point Energies= -462.602061
Sum of electronic and thermal Energies= -462.591646
Sum of electronic and thermal Enthalpies= -462.590702
Sum of electronic and thermal Free Energies= -462.638049
HF=-462.7986958

B[52]

C	-4.32661400	-3.80931400	-0.91340900
H	-3.35746700	-3.52047700	-1.33028500
C	-4.37845700	-4.47497600	0.24372700
H	-5.33730900	-4.77357100	0.67939400
H	-5.23044300	-3.53986600	-1.46471500
C	-3.12388400	-4.83285400	0.98130800
O	-2.00538000	-4.54064300	0.57027400
N	-3.32532000	-5.50719900	2.14216800
H	-4.24966800	-5.74567700	2.47745900
H	-2.52309400	-5.78274200	2.69697000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.079033 (Hartree/Particle)
Thermal correction to Energy= 0.084510
Thermal correction to Enthalpy= 0.085454
Thermal correction to Gibbs Free Energy= 0.050766
Sum of electronic and zero-point Energies= -247.057752
Sum of electronic and thermal Energies= -247.052274
Sum of electronic and thermal Enthalpies= -247.051330
Sum of electronic and thermal Free Energies= -247.086019
HF=-247.1367843

B-TS-C[52]

C	-3.94966300	-3.88942200	-1.28334500
H	-2.95594900	-4.17430800	-1.63197800
C	-4.35036500	-4.25870200	-0.03803200
H	-5.29630500	-3.89248100	0.37170600
H	-4.47491200	-3.10344100	-1.82692200
C	-4.80959300	-5.48684900	-2.84993100
C	-6.04517100	-5.93991800	-2.13642400
H	-6.57195500	-6.71508800	-2.73043200
H	-5.80629000	-6.38523100	-1.15793300
H	-6.75456900	-5.11260000	-1.97681300
C	-3.65988100	-6.44830700	-2.87458300
H	-2.76436400	-6.00415600	-3.33743400
H	-3.39290000	-6.78301300	-1.86086200
H	-3.92234100	-7.34823300	-3.46949200
C	-4.98948200	-4.60112200	-4.04459000
H	-5.31791400	-5.19592600	-4.92288300
H	-5.75690100	-3.82907700	-3.87522900
H	-4.04802000	-4.10513900	-4.33192800
C	-3.57249800	-5.23223700	0.75916700
O	-2.52825300	-5.75357500	0.35944900
N	-4.09954300	-5.53280200	1.97986600
H	-3.59994500	-6.17412100	2.58426600
H	-4.93206700	-5.08149100	2.33535800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.196947 (Hartree/Particle)
Thermal correction to Energy= 0.208958
Thermal correction to Enthalpy= 0.209902
Thermal correction to Gibbs Free Energy= 0.158381
Sum of electronic and zero-point Energies= -404.644342
Sum of electronic and thermal Energies= -404.632331
Sum of electronic and thermal Enthalpies= -404.631387
Sum of electronic and thermal Free Energies= -404.682908
HF=-404.8412892

C[52]

C	-4.32284300	-3.95931800	-1.10458200
H	-3.29235200	-3.62056200	-1.29117200
C	-4.38261800	-4.53911300	0.25759200
H	-5.34873900	-4.68041400	0.75095400
H	-4.99041000	-3.08066900	-1.16020500
C	-4.73259300	-4.92788700	-2.26382400
C	-6.20458300	-5.34094500	-2.11539300
H	-6.51022000	-5.99156000	-2.95075700
H	-6.37618900	-5.89703100	-1.18034300
H	-6.86713100	-4.45990400	-2.11416900
C	-3.83801400	-6.17646100	-2.24381100
H	-2.77274900	-5.90360800	-2.29331500
H	-3.98908800	-6.76157100	-1.32284200
H	-4.06866500	-6.83063300	-3.10024300
C	-4.54157300	-4.17855700	-3.59021700
H	-4.82472300	-4.81624500	-4.44332600
H	-5.16285500	-3.26888900	-3.62666200
H	-3.49051300	-3.87693000	-3.72641300
C	-3.16636000	-4.98399000	0.94114400
O	-2.04296100	-4.86955200	0.43797900
N	-3.34956900	-5.54175000	2.17364400
H	-2.54078100	-5.86725200	2.68912600
H	-4.26449400	-5.64183600	2.59287000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.200702 (Hartree/Particle)
Thermal correction to Energy= 0.212116
Thermal correction to Enthalpy= 0.213061
Thermal correction to Gibbs Free Energy= 0.163209
Sum of electronic and zero-point Energies= -404.680086
Sum of electronic and thermal Energies= -404.668671
Sum of electronic and thermal Enthalpies= -404.667727
Sum of electronic and thermal Free Energies= -404.717578
HF=-404.8807879

B[53]

C	-3.34273300	-3.61119700	-1.46426900
H	-2.76204300	-4.05002500	-2.27991300
C	-3.18618900	-4.05918600	-0.21405800
H	-3.76480000	-3.62146000	0.59774400
H	-4.04439000	-2.80720800	-1.69825400
C	-2.21718700	-5.16312800	0.07765200
O	-1.55665700	-5.67845000	-0.82528100
N	-2.07152000	-5.59613800	1.36220600
H	-1.38715400	-6.34516400	1.41988400
C	-2.69170500	-5.20364700	2.64781200
C	-2.37031500	-3.74084500	3.00100300
C	-4.20906000	-5.45935700	2.63761100
C	-2.04792300	-6.11532100	3.70465200
H	-1.28154600	-3.58073200	3.00674900
H	-2.81459500	-3.02968100	2.29165300

H	-2.76136700	-3.50181500	4.00170400
H	-4.41631200	-6.51102200	2.38830300
H	-4.63238500	-5.24848700	3.63148900
H	-4.73664800	-4.82752200	1.91038600
H	-2.45584600	-5.88938100	4.70000800
H	-2.25028300	-7.17512600	3.48339300
H	-0.95724000	-5.96579400	3.73881700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.191313 (Hartree/Particle)
Thermal correction to Energy= 0.201941
Thermal correction to Enthalpy= 0.202885
Thermal correction to Gibbs Free Energy= 0.155604
Sum of electronic and zero-point Energies= -404.100048
Sum of electronic and thermal Energies= -404.089420
Sum of electronic and thermal Enthalpies= -404.088476
Sum of electronic and thermal Free Energies= -404.135757
HF=-404.2913611

B-TS-C[53]

C	-3.46892500	-3.72955100	-1.51792400
H	-2.81625100	-4.08518700	-2.31559600
C	-3.24369800	-4.12511400	-0.23653800
H	-3.82845700	-3.68849000	0.57026300
H	-4.11406200	-2.87557600	-1.72669500
C	-5.15998000	-5.18078200	-2.43715500
C	-5.86479900	-4.21213200	-3.33630900
H	-6.65484100	-4.72918700	-3.92097000
H	-6.36038200	-3.40765500	-2.76978600
H	-5.17699600	-3.75642300	-4.06713300
C	-5.87023600	-5.60410200	-1.18946700
H	-5.19518300	-6.13226900	-0.49857500
H	-6.31041300	-4.74729600	-0.65543100
H	-6.69910700	-6.30013100	-1.43412000
C	-4.27392100	-6.20216300	-3.08355500
H	-4.87921200	-7.04783400	-3.47270400
H	-3.71928800	-5.78156900	-3.93735200
H	-3.54558700	-6.61215800	-2.36777100
C	-2.28300000	-5.20929600	0.05691100
O	-1.64527100	-5.76748300	-0.84646700
N	-2.09407400	-5.61294200	1.35089200
H	-1.41779100	-6.36893100	1.40313500
C	-2.69567000	-5.20513000	2.63726000
C	-2.39023500	-3.73105600	2.95706000
C	-4.21037800	-5.47963000	2.65912400
C	-2.02294000	-6.08627200	3.70183900
H	-1.30341100	-3.55754200	2.94843300
H	-2.84936600	-3.04311300	2.23462300
H	-2.77461400	-3.47456600	3.95618900
H	-4.40780400	-6.53937900	2.43666100
H	-4.62149400	-5.25180500	3.65452700
H	-4.75578300	-4.87263200	1.92438000
H	-2.41605100	-5.84535300	4.69978800
H	-2.21558700	-7.15295300	3.50568200
H	-0.93368200	-5.92329200	3.71302300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.309387 (Hartree/Particle)
Thermal correction to Energy= 0.326461
Thermal correction to Enthalpy= 0.327405
Thermal correction to Gibbs Free Energy= 0.264459
Sum of electronic and zero-point Energies= -561.687804
Sum of electronic and thermal Energies= -561.670730
Sum of electronic and thermal Enthalpies= -561.669786
Sum of electronic and thermal Free Energies= -561.732732
HF=-561.9971912

C[53]

C	-3.65348000	-3.71505200	-1.50982100
H	-2.77549300	-3.78703000	-2.16835000
C	-3.24192200	-4.07583700	-0.13180000
H	-3.87701400	-3.78670600	0.70324500
H	-4.01457300	-2.67132500	-1.52375000
C	-4.78992200	-4.60790200	-2.11136600
C	-5.03824300	-4.14189000	-3.55306200
H	-5.83907900	-4.73535500	-4.02323800
H	-5.34035700	-3.08232700	-3.58223600
H	-4.12937200	-4.25215700	-4.16623500
C	-6.07983200	-4.44999100	-1.29217500
H	-5.94636800	-4.79666000	-0.25536300
H	-6.40464200	-3.39717600	-1.25932200
H	-6.89619400	-5.04161800	-1.73709900
C	-4.35414400	-6.08099800	-2.11320600
H	-5.11680500	-6.70863400	-2.60202000
H	-3.40164100	-6.21365400	-2.64868900
H	-4.21510700	-6.45833200	-1.08771600
C	-2.02732600	-4.85548000	0.10059800
O	-1.25264400	-5.11520000	-0.83398200
N	-1.72931400	-5.29880400	1.36362600
H	-0.86340200	-5.82938000	1.37103700
C	-2.49411800	-5.30736100	2.62744100
C	-2.67448900	-3.88324000	3.18280100
C	-3.85043300	-6.01502400	2.45517800
C	-1.64100900	-6.11412500	3.61891300
H	-1.69553200	-3.39448100	3.30052200
H	-3.29164200	-3.25250100	2.52854700
H	-3.16479900	-3.92134100	4.16755200
H	-3.70206500	-7.03372800	2.06571900
H	-4.36636600	-6.08545200	3.42487000
H	-4.51385400	-5.48061000	1.76173300
H	-2.14107400	-6.16680700	4.59643800
H	-1.48737900	-7.14268800	3.25603100
H	-0.65621900	-5.64202300	3.76189300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.313095 (Hartree/Particle)
Thermal correction to Energy= 0.329563
Thermal correction to Enthalpy= 0.330507
Thermal correction to Gibbs Free Energy= 0.268944
Sum of electronic and zero-point Energies= -561.724075
Sum of electronic and thermal Energies= -561.707606
Sum of electronic and thermal Enthalpies= -561.706662

Sum of electronic and thermal Free Energies= -561.768225
HF=-562.0371696

B[49]

C	-4.29833200	-3.78258200	-0.89752700
H	-3.32638000	-3.75874600	-1.39857100
C	-4.42262100	-4.35320000	0.30518200
H	-5.37775200	-4.39497900	0.83417600
H	-5.15221600	-3.33021300	-1.40701400
C	-3.25143500	-4.96411200	0.98475100
O	-2.12262700	-5.00648000	0.54487400
O	-3.58789300	-5.48230000	2.17940400
H	-2.78314700	-5.86475900	2.57171600

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.067257 (Hartree/Particle)
Thermal correction to Energy= 0.072257
Thermal correction to Enthalpy= 0.073201
Thermal correction to Gibbs Free Energy= 0.039266
Sum of electronic and zero-point Energies= -266.917836
Sum of electronic and thermal Energies= -266.912836
Sum of electronic and thermal Enthalpies= -266.911892
Sum of electronic and thermal Free Energies= -266.945827
HF=-266.9850931

B-TS-C[49]

C	-4.63734400	-3.79275400	-1.07318800
H	-3.71081900	-3.54542200	-1.59369200
C	-4.58831700	-4.43211800	0.11888400
H	-5.48742700	-4.63420200	0.70488600
H	-5.56346500	-3.35079000	-1.44200500
C	-4.93229500	-5.52507900	-2.86675800
C	-6.40598700	-5.74679200	-2.73479100
H	-6.74076300	-6.55652500	-3.41708700
H	-6.67863400	-6.05815000	-1.71333900
H	-6.98603000	-4.84752900	-2.99646500
C	-4.02808500	-6.58261300	-2.32049900
H	-2.99232700	-6.22607700	-2.21695100
H	-4.37142000	-6.93695500	-1.33534500
H	-4.01114300	-7.46520000	-2.99383600
C	-4.44788600	-4.71371600	-4.02604500
H	-4.54756500	-5.28655000	-4.97247100
H	-5.03382400	-3.78888000	-4.15435300
H	-3.38389100	-4.44660300	-3.92608900
C	-3.31465400	-4.94176000	0.64277000
O	-2.22494200	-4.82934100	0.11004900
O	-3.46812000	-5.57938900	1.82449200
H	-2.58654800	-5.88379900	2.10133400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.185049 (Hartree/Particle)
Thermal correction to Energy= 0.196666
Thermal correction to Enthalpy= 0.197610
Thermal correction to Gibbs Free Energy= 0.146509
Sum of electronic and zero-point Energies= -424.506644
Sum of electronic and thermal Energies= -424.495027
Sum of electronic and thermal Enthalpies= -424.494083
Sum of electronic and thermal Free Energies= -424.545184
HF=-424.6916931

C[49]

C	-4.36394100	-3.97578600	-1.09652700
H	-3.33631400	-3.61492200	-1.25523200
C	-4.45664300	-4.57712900	0.25330400
H	-5.42455000	-4.74234700	0.73178200
H	-5.04572500	-3.10885000	-1.15370400
C	-4.73117600	-4.93457000	-2.27990400
C	-6.19415100	-5.38715500	-2.16213700
H	-6.47024800	-6.02399300	-3.01789200
H	-6.36553600	-5.97078200	-1.24411300
H	-6.87853600	-4.52324100	-2.14975200
C	-3.80353700	-6.15881200	-2.26803300
H	-2.74506600	-5.85748000	-2.30190300
H	-3.95038700	-6.76533600	-1.36036400
H	-4.00590700	-6.80340300	-3.13848500
C	-4.53792000	-4.15392300	-3.58769400
H	-4.78725900	-4.78409600	-4.45657300
H	-5.18506100	-3.26246600	-3.61884300
H	-3.49387300	-3.81990500	-3.69943400
C	-3.27223700	-5.01549300	0.96766900
O	-2.12682000	-4.92205900	0.54994300
O	-3.55467000	-5.55760700	2.17442100
H	-2.70910600	-5.82212500	2.57574900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.189390 (Hartree/Particle)
Thermal correction to Energy= 0.200058
Thermal correction to Enthalpy= 0.201002
Thermal correction to Gibbs Free Energy= 0.152764
Sum of electronic and zero-point Energies= -424.541233
Sum of electronic and thermal Energies= -424.530565
Sum of electronic and thermal Enthalpies= -424.529621
Sum of electronic and thermal Free Energies= -424.577859
HF=-424.7306232

B[54]

C	-4.29476500	-3.72816200	-1.00633700
H	-3.30791000	-3.71932700	-1.47891600
C	-4.45121300	-4.29402900	0.19646900
H	-5.42856700	-4.31437400	0.68855500
H	-5.12782900	-3.26739700	-1.54264500
C	-3.30344100	-4.92143700	0.92119900
O	-2.17937200	-4.94719300	0.44943800
C	-2.42599700	-6.14882400	2.97560300
H	-1.63432400	-5.40334700	3.14489400
H	-2.71764800	-6.57025000	3.94905400
H	-1.99148500	-6.95520100	2.36562500
C	-3.62318400	-5.52190200	2.27534600
H	-4.43641900	-6.25585900	2.12385800
H	-4.08060100	-4.72271900	2.88779500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.117470 (Hartree/Particle)
Thermal correction to Energy= 0.124535
Thermal correction to Enthalpy= 0.125480
Thermal correction to Gibbs Free Energy= 0.086478
Sum of electronic and zero-point Energies= -270.258029
Sum of electronic and thermal Energies= -270.250964
Sum of electronic and thermal Enthalpies= -270.250020
Sum of electronic and thermal Free Energies= -270.289022
HF=-270.3754997

B-TS-C[54]

C	-4.68436300	-3.73160000	-1.08349500
H	-3.75427000	-3.50917800	-1.60973300
C	-4.64145400	-4.38227300	0.09915400
H	-5.55525400	-4.57076300	0.67056700
H	-5.60865200	-3.30305200	-1.47336300
C	-4.95922000	-5.54104300	-2.95125600
C	-6.43923300	-5.72850200	-2.85180900
H	-6.78142400	-6.53848500	-3.53113900
H	-6.74264500	-6.02052200	-1.83300100
H	-6.99227800	-4.81903400	-3.13646000
C	-4.08472600	-6.59128400	-2.34852300
H	-3.04828700	-6.24268300	-2.22607400
H	-4.45864500	-6.90884100	-1.36155800
H	-4.05789400	-7.49811100	-2.98959500
C	-4.42297200	-4.73299700	-4.08862400
H	-4.48816500	-5.29957700	-5.04252500
H	-4.99501400	-3.80223200	-4.23714900
H	-3.36154400	-4.47479900	-3.94536100
C	-3.37097600	-4.90757800	0.64355100
O	-2.30145700	-4.77337000	0.06027700
C	-2.12871600	-6.15658400	2.48880900
H	-1.41262300	-5.33310200	2.63155000
H	-2.25316200	-6.67660300	3.45055300
H	-1.67811300	-6.85930100	1.77156800
C	-3.46254200	-5.63544800	1.97428400
H	-4.19448700	-6.45483000	1.85021200
H	-3.93440000	-4.94619500	2.69859200

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.235017 (Hartree/Particle)
Thermal correction to Energy= 0.248877
Thermal correction to Enthalpy= 0.249821
Thermal correction to Gibbs Free Energy= 0.193154
Sum of electronic and zero-point Energies= -427.847354
Sum of electronic and thermal Energies= -427.833495
Sum of electronic and thermal Enthalpies= -427.832550
Sum of electronic and thermal Free Energies= -427.889217
HF=-428.0823713

C[54]

C	-4.37469900	-3.96469100	-1.14263200
H	-3.33804800	-3.62456700	-1.28659500
C	-4.49400000	-4.55808600	0.21052500
H	-5.48447100	-4.70565800	0.65184300
H	-5.04112100	-3.08662700	-1.21410100
C	-4.74078300	-4.92468700	-2.32382100
C	-6.20959200	-5.36229500	-2.22042700
H	-6.48428800	-5.99639900	-3.07874200
H	-6.39606500	-5.94413900	-1.30418900
H	-6.88521200	-4.49138000	-2.21451800
C	-3.82637400	-6.15857600	-2.29609200
H	-2.76478300	-5.86797800	-2.32543700
H	-3.98405900	-6.75435300	-1.38317300
H	-4.02985400	-6.80890200	-3.16208700
C	-4.52583400	-4.15430600	-3.63454300
H	-4.76890600	-4.78779500	-4.50288000
H	-5.16570400	-3.25814500	-3.67911800
H	-3.47802800	-3.82855100	-3.73490100
C	-3.34022800	-4.99736200	0.96546000
O	-2.19425400	-4.88267400	0.51379800
C	-2.32606100	-6.05512600	3.05254700
H	-1.64584800	-5.20411700	3.20927900
H	-2.56303200	-6.49312700	4.03380600
H	-1.77815100	-6.80557700	2.46263000
C	-3.59399400	-5.61585400	2.33376900
H	-4.28725100	-6.46524500	2.19582400
H	-4.15962800	-4.88180900	2.93576300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.239853 (Hartree/Particle)
Thermal correction to Energy= 0.252557
Thermal correction to Enthalpy= 0.253502
Thermal correction to Gibbs Free Energy= 0.200159
Sum of electronic and zero-point Energies= -427.884509
Sum of electronic and thermal Energies= -427.871804
Sum of electronic and thermal Enthalpies= -427.870860
Sum of electronic and thermal Free Energies= -427.924202
HF=-428.1243616

B[57]

C	-4.21251500	-4.28670700	-1.36050400
H	-3.54196500	-4.91968400	-1.94951000
C	-4.16423900	-4.29737100	-0.02480900
H	-4.82260700	-3.67119400	0.58614900
H	-4.91794900	-3.65160000	-1.90422100
O	-2.13794500	-6.20377000	-0.03064500
O	-3.88470400	-6.03299800	1.95021500
O	-2.09586800	-4.29652500	1.75663900
C	-3.32671100	-7.05340400	2.80934200
C	-2.90743300	-6.47528400	4.14696600
H	-2.48111900	-7.53506600	2.29296100
H	-4.11975900	-7.80579700	2.92999600
H	-2.54767000	-7.28130100	4.80579200
H	-2.10161800	-5.73869200	4.01808800
H	-3.75826600	-5.97926200	4.63896000
C	-0.92989100	-3.64906000	1.21337800
C	-0.05807700	-3.18352900	2.35935300
H	-1.25472600	-2.79795500	0.59008600
H	-0.39499300	-4.36012900	0.56451000

H	0.82864600	-2.66046300	1.96909800
H	-0.60979100	-2.49109200	3.01357300
H	0.27978000	-4.03969600	2.96331900
P	-2.96959900	-5.31481800	0.83604600

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.189850 (Hartree/Particle)
Thermal correction to Energy= 0.202904
Thermal correction to Enthalpy= 0.203848
Thermal correction to Gibbs Free Energy= 0.148051
Sum of electronic and zero-point Energies= -802.948741
Sum of electronic and thermal Energies= -802.935687
Sum of electronic and thermal Enthalpies= -802.934743
Sum of electronic and thermal Free Energies= -802.990540
HF=-803.1385909

B-TS-C[57]

C	-4.10219800	-4.22923600	-1.33902500
H	-3.47284400	-4.92976300	-1.89083900
C	-3.92449900	-4.05971700	0.00316800
H	-4.45912000	-3.28249200	0.55714200
H	-4.63105500	-3.47220200	-1.92139600
O	-2.26060200	-6.27275500	0.17056500
O	-3.96200900	-5.69200400	2.10269900
O	-1.91388000	-4.29604300	1.84687400
C	-3.56504300	-6.74115500	3.01261800
C	-3.06755300	-6.16955900	4.32626800
H	-2.79873900	-7.36636200	2.52728900
H	-4.46082500	-7.36211800	3.16107600
H	-2.82981600	-6.98730400	5.02495700
H	-2.16301000	-5.56506600	4.16848000
H	-3.83714400	-5.53187100	4.78816200
C	-0.71166500	-3.78955400	1.24306900
C	0.15192600	-3.18168700	2.32695700
H	-0.97956500	-3.03582900	0.48151900
H	-0.19142800	-4.61446200	0.72994600
H	1.07386300	-2.76959800	1.88840800
H	-0.38292800	-2.36805000	2.84064400
H	0.43080900	-3.94102300	3.07380200
P	-2.94286900	-5.18879300	0.94836800
C	-5.87714500	-5.72790600	-1.67615400
C	-6.67740300	-5.51503000	-0.42769100
H	-7.56614000	-6.17840900	-0.42875000
H	-6.09002400	-5.74924500	0.47278800
H	-7.04202100	-4.47910400	-0.34579400
C	-5.11654000	-7.01768800	-1.76583600
H	-4.50108000	-7.06844800	-2.67789800
H	-4.45579100	-7.16523500	-0.89824900
H	-5.82190500	-7.87341000	-1.79875700
C	-6.43866600	-5.18029200	-2.95334400
H	-7.26397200	-5.82693500	-3.31744400
H	-6.85606800	-4.16948600	-2.82196900
H	-5.68216400	-5.14966800	-3.75415800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.308178 (Hartree/Particle)
Thermal correction to Energy= 0.327564
Thermal correction to Enthalpy= 0.328508
Thermal correction to Gibbs Free Energy= 0.257760
Sum of electronic and zero-point Energies= -960.538331
Sum of electronic and thermal Energies= -960.518945
Sum of electronic and thermal Enthalpies= -960.518001
Sum of electronic and thermal Free Energies= -960.588749
HF=-960.8465089

C[57]

C	-4.11628200	-4.09356200	-0.95005000
H	-3.25888400	-4.49449100	-1.51370000
C	-3.82739100	-4.17556000	0.50607300
H	-4.36128800	-3.54121300	1.22007700
H	-4.24650400	-3.03588300	-1.23769700
O	-1.93238200	-6.14898100	0.14049400
O	-3.63006100	-6.22689300	2.16964700
O	-1.73979800	-4.59124200	2.22861700
C	-3.08955900	-7.37969100	2.85514000
C	-2.70942800	-7.03535900	4.28174500
H	-2.22855600	-7.76675100	2.28712700
H	-3.88066400	-8.14333500	2.82469600
H	-2.35528300	-7.93834800	4.80372300
H	-1.91000600	-6.28084800	4.29874300
H	-3.57775000	-6.63696300	4.82891400
C	-0.46044300	-4.07415000	1.81650300
C	-0.59046800	-2.72596600	1.13179100
H	0.02569200	-4.80923200	1.15641300
H	0.13210300	-3.99370800	2.73941300
H	0.40804800	-2.31788800	0.90965200
H	-1.14051400	-2.81439800	0.18144700
H	-1.12442700	-2.01073500	1.77611000
P	-2.69842600	-5.36950200	1.16340600
C	-5.39589400	-4.87008000	-1.41590200
C	-6.64193600	-4.28590300	-0.73498200
H	-7.55107000	-4.79776200	-1.08952000
H	-6.59631100	-4.40553500	0.35881100
H	-6.75096300	-3.21164400	-0.95679500
C	-5.26308900	-6.36086000	-1.06825500
H	-4.33862000	-6.78677500	-1.48752700
H	-5.23634200	-6.51770500	0.02083900
H	-6.11901000	-6.92626600	-1.47044900
C	-5.51059400	-4.70242600	-2.93749100
H	-6.40260900	-5.22458000	-3.31952400
H	-5.59450900	-3.63965100	-3.21687400
H	-4.62849400	-5.11975800	-3.44933000

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.312029 (Hartree/Particle)
Thermal correction to Energy= 0.330780
Thermal correction to Enthalpy= 0.331724
Thermal correction to Gibbs Free Energy= 0.262579
Sum of electronic and zero-point Energies= -960.569876
Sum of electronic and thermal Energies= -960.551125
Sum of electronic and thermal Enthalpies= -960.550181
Sum of electronic and thermal Free Energies= -960.619326

HF=-960.8819047

B[56]

C	-4.77335900	-4.32150700	-1.16309700
H	-4.19941800	-5.09344900	-1.68284100
C	-4.46428800	-3.97443800	0.08358900
H	-4.97514300	-3.21458500	0.68036900
H	-5.60062500	-3.84039400	-1.69147700
S	-3.06668500	-4.72549700	0.90306700
O	-2.45153500	-5.69464400	-0.02271400
O	-2.25932200	-3.63192500	1.47360700
C	-3.79556500	-5.63854200	2.26120000
C	-4.24559200	-6.94279000	2.03704800
C	-3.88898100	-5.02778500	3.51386000
C	-4.81490200	-7.64679100	3.09930600
H	-4.14081100	-7.39399500	1.04931300
C	-4.46064000	-5.74414200	4.56822000
H	-3.51003200	-4.01444800	3.65286000
C	-4.92334000	-7.04775400	4.36010900
H	-5.17056300	-8.66765000	2.94483400
H	-4.54061200	-5.28436900	5.55549300
H	-5.36892300	-7.60385300	5.18791600

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.143221 (Hartree/Particle)
Thermal correction to Energy= 0.153200
Thermal correction to Enthalpy= 0.154145
Thermal correction to Gibbs Free Energy= 0.106958
Sum of electronic and zero-point Energies= -857.660791
Sum of electronic and thermal Energies= -857.650811
Sum of electronic and thermal Enthalpies= -857.649867
Sum of electronic and thermal Free Energies= -857.697054
HF=-857.8040116

B-TS-C[56]

C	-5.71322600	-4.85997900	-0.88427700
H	-5.18967200	-3.90389300	-0.92196900
C	-5.25344900	-5.85522000	-0.08502600
H	-5.75649100	-6.81041000	0.07858500
H	-6.74209600	-4.89494000	-1.24552200
C	-4.94695100	-5.27340100	-3.09219100
C	-6.10694900	-4.72368700	-3.86428300
H	-5.89659600	-4.76954200	-4.95304300
H	-7.03008900	-5.29900700	-3.69119200
H	-6.29702800	-3.66551800	-3.62228700
C	-4.78458800	-6.76123500	-3.04857700
H	-4.06802200	-7.06427800	-2.27015600
H	-5.74143600	-7.27417600	-2.86407200
H	-4.39565300	-7.12829100	-4.02005500
C	-3.68443700	-4.46558500	-3.08724200
H	-3.12926300	-4.62674400	-4.03423200
H	-3.88630300	-3.38568600	-3.00875600
H	-3.01870000	-4.75362800	-2.26061500
S	-3.61682800	-5.79313600	0.56128900
O	-2.88592200	-6.99493300	0.09958500
O	-3.04678900	-4.45587400	0.28768100
C	-3.81629900	-5.94706700	2.33529200
C	-3.75181300	-7.21391700	2.92061500
C	-4.03199200	-4.79327200	3.09471800
C	-3.92089500	-7.32538400	4.30295500
H	-3.56267200	-8.08939300	2.29815600
C	-4.19771400	-4.91861700	4.47494100
H	-4.05974300	-3.81807500	2.60649700
C	-4.14474300	-6.18167200	5.07675200
H	-3.87224300	-8.30790800	4.77730400
H	-4.36422600	-4.02764600	5.08416700
H	-4.27477100	-6.27385200	6.15735700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.261634 (Hartree/Particle)
Thermal correction to Energy= 0.277997
Thermal correction to Enthalpy= 0.278941
Thermal correction to Gibbs Free Energy= 0.216065
Sum of electronic and zero-point Energies= -1015.252722
Sum of electronic and thermal Energies= -1015.236360
Sum of electronic and thermal Enthalpies= -1015.235415
Sum of electronic and thermal Free Energies= -1015.298291
HF=-1015.5143562

C[56]

C	-4.93940100	-4.28736100	-0.83907500
H	-4.09622000	-3.63183400	-0.57106100
C	-4.98856700	-5.42369000	0.10734700
H	-5.88008300	-6.03052200	0.28452700
H	-5.87181600	-3.70753200	-0.72796600
C	-4.79611900	-4.67764500	-2.35160300
C	-5.96850000	-5.57408400	-2.77504100
H	-5.91018700	-5.79897400	-3.85191500
H	-5.95842400	-6.53287800	-2.23332200
H	-6.93680100	-5.08315600	-2.58425100
C	-3.46783600	-5.41298400	-2.58260600
H	-2.61155500	-4.79558900	-2.27086300
H	-3.42393600	-6.35399500	-2.01400300
H	-3.34745900	-5.65588100	-3.65042100
C	-4.81673900	-3.37581900	-3.16463600
H	-4.70859500	-3.59026900	-4.23988900
H	-5.76318700	-2.82976500	-3.02146300
H	-3.99093300	-2.70975100	-2.86727900
S	-3.52953000	-6.07025000	0.83975800
O	-3.34617200	-7.45836200	0.35939100
O	-2.44112000	-5.08958400	0.65542500
C	-3.91216100	-6.15748200	2.58499000
C	-3.65881200	-5.04096700	3.38789400
C	-4.45632300	-7.33500500	3.10535100
C	-3.96962700	-5.10814200	4.74695800
H	-3.21757700	-4.14464200	2.94979400
C	-4.76371400	-7.38733600	4.46663400
H	-4.62191700	-8.19188600	2.45107600
C	-4.52268600	-6.27697100	5.28338200
H	-3.77570700	-4.24764900	5.39075200
H	-5.18743400	-8.29956800	4.89189000
H	-4.76374800	-6.32387700	6.34767700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.265352 (Hartree/Particle)
Thermal correction to Energy= 0.281141

Thermal correction to Enthalpy= 0.282085
Thermal correction to Gibbs Free Energy= 0.220995
Sum of electronic and zero-point Energies= -1015.283243
Sum of electronic and thermal Energies= -1015.267455
Sum of electronic and thermal Enthalpies= -1015.266511
Sum of electronic and thermal Free Energies= -1015.327601
HF=-1015.5485956

B[55]

C	-4.74436700	-4.17487400	-1.11187600
H	-4.12203200	-4.86581000	-1.68723800
C	-4.48163000	-3.94053000	0.17126700
H	-5.03909300	-3.26263100	0.82281900
H	-5.57775600	-3.67865600	-1.61628100
S	-3.07125900	-4.71551300	0.94600600
O	-2.34181400	-5.49949700	-0.07097100
O	-2.35174300	-3.67047800	1.70083300
C	-3.78643300	-5.87518300	2.13884300
H	-4.44945300	-5.27972700	2.78375000
H	-4.38934300	-6.57893900	1.54697600
C	-2.67057300	-6.55790400	2.91774100
H	-2.07035900	-5.81730400	3.46530900
H	-3.10235400	-7.26340900	3.64247300
H	-2.00874000	-7.11521400	2.23926400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.118171 (Hartree/Particle)
Thermal correction to Energy= 0.126491
Thermal correction to Enthalpy= 0.127436
Thermal correction to Gibbs Free Energy= 0.085281
Sum of electronic and zero-point Energies= -705.358909
Sum of electronic and thermal Energies= -705.350589
Sum of electronic and thermal Enthalpies= -705.349645
Sum of electronic and thermal Free Energies= -705.391799
HF=-705.4770802

B-TS-C[55]

C	-5.53420600	-4.72717700	-0.67583800
H	-4.97529000	-3.81490000	-0.88876900
C	-5.04270700	-5.63293900	0.20739200
H	-5.56629500	-6.53531500	0.53022600
H	-6.59347900	-4.75111100	-0.93582800
C	-5.01708900	-5.47366500	-2.86322900
C	-6.20817200	-4.93785000	-3.59709900
H	-6.10877600	-5.13918500	-4.68393000
H	-7.14607900	-5.41188600	-3.26722300
H	-6.30315900	-3.84578100	-3.48403200
C	-4.95011600	-6.95225200	-2.63541800
H	-4.17627000	-7.20915900	-1.89625800
H	-5.91403800	-7.35973700	-2.29239900
H	-4.69192300	-7.46944100	-3.58176100
C	-3.70890900	-4.77490100	-3.08032500
H	-3.26276800	-5.10023600	-4.04265900
H	-3.82893900	-3.68125500	-3.13069500
H	-2.98603300	-5.00660200	-2.28481000
S	-3.34438400	-5.57943200	0.67193900
O	-2.70641400	-6.86176500	0.28615900
O	-2.74187100	-4.32172700	0.17185100
C	-3.34351800	-5.50642200	2.48079200
H	-3.87685400	-4.58050200	2.74015200
H	-3.93349800	-6.37073200	2.82001400
C	-1.91363800	-5.53335300	3.00165300
H	-1.34410600	-4.67672800	2.61306800
H	-1.91604400	-5.48189000	4.10031200
H	-1.40728900	-6.45958700	2.69490800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.236530 (Hartree/Particle)
Thermal correction to Energy= 0.251222
Thermal correction to Enthalpy= 0.252166
Thermal correction to Gibbs Free Energy= 0.193975
Sum of electronic and zero-point Energies= -862.950880
Sum of electronic and thermal Energies= -862.936188
Sum of electronic and thermal Enthalpies= -862.935244
Sum of electronic and thermal Free Energies= -862.993435
HF=-863.1874102

C[55]

C	-4.56687300	-4.03659400	-0.89429200
H	-3.54133900	-3.63591100	-0.87906200
C	-4.77873800	-4.86255300	0.31540100
H	-5.76623800	-5.11129800	0.71329200
H	-5.26722900	-3.18464100	-0.85211700
C	-4.78790700	-4.76785000	-2.26432800
C	-6.21103500	-5.34024600	-2.33003100
H	-6.39619900	-5.79557900	-3.31593600
H	-6.36690800	-6.12012500	-1.56820000
H	-6.96688000	-4.55314500	-2.17424200
C	-3.76316500	-5.89991000	-2.42925900
H	-2.73314300	-5.51611500	-2.36999900
H	-3.87798200	-6.66511900	-1.64721900
H	-3.89244100	-6.39066400	-3.40714800
C	-4.59364200	-3.72659300	-3.37520100
H	-4.72396800	-4.19030900	-4.36605000
H	-5.32346100	-2.90567100	-3.28638500
H	-3.58296100	-3.28952200	-3.33599600
S	-3.45793300	-5.76956500	1.03885200
O	-3.73472000	-7.21628800	0.86278900
O	-2.17730800	-5.23070100	0.53279300
C	-3.55647300	-5.41922900	2.81144600
H	-3.42344800	-4.33218200	2.90959800
H	-4.57706200	-5.69040100	3.11886400
C	-2.49047600	-6.21497700	3.55237900
H	-1.48685400	-5.94821800	3.19107900
H	-2.54494400	-5.99361900	4.62822600
H	-2.64124600	-7.29412000	3.40797100

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.240289 (Hartree/Particle)
Thermal correction to Energy= 0.254387
Thermal correction to Enthalpy= 0.255331
Thermal correction to Gibbs Free Energy= 0.199156

Sum of electronic and zero-point Energies= -862.980808
Sum of electronic and thermal Energies= -862.966710
Sum of electronic and thermal Enthalpies= -862.965766
Sum of electronic and thermal Free Energies= -863.021941
HF=-863.2210973

Figure A3.7
F-TS-H^{R}

Ni	-1.36141200	1.24562200	-0.37638400
C	-3.11461200	2.00729900	0.08091300
C	-4.99910900	4.06136700	-0.38938700
C	-3.18896800	3.12798600	0.93047400
C	-4.04774400	1.90396500	-0.96922700
C	-4.96709500	2.92740900	-1.20857600
C	-4.10561600	4.15055300	0.68545700
H	-2.53735500	3.17337100	1.80109900
H	-4.03787300	1.03807900	-1.63369000
H	-5.66218800	2.83663100	-2.04741500
H	-4.13007900	5.01931400	1.34896000
H	-5.72167000	4.85884700	-0.57665800
C	-3.09124700	-0.93581600	0.22285500
H	-2.19009100	-1.56112800	0.20962900
C	-2.77547700	0.33702800	1.00186300
H	-3.64644600	0.65482500	1.57889000
H	-3.32768600	-0.70579100	-0.82759600
C	-4.26514500	-1.77757600	0.78735900
C	-5.58911200	-1.00704700	0.66207900
H	-6.42551900	-1.60731500	1.05457700
H	-5.57065000	-0.06052100	1.22543800
H	-5.80843400	-0.76396800	-0.38954400
C	-4.01024800	-2.14135100	2.25921200
H	-3.04806000	-2.66249000	2.37789400
H	-3.99007100	-1.24876000	2.90457600
H	-4.80908800	-2.79942100	2.63713500
C	-4.35042400	-3.06677500	-0.04447100
H	-5.18250500	-3.70298400	0.29752800
H	-4.51381500	-2.83978100	-1.11060300
H	-3.41982800	-3.65149300	0.03758000
C	-1.67749300	0.18359500	2.01861200
O	-0.90517200	-0.74887300	2.11694700
O	-1.68481600	1.20383800	2.90174600
C	-0.67945900	1.17284100	3.91414700
H	0.32386900	1.19998300	3.46473900
H	-0.84100500	2.06358600	4.53220600
H	-0.76938200	0.26350400	4.52578700
Br	-0.80119300	2.30851600	-2.56719200
C	1.35400700	1.51713100	0.37372700
C	2.26462900	3.46989500	0.90428600
C	0.72502000	3.60586100	0.78049900
N	0.28971000	2.20674000	0.56943000
H	2.82970500	4.14569800	0.25125500
H	0.45231300	4.14146300	-0.14481400
C	0.29117800	-1.67083100	-0.97424600
C	1.82768100	-1.87208600	-0.86202600
C	1.24685800	0.13810800	-0.11864000
N	0.11324700	-0.27861300	-0.53199100
H	-0.23221800	-2.31013000	-0.24449200
H	2.32277900	-1.91724100	-1.84367600
H	2.61381300	3.57625200	1.94264600
H	2.12131600	-2.73901100	-0.25810700
O	2.54047600	2.10283100	0.48444100
O	2.30256500	-0.66932200	-0.18465100
C	0.09288700	4.29931600	1.97576600
H	0.53307900	5.30172200	2.09177900
H	-0.98720600	4.42019600	1.83570400
H	0.27381500	3.73370500	2.90109500
C	-0.28053000	-1.90098000	-2.36537000
H	-0.10613200	-2.94011600	-2.68357000
H	-1.36419300	-1.71535000	-2.36816300
H	0.18728400	-1.22036900	-3.09234400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.513653 (Hartree/Particle)
Thermal correction to Energy= 0.546913
Thermal correction to Enthalpy= 0.547857
Thermal correction to Gibbs Free Energy= 0.446030
Sum of electronic and zero-point Energies= -5348.812342
Sum of electronic and thermal Energies= -5348.779082
Sum of electronic and thermal Enthalpies= -5348.778138
Sum of electronic and thermal Free Energies= -5348.879965
HF=-5349.325995

Figure A3.8
^{1}G-C^{R}

Ni	-0.70885300	0.14705700	-0.57870400
C	-1.24483000	1.78858300	-1.32173600
C	-1.89610100	4.29971600	-2.46436300
C	-2.16732100	2.64953700	-0.70363400
C	-0.66454600	2.20939000	-2.53086100
C	-0.98791700	3.44813800	-3.10117200
C	-2.48431900	3.89422800	-1.26102700
H	-2.64997600	2.34801100	0.22788500
H	0.05941900	1.56706900	-3.04317600
H	-0.52434400	3.74950600	-4.04526600
H	-3.19959700	4.54885800	-0.75420200
Br	-2.82026900	-0.80394300	-0.96925700
C	-3.75426900	1.23963800	2.61779100
H	-2.94278800	1.98338900	2.64672800
H	-3.95454800	0.99398000	1.56344300
H	-4.65387600	1.71782400	3.03745500
C	-3.39782500	-0.02491200	3.41373900
C	-2.17804400	-0.74684800	2.77092400
H	-1.99446100	-1.69522200	3.29785200
H	-2.45966600	-0.99484800	1.72926500
C	-0.91900900	0.02684000	2.72736400
C	-4.58451500	-0.99900500	3.37142500
H	-4.36058600	-1.92088900	3.93231600
H	-5.48321800	-0.54124300	3.81530600
H	-4.82275800	-1.28249200	2.33371700
H	-0.88358500	1.02282400	2.28385000
C	0.30943500	-0.51564500	3.26174800
O	0.43211200	-1.61723100	3.78269100
O	1.36426000	0.32562700	3.10523400
C	2.61634700	-0.11832900	3.63300800
H	2.94917300	-1.03315100	3.12270700
H	3.32800000	0.69439600	3.44974100

H	2.53264100	-0.31888800	4.71113000
C	-3.07585300	0.34142300	4.87009200
H	-2.80788200	-0.55417600	5.45404700
H	-2.22925100	1.04502000	4.92543900
H	-3.94314700	0.81719500	5.35588200
H	-2.14577500	5.26933500	-2.90300400
C	1.91805400	-0.05487300	0.22480200
C	3.23670700	1.71961500	0.05094300
C	1.76402000	2.12619400	-0.21846900
N	1.07964600	0.81491500	-0.22173900
H	3.86903600	1.74652500	-0.84684300
H	1.65283600	2.58424300	-1.21014400
C	-0.17012500	-2.98623800	0.48790000
C	1.10969000	-3.46479000	1.23019700
C	1.39119700	-1.40003200	0.46494500
N	0.15424500	-1.58177900	0.17420700
H	-1.03875700	-2.99360000	1.16171000
H	1.54008500	-4.38632800	0.81930200
H	3.70988500	2.28831900	0.86064600
H	0.97232800	-3.54497000	2.31511900
O	3.15693500	0.32031400	0.48095700
O	2.08356900	-2.38589600	1.00914200
C	1.16967300	3.04017600	0.84834400
H	1.70793900	4.00030900	0.85657900
H	0.11077000	3.23374000	0.63235500
H	1.25358600	2.57358300	1.84101800
C	-0.49536400	-3.77215400	-0.77759400
H	-0.72883600	-4.81669000	-0.52017200
H	-1.36432200	-3.32438100	-1.27830300
H	0.36048200	-3.76478200	-1.47090700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.513178 (Hartree/Particle)
Thermal correction to Energy= 0.547040
Thermal correction to Enthalpy= 0.547984
Thermal correction to Gibbs Free Energy= 0.444939
Sum of electronic and zero-point Energies= -5348.817365
Sum of electronic and thermal Energies= -5348.783502
Sum of electronic and thermal Enthalpies= -5348.782558
Sum of electronic and thermal Free Energies= -5348.885604
HF=-5349.3305428

Figure A3.9
^{2}F'-TS-H^R-B^{CF3}-Conf1

Ni	-0.70885300	0.14705700	-0.57870400
C	-1.24483000	1.78858300	-1.32173600
C	-1.89610100	4.29971600	-2.46436300
C	-2.16732100	2.64953700	-0.70363400
C	-0.66454600	2.20939000	-2.53086100
C	-0.98791700	3.44813800	-3.10117200
C	-2.48431900	3.89422800	-1.26102700
H	-2.64997600	2.34801100	0.22788500
H	0.05941900	1.56706900	-3.04317600
H	-0.52434400	3.74950600	-4.04526600
H	-3.19959700	4.54885800	-0.75420200
Br	-2.82026900	-0.80394300	-0.96925700
C	-3.75426900	1.23963800	2.61779100
H	-2.94278800	1.98338900	2.64672800
H	-3.95454800	0.99398000	1.56344300
H	-4.65387600	1.71782400	3.03745500
C	-3.39782500	-0.02491200	3.41373900
C	-2.17804400	-0.74684800	2.77092400
H	-1.99446100	-1.69522200	3.29785200
H	-2.45966600	-0.99484800	1.72926500
C	-0.91900900	0.02684000	2.72736400
C	-4.58451500	-0.99900500	3.37142500
H	-4.36058600	-1.92088900	3.93231600
H	-5.48321800	-0.54124300	3.81530600
H	-4.82275800	-1.28249200	2.33371700
H	-0.88358500	1.02282400	2.28385000
C	0.30943500	-0.51564500	3.26174800
O	0.43211200	-1.61723100	3.78269100
O	1.36426000	0.32562700	3.10523400
C	2.61634700	-0.11832900	3.63300800
H	2.94917300	-1.03315100	3.12270700
H	3.32800000	0.69439600	3.44974100
H	2.53264100	-0.31888800	4.71113000
C	-3.07585300	0.34142300	4.87009200
H	-2.80788200	-0.55417600	5.45404700
H	-2.22925100	1.04502000	4.92543900
H	-3.94314700	0.81719500	5.35588200
H	-2.14577500	5.26933500	-2.90300400
C	1.91805400	-0.05487300	0.22480200
C	3.23670700	1.71961500	0.05094300
C	1.76402000	2.12619400	-0.21846900
N	1.07964600	0.81491500	-0.22173900
H	3.86903600	1.74652500	-0.84684300
H	1.65283600	2.58424300	-1.21014400
C	-0.17012500	-2.98623800	0.48790000
C	1.10969000	-3.46479000	1.23019700
C	1.39119700	-1.40003200	0.46494500
N	0.15424500	-1.58177900	0.17420700
H	-1.03875700	-2.99360000	1.16171000
H	1.54008500	-4.38632800	0.81930200
H	3.70988500	2.28831900	0.86064600
H	0.97232800	-3.54497000	2.31511900
O	3.15693500	0.32031400	0.48095700
O	2.08356900	-2.38589600	1.00914200
C	1.16967300	3.04017600	0.84834400
H	1.70793900	4.00030900	0.85657900
H	0.11077000	3.23374000	0.63235500
H	1.25358600	2.57358300	1.84101800
C	-0.49536400	-3.77215400	-0.77759400
H	-0.72883600	-4.81669000	-0.52017200
H	-1.36432200	-3.32438100	-1.27830300
H	0.36048200	-3.76478200	-1.47090700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.689324 (Hartree/Particle)
Thermal correction to Energy= 0.734093
Thermal correction to Enthalpy= 0.735038
Thermal correction to Gibbs Free Energy= 0.606265
Sum of electronic and zero-point Energies= -5921.190128
Sum of electronic and thermal Energies= -5921.145359
Sum of electronic and thermal Enthalpies= -5921.144415
Sum of electronic and thermal Free Energies= -5921.273188

HF=-5921.8794522

^{2}F'-TS-H^R-B^{CF3}-Conf2

Ni	-1.40461300	1.04075000	-0.23681400
C	-1.83144800	0.77974100	1.62486400
C	-1.44466200	1.68637600	4.25465600
C	-0.77235400	0.27962500	2.40411600
C	-2.74785200	1.66885100	2.21623100
C	-2.55352400	2.12216100	3.51653900
C	-0.56228100	0.75249400	3.69854300
H	-0.10387600	-0.47890800	1.99820000
H	-3.59812200	2.03168700	1.63715700
H	-3.26081600	2.82715500	3.95554200
H	0.28855400	0.39102500	4.27804800
C	-2.87592700	-0.99060700	-1.04301500
H	-2.12216500	-1.77910000	-1.13324000
C	-2.88921000	-0.50536800	0.41422700
H	-3.82809900	-0.00866400	0.66135300
H	-2.60503800	-0.19098400	-1.75017100
C	-4.23450000	-1.56604400	-1.54044400
C	-5.31352600	-0.47353900	-1.57748900
H	-6.24631600	-0.87242300	-2.00748100
H	-5.55045300	-0.09694200	-0.57028300
H	-4.98635100	0.38626400	-2.18088700
C	-4.70208100	-2.73144000	-0.65400200
H	-3.92865800	-3.51189400	-0.57985100
H	-4.94746600	-2.39797100	0.36562300
H	-5.61055700	-3.19075000	-1.07547600
C	-3.99206000	-2.08538200	-2.96789900
H	-4.92054200	-2.49132100	-3.40021100
H	-3.63519300	-1.27846000	-3.62810700
H	-3.23675600	-2.88778900	-2.97473700
C	-2.62188700	-1.63285600	1.35735100
O	-1.76983300	-2.48681200	1.19878700
O	-3.42160900	-1.59950300	2.43355700
C	-3.16326000	-2.56716700	3.45226800
H	-2.14928400	-2.43250600	3.85777200
H	-3.90993200	-2.39235000	4.23539500
H	-3.25748900	-3.58822000	3.05511200
Br	-2.92666400	2.63515600	-1.35025300
C	1.51023400	1.74589200	0.02299500
C	2.47003400	3.63227700	0.68036500
C	0.94865200	3.84443200	0.44797900
N	0.46997700	2.48026700	0.12577000
H	3.11465700	4.30484200	0.10248500
H	0.77418200	4.46230200	-0.45085500
C	0.51559500	-1.57219500	-1.08437000
C	1.99297200	-1.78391300	-0.68042400
C	1.40056000	0.32940800	-0.35419400
N	0.25869500	-0.19375800	-0.61300400
H	-0.14335200	-2.25263200	-0.52937400
H	2.62046200	-2.23561900	-1.45694800
H	2.74422400	3.68035500	1.74473300
H	2.10481500	-2.34474800	0.25820200
O	2.71663100	2.27015700	0.23393900
O	2.48498400	-0.42946800	-0.43696400
C	0.23136100	4.51709200	1.62807700
H	0.32613800	3.84215000	2.49925100
C	0.23142300	-1.69569700	-2.59808400
H	-0.79806900	-1.33327300	-2.73959900
C	0.91995700	5.84695200	1.96014400
H	0.45088000	6.32291000	2.83242600
H	1.98732900	5.72251300	2.19817400
H	0.84131700	6.54755500	1.11152300
C	-1.25964200	4.70440900	1.32439800
H	-1.68486200	3.72797400	1.06518500
H	-1.36320400	5.32018200	0.41306700
C	-2.05969200	5.33263100	2.46426400
H	-1.83053400	6.40181400	2.59520700
H	-3.14105100	5.24879600	2.27290700
H	-1.84900000	4.83019400	3.42084500
C	1.14602900	-0.81081500	-3.44881900
H	1.09839100	0.24028200	-3.12577900
H	2.19754900	-1.13824300	-3.40656800
H	0.83824400	-0.83511400	-4.50366700
C	0.25694500	-3.17715900	-3.00835600
H	-0.38919600	-3.73892500	-2.31155100
H	1.27579100	-3.58245000	-2.87068600
C	-0.20718200	-3.43916300	-4.44040600
H	0.47005100	-2.98948600	-5.18255100
H	-0.25186200	-4.51973400	-4.64683900
H	-1.21365300	-3.02277300	-4.61071400
C	-1.18250400	2.27877400	5.60584700
F	-0.61670300	3.50936400	5.50664500
F	-2.31196200	2.44370900	6.32125800
F	-0.34366900	1.53276600	6.34616500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.689454 (Hartree/Particle)
Thermal correction to Energy= 0.733978
Thermal correction to Enthalpy= 0.734922
Thermal correction to Gibbs Free Energy= 0.607791
Sum of electronic and zero-point Energies= -5921.186304
Sum of electronic and thermal Energies= -5921.141781
Sum of electronic and thermal Enthalpies= -5921.140837
Sum of electronic and thermal Free Energies= -5921.267968
HF=-5921.8757585

^{2}F'-TS-H^R-B^{CF3}-Conf3

Ni	-1.27276600	1.20200200	-0.21710100
C	-1.68621200	0.83628300	1.63416200
C	-1.22829300	1.40941400	4.35574800
C	-0.72365900	0.11767800	2.37138300
C	-2.45083000	1.81239700	2.30456800
C	-2.21405900	2.10627000	3.64319100
C	-0.48776300	0.41058100	3.71314600
H	-0.16467600	-0.68915700	1.90031300
H	-3.21841100	2.35913700	1.75539100
H	-2.80252200	2.88079400	4.13912400
H	0.27462100	-0.14384500	4.26260700
C	-2.77982800	-0.61644600	-1.10379300
H	-2.08315200	-1.45746500	-1.17493100
C	-2.85136600	-0.19336400	0.37310600
H	-3.74490800	0.39723800	0.58248800
H	-2.39599400	0.18102400	-1.76582500
C	-4.13806800	-1.06080900	-1.72502700
C	-5.13573900	0.10526400	-1.77569900
H	-6.06147300	-0.20968100	-2.28372500
H	-5.41296900	0.45090800	-0.76796200
H	-4.71373600	0.96769100	-2.31175300

C	-4.75273600	-2.23207400	-0.94171100
H	-4.04642900	-3.07177900	-0.85496100
H	-5.05242600	-1.93248700	0.07397600
H	-5.65737500	-2.59679300	-1.45394900
C	-3.82954600	-1.52387200	-3.15924900
H	-4.75048200	-1.83718700	-3.67627400
H	-3.36969900	-0.71317900	-3.74716700
H	-3.13425900	-2.37905100	-3.15978800
C	-2.79795000	-1.39998700	1.25779900
O	-2.06622000	-2.35639300	1.08904500
O	-3.64595600	-1.30847200	2.29183900
C	-3.58917500	-2.35901500	3.25897200
H	-2.58796800	-2.40635000	3.71250000
H	-4.33855800	-2.11352000	4.02017900
H	-3.81894000	-3.32934000	2.79538900
Br	-2.79285500	3.02392700	-1.06950500
C	1.48996700	1.88161900	-0.28586700
C	2.13446000	4.00661700	-0.21841500
C	0.59788900	3.90017100	-0.00961900
N	0.35433400	2.46280400	-0.19074200
H	2.41012000	4.46511600	-1.17753200
H	0.04997400	4.42661900	-0.80165700
C	0.67466800	-1.60070800	-0.84951700
C	2.16581200	-1.68972600	-0.44049800
C	1.49157300	0.42165400	-0.44551700
N	0.36682500	-0.17640000	-0.60337800
H	0.03795200	-2.21108000	-0.19380400
H	2.80280800	-2.23412200	-1.14665400
H	2.66734200	4.51210000	0.59593100
H	2.31177100	-2.08994400	0.57260700
O	2.59507800	2.61507800	-0.25351900
O	2.60753900	-0.29423800	-0.42347600
C	0.07012500	4.37973200	1.35679100
H	-0.98925400	4.07643800	1.36895300
C	0.38633300	-1.98560700	-2.31880400
H	-0.66306300	-1.70821800	-2.49998500
C	0.77582100	3.69324800	2.52612700
H	0.29868000	3.96339300	3.47834300
H	0.72584400	2.59908600	2.44096600
H	1.83604400	3.98780900	2.59630300
C	0.12572800	5.91036800	1.48432700
H	1.17898000	6.24635900	1.46079400
H	-0.24160200	6.16717100	2.49224500
C	-0.68854200	6.67794600	0.44213300
H	-1.72550300	6.30748000	0.39759300
H	-0.72149000	7.75201000	0.68247400
H	-0.26404300	6.58589700	-0.57025600
C	1.24326000	-1.20370800	-3.31738900
H	1.13923500	-0.11813700	-3.16916000
H	2.31177100	-1.46220900	-3.23834200
H	0.93079200	-1.41784500	-4.34921400
C	0.49138800	-3.51052100	-2.48475500
H	-0.10405700	-3.98602600	-1.68632400
H	1.53582300	-3.83083300	-2.31816500
C	0.01022800	-4.02731000	-3.83998500
H	0.63686700	-3.66174000	-4.66787600
H	0.03221900	-5.12764800	-3.87085000
H	-1.02594900	-3.70697700	-4.03890300
C	-0.93544000	1.78434900	5.77646900
F	-2.05386300	2.08801600	6.46471400
F	-0.13679500	2.87791300	5.85756200
F	-0.30525900	0.80387900	6.44949700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.688670 (Hartree/Particle)
Thermal correction to Energy= 0.733336
Thermal correction to Enthalpy= 0.734280
Thermal correction to Gibbs Free Energy= 0.607040
Sum of electronic and zero-point Energies= -5921.190432
Sum of electronic and thermal Energies= -5921.145766
Sum of electronic and thermal Enthalpies= -5921.144822
Sum of electronic and thermal Free Energies= -5921.272062
HF=-5921.8791022

^{2}F'-TS-H^R-B^{CF3}-Conf4

Ni	-1.33949400	1.40341200	-0.39650900
C	-1.66275700	1.04445100	1.48161800
C	-1.16578700	1.74532000	4.16268100
C	-0.61926200	0.43259300	2.20372400
C	-2.49239000	1.96824100	2.14872000
C	-2.23503900	2.32807800	3.46782700
C	-0.36409000	0.79068600	3.52644000
H	-0.00907800	-0.33812700	1.73557700
H	-3.32435800	2.42683400	1.61238800
H	-2.87177600	3.06444200	3.96219400
H	0.46200100	0.32363800	4.06488800
C	-2.75712900	-0.66077900	-1.16840300
H	-1.96837700	-1.41673700	-1.24560200
C	-2.81866800	-0.19281600	0.29057500
H	-3.74199500	0.33889300	0.52597500
H	-2.49501100	0.15469700	-1.86543300
C	-4.08402400	-1.26890900	-1.71220200
C	-5.19451300	-0.20837200	-1.75291900
H	-6.10130600	-0.62324600	-2.22167400
H	-5.47192800	0.13276300	-0.74362300
H	-4.87737900	0.67753800	-2.32326900
C	-4.53944200	-2.46568600	-0.86197100
H	-3.74805800	-3.22674300	-0.78432800
H	-4.81843400	-2.15982400	0.15795500
H	-5.42596900	-2.93784900	-1.31477200
C	-3.79182300	-1.74923700	-3.14367500
H	-4.69511200	-2.17957500	-3.60472000
H	-3.45051500	-0.91598700	-3.77887800
H	-3.00713500	-2.52287700	-3.15067600
C	-2.58909200	-1.32764700	1.23243600
O	-1.77017300	-2.21273500	1.07123600
O	-3.38232600	-1.26140600	2.31179500
C	-3.15226000	-2.23413700	3.33271200
H	-2.12968800	-2.13748400	3.72716500
H	-3.88354100	-2.02661700	4.12233400
H	-3.29072900	-3.25236000	2.94126800
Br	-3.02260000	3.04959700	-1.27819500
C	1.44630300	2.16501900	-0.62586600
C	1.98143800	4.32444800	-0.65352000
C	0.45651200	4.14862500	-0.41283200
N	0.28527400	2.69456900	-0.52716700
H	2.21760800	4.76525500	-1.63112200
H	-0.12940500	4.61282200	-1.21691300
C	0.89175200	-1.40904800	-0.92261900
C	2.39565500	-1.34743000	-0.54959800

C	1.54771400	0.69787300	-0.70178000
N	0.47832600	0.00096400	-0.80400300
H	0.31908800	-1.99094500	-0.18886000
H	3.06081400	-1.88939100	-1.23159600
H	2.50221000	4.88117900	0.13498200
H	2.59444600	-1.66082800	0.48487100
O	2.50991900	2.95733000	-0.65328200
O	2.72159100	0.07662500	-0.64079100
C	-0.07833600	4.65539400	0.94145800
H	-1.12135800	4.30025200	0.97905500
C	0.59167300	-1.95447500	-2.33810400
H	-0.46619500	-1.71596700	-2.53079000
C	1.41848600	-1.26631500	-3.42663400
H	1.08340100	-1.59723900	-4.42132200
H	1.30830200	-0.17158400	-3.38978100
H	2.49089100	-1.50704900	-3.34820600
C	0.73941400	-3.48521300	-2.37616600
H	1.73334200	-3.76840400	-1.98388800
H	0.73772500	-3.80390500	-3.43190000
C	-0.35723800	-4.24100400	-1.62408700
H	-1.34431700	-4.04666600	-2.07439800
H	-0.18331000	-5.32766000	-1.65946500
H	-0.42360800	-3.94602800	-0.56598500
C	0.67326600	4.05021300	2.12711400
H	0.19309900	4.33292500	3.07439700
H	0.67663800	2.95254900	2.08409400
H	1.71825400	4.39900600	2.17290000
C	-0.09884600	6.19054500	1.00936300
H	0.93538700	6.57795000	0.95386900
H	-0.46262800	6.46783100	2.01309000
C	-0.96858300	6.87377100	-0.04660000
H	-1.98637800	6.45117100	-0.05528600
H	-1.05095600	7.95384900	0.15105100
H	-0.55799900	6.76138700	-1.06269100
C	-0.85238200	2.19902300	5.55609100
F	-1.96528100	2.43929200	6.27710500
F	-0.11931600	1.30026200	6.23876400
F	-0.14346000	3.35536500	5.56262800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.689511 (Hartree/Particle)
Thermal correction to Energy= 0.734150
Thermal correction to Enthalpy= 0.735094
Thermal correction to Gibbs Free Energy= 0.607734
Sum of electronic and zero-point Energies= -5921.190816
Sum of electronic and thermal Energies= -5921.146177
Sum of electronic and thermal Enthalpies= -5921.145233
Sum of electronic and thermal Free Energies= -5921.272594
HF=-5921.8803271

^{2}F'-TS-H^R-B^{CF3}-Conf5

Ni	-1.40120300	1.24041200	-0.22186400
C	-1.82410400	0.83531400	1.62402700
C	-1.48091500	1.41755300	4.35766300
C	-0.82231700	0.18996000	2.37702100
C	-2.68755400	1.73071700	2.28365000
C	-2.50861900	2.03148900	3.63133000
C	-0.64336700	0.48894800	3.72541200
H	-0.18222200	-0.55760600	1.91087300
H	-3.48971300	2.21315400	1.72308800
H	-3.16533100	2.75493700	4.11724300
H	0.15877900	0.00513400	4.28557300
C	-2.87185000	-0.79679100	-1.11224300
H	-2.12941200	-1.60006900	-1.16088400
C	-2.96383500	-0.33129400	0.34404400
H	-3.87413400	0.23519300	0.54664100
H	-2.53566700	0.00366700	-1.79107800
C	-4.20752100	-1.33403000	-1.70739300
C	-5.25338200	-0.21360800	-1.80656300
H	-6.16595700	-0.58614000	-2.29925200
H	-5.54431200	0.16326600	-0.81391900
H	-4.86655500	0.64152900	-2.38034000
C	-4.76763500	-2.49360900	-0.86807000
H	-4.02462400	-3.29713600	-0.74883200
H	-5.07357000	-2.16173000	0.13578900
H	-5.65830400	-2.92071900	-1.35616600
C	-3.88170800	-1.84810200	-3.11991400
H	-4.78902400	-2.22352500	-3.61954000
H	-3.45724900	-1.04635700	-3.74554800
H	-3.15063900	-2.67191800	-3.08285600
C	-2.81952200	-1.48118600	1.28571200
O	-2.03068900	-2.39767600	1.14986600
O	-3.65282800	-1.39179600	2.33306300
C	-3.49459500	-2.37132400	3.36073100
H	-2.48598700	-2.30617200	3.79557800
H	-4.24912200	-2.14010200	4.12140600
H	-3.64988700	-3.38487700	2.96359300
Br	-2.96399400	2.87802700	-1.25049700
C	1.44259900	1.96256100	-0.26680200
C	2.22703800	4.03810600	-0.22572800
C	0.69550100	4.03168500	0.03796900
N	0.34554300	2.60515700	-0.12662600
H	2.50031500	4.49001200	-1.18888300
H	0.16136900	4.60102700	-0.73659200
C	0.60710900	-1.51424400	-0.89153400
C	2.09145600	-1.60936800	-0.46406500
C	1.41474600	0.50207900	-0.44068500
N	0.29508500	-0.09632600	-0.61599300
H	-0.03606900	-2.14078300	-0.25794300
H	2.73801000	-2.14575600	-1.16752100
H	2.81129600	4.50349800	0.57833700
H	2.22307000	-2.02097100	0.54654600
O	2.59341000	2.62616600	-0.28570300
O	2.53159600	-0.21419600	-0.42498200
C	0.30127300	4.59147000	1.42217300
H	0.83687500	5.55631600	1.50196500
C	0.34014300	-1.85833600	-2.37518300
H	-0.69837000	-1.55176600	-2.57036900
C	-1.19845100	4.87712100	1.48948800
H	-1.48104700	5.29987000	2.46453300
H	-1.49667600	5.59426100	0.70949400
H	-1.77632900	3.95930900	1.32762800
C	0.79463500	3.67757100	2.55469700
H	1.85534500	3.42349700	2.38206500
H	0.24531100	2.72680200	2.50338300
C	0.65903000	4.27017100	3.95551600
H	-0.39293100	4.44384000	4.22566900
H	1.07390800	3.58509900	4.70984200
H	1.19289700	5.23166300	4.03925200
C	1.23422400	-1.07433400	-3.33913500

H	1.15897800	0.00951500	-3.16329100
H	2.29363000	-1.36571300	-3.25348600
H	0.93011400	-1.25073900	-4.38051300
C	0.41496900	-3.38131800	-2.57212500
H	-0.22642000	-3.85834300	-1.81101200
H	1.44284800	-3.73128800	-2.36641100
C	-0.01698500	-3.85750000	-3.95836300
H	0.65926000	-3.49679700	-4.74844700
H	-0.02691000	-4.95726400	-4.00965900
H	-1.03212800	-3.50128900	-4.19951300
C	-1.30648800	1.71038600	5.81743000
F	-1.74917600	2.93971100	6.14821900
F	-0.01346000	1.63771800	6.19903600
F	-1.98090500	0.83789200	6.59976300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.689968 (Hartree/Particle)
Thermal correction to Energy= 0.734447
Thermal correction to Enthalpy= 0.735392
Thermal correction to Gibbs Free Energy= 0.609158
Sum of electronic and zero-point Energies= -5921.189751
Sum of electronic and thermal Energies= -5921.145271
Sum of electronic and thermal Enthalpies= -5921.144327
Sum of electronic and thermal Free Energies= -5921.270561
HF=-5921.8797183

^{2}F'-TS-H^S-*B*^{CF3}-Conf1

Ni	-0.82619500	0.87376900	-0.28106300
C	-1.90446500	1.49558700	1.17765500
C	-2.29358900	3.32873300	3.26108400
C	-1.43687100	1.20734700	2.46819900
C	-2.63589400	2.67589000	0.95386000
C	-2.81610500	3.59308100	1.98703900
C	-1.62035800	2.12466500	3.50170300
H	-0.88494600	0.28620100	2.66465400
H	-3.03853800	2.87863900	-0.03943000
H	-3.35113700	4.52504600	1.79925500
H	-1.20972800	1.91374300	4.49104400
Br	-1.03932700	2.21171100	-2.37383600
C	-2.34849900	-1.49361400	0.84621400
H	-1.58924600	-1.33997500	1.62519700
C	-2.75125600	-0.17554200	0.21527500
H	-3.60919300	0.27278400	0.71484600
H	-1.88162800	-2.11436000	0.07266000
C	-3.51527700	-2.29585600	1.47964300
C	-2.94557200	-3.65017700	1.93091400
H	-3.72226600	-4.26604300	2.41217200
H	-2.54689200	-4.21583300	1.07290000
H	-2.12565900	-3.51292700	2.65488900
C	-4.63392400	-2.53324300	0.45223900
H	-5.10340700	-1.58916300	0.13363300
H	-4.24531400	-3.03543700	-0.44725100
H	-5.42693100	-3.16531700	0.88312400
C	-4.07614300	-1.55076900	2.70130800
H	-4.88506700	-2.13118300	3.17323300
H	-3.29171700	-1.38360600	3.45677500
H	-4.49256200	-0.56817900	2.42873400
C	-3.09164100	-0.25268600	-1.23872800
O	-2.66934500	-1.07697800	-2.02912900
O	-4.00321100	0.67714500	-1.57048400
C	-4.37033100	0.74905300	-2.94985500
H	-4.77293400	-0.21449900	-3.29461200
H	-5.13800400	1.52883000	-3.01940100
H	-3.49409800	1.02241300	-3.55435100
C	2.04717100	1.12723700	0.25068300
C	3.02526700	3.12036700	0.16849300
C	1.48031100	3.27598700	0.22082800
N	1.02244600	1.88224600	0.14787000
H	3.45472300	3.40003800	-0.80290600
H	1.10289800	3.79367200	-0.67306200
C	0.83131400	-2.26413600	-0.14451300
C	2.34076000	-2.49892600	0.12753700
C	1.85927600	-0.33212900	0.20465200
N	0.67736500	-0.81834200	0.10358400
H	0.22111300	-2.81978300	0.58082100
H	2.86590300	-3.04538000	-0.66503900
H	3.56042500	3.64138200	0.97096600
H	2.53526800	-2.97859600	1.09640800
O	3.24976400	1.68306600	0.34381800
O	2.90262400	-1.15134000	0.18517400
C	0.91503500	3.97985900	1.47081800
H	-0.17090700	3.80704600	1.42899800
C	0.34234800	-2.61731900	-1.56502200
H	-0.70192000	-2.26997800	-1.61488100
C	1.11541800	-1.86600900	-2.65218300
H	0.70141700	-2.08841200	-3.64587400
H	1.03852900	-0.77707300	-2.51241400
H	2.18323500	-2.14089000	-2.67236200
C	0.33684400	-4.14244500	-1.75543000
H	-0.15702100	-4.59919600	-0.87955500
H	1.37350000	-4.52616100	-1.75507500
C	-0.37893500	-4.60576700	-3.02399400
H	0.13308000	-4.26046700	-3.93533700
H	-0.42815800	-5.70486800	-3.07028400
H	-1.41096000	-4.21947500	-3.05535700
C	1.44078300	3.37637500	2.77565000
H	0.87024800	3.75497400	3.63389500
H	1.33591700	2.28182100	2.78131300
H	2.50150300	3.62553000	2.94407300
C	1.14786200	5.49599100	1.37708600
H	0.80069100	5.84118400	0.38784600
H	2.23322700	5.70471600	1.40906500
C	0.43980900	6.30384400	2.46441600
H	0.80781400	6.05347300	3.47097000
H	0.59472900	7.38371400	2.31449200
H	-0.64533000	6.11592100	2.45614900
C	-2.45404900	4.31318900	4.38052600
F	-1.29993200	4.48368200	5.06696900
F	-2.83427200	5.52944200	3.94504300
F	-3.37296500	3.91930200	5.28804200

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.689599 (Hartree/Particle)
Thermal correction to Energy= 0.734283
Thermal correction to Enthalpy= 0.735227
Thermal correction to Gibbs Free Energy= 0.607733
Sum of electronic and zero-point Energies= -5921.192377
Sum of electronic and thermal Energies= -5921.147694

Sum of electronic and thermal Enthalpies= -5921.146750
Sum of electronic and thermal Free Energies= -5921.274243
HF=-5921.8819765

^{2}F'-TS-H^S-B^{CF3}-Conf2

Ni	-0.79270500	0.87234400	-0.28770200
C	-1.89849200	1.52525000	1.13560400
C	-2.31182300	3.39932600	3.17681400
C	-1.47025400	1.25127500	2.44242000
C	-2.60985700	2.71069100	0.87359300
C	-2.79757400	3.64996900	1.88469800
C	-1.66526400	2.18964700	3.45580000
H	-0.94306600	0.32293200	2.67040500
H	-2.98835600	2.89939900	-0.13167600
H	-3.31724100	4.58492700	1.66899400
H	-1.29287100	1.98719700	4.46151800
Br	-0.95374600	2.21175000	-2.38945500
C	-2.33284600	-1.47485200	0.81909600
H	-1.58506800	-1.31688800	1.60855500
C	-2.72910400	-0.15964400	0.17735500
H	-3.59293600	0.29143500	0.66447000
H	-1.85218900	-2.09658400	0.05480300
C	-3.50676500	-2.27804200	1.43785000
C	-2.94059000	-3.62987800	1.90087300
H	-3.72264700	-4.24602100	2.37300300
H	-2.52877900	-4.19712400	1.05013700
H	-2.13115600	-3.48882400	2.63582000
C	-4.60994600	-2.52050300	0.39506100
H	-5.07700500	-1.57824000	0.06758200
H	-4.20726200	-3.02374100	-0.49760100
H	-5.40758600	-3.15342700	0.81602700
C	-4.08672100	-1.53089000	2.64924700
H	-4.90149100	-2.11145800	3.11080000
H	-3.31372000	-1.36057700	3.41571900
H	-4.50069200	-0.54970000	2.36803500
C	-3.04819300	-0.24003800	-1.28111200
O	-2.61799700	-1.06879300	-2.06246100
O	-3.94792300	0.69516400	-1.62987700
C	-4.29087600	0.76765200	-3.01548600
H	-4.68923000	-0.19507400	-3.36731500
H	-5.05563100	1.54898400	-3.09841600
H	-3.40365900	1.03939200	-3.60456600
C	2.07574800	1.09845000	0.26417400
C	3.04292800	3.09797600	0.19414000
C	1.49857300	3.24506800	0.25483600
N	1.04863600	1.85031200	0.16323000
H	3.46441100	3.37846900	-0.78065200
H	1.11558000	3.76588600	-0.63258300
C	0.86393900	-2.29216000	-0.15175300
C	2.37317300	-2.52767200	0.12387100
C	1.89041800	-0.36112700	0.20712300
N	0.70947600	-0.84706700	0.09644500
H	0.25132700	-2.84727400	0.57241800
H	2.90106100	-3.06913800	-0.67035300
H	3.58118000	3.62237000	0.99233000
H	2.56499500	-3.01319500	1.09033900
O	3.27477000	1.66082600	0.36814800
O	2.93440700	-1.18018600	0.19127500
C	0.93155200	3.91625800	1.52233000
H	-0.14754000	3.70946300	1.49510200
C	0.37773200	-2.64633800	-1.57300000
H	-0.66704400	-2.30050500	-1.62451900
C	1.15131900	-1.89337900	-2.65859100
H	0.73882600	-2.11514100	-3.65306100
H	1.07347900	-0.80469100	-2.51743500
H	2.21939300	-2.16742200	-2.67759000
C	0.37554300	-4.17145900	-1.76330800
H	-0.11998900	-4.62901100	-0.88878800
H	1.41297300	-4.55306800	-1.75976000
C	-0.33517800	-4.63674600	-3.03397100
H	0.17884800	-4.29038600	-3.94377700
H	-0.38156300	-5.73598100	-3.08016600
H	-1.36810300	-4.25311500	-3.06875400
C	1.49109500	3.31359200	2.81228300
H	0.94209800	3.71328400	3.67664800
H	1.38182200	2.21925100	2.83153000
H	2.55624100	3.55883200	2.95456100
C	1.10233900	5.44303200	1.49348700
H	2.17692300	5.69852800	1.44253800
H	0.74618200	5.82837700	2.46298100
C	0.33990000	6.14711700	0.37093500
H	-0.72999300	5.88275100	0.39865800
H	0.41944700	7.24118900	0.46624400
H	0.71931300	5.87958800	-0.62793500
C	-2.39841500	4.45346300	4.23816600
F	-1.25269100	5.18107700	4.31414200
F	-3.39063100	5.33305500	4.01501600
F	-2.59012600	3.93245800	5.46525700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.689275 (Hartree/Particle)
Thermal correction to Energy= 0.734101
Thermal correction to Enthalpy= 0.735045
Thermal correction to Gibbs Free Energy= 0.606568
Sum of electronic and zero-point Energies= -5921.192282
Sum of electronic and thermal Energies= -5921.147455
Sum of electronic and thermal Enthalpies= -5921.146511
Sum of electronic and thermal Free Energies= -5921.274988
HF=-5921.8815562

^{2}F'-TS-H^S-B^{CF3}-Conf3

Ni	-0.46516300	0.33638200	-0.04343600
C	-1.30856200	0.71486800	1.63206500
C	-1.38726100	2.24632000	3.97952700
C	-0.64745700	0.27284600	2.78699700
C	-2.07088400	1.89747600	1.68182400
C	-2.09556700	2.66542100	2.84284400
C	-0.67684800	1.04063000	3.95099800
H	-0.07219900	-0.65450300	2.77517000
H	-2.62568900	2.21529800	0.79832400
H	-2.66181600	3.59793700	2.86622000
H	-0.12741800	0.70837600	4.83353200
Br	-1.02320800	1.94752900	-1.86580900
C	-1.74879300	-2.18533200	0.94778800
H	-0.86135200	-2.13679900	1.59357400
C	-2.23506100	-0.79225300	0.58859600
H	-3.02107600	-0.46662900	1.26971300
H	-1.43690700	-2.68720700	0.02439200

C	-2.80148300	-3.07585200	1.65839800
C	-2.18054900	-4.47057400	1.83576400
H	-2.87403800	-5.14779200	2.35970500
H	-1.93730200	-4.92157200	0.86098200
H	-1.25005500	-4.41738700	2.42447200
C	-4.07568200	-3.19399100	0.80611000
H	-4.58329300	-2.22322600	0.69148700
H	-3.84371800	-3.57297400	-0.20139500
H	-4.79285700	-3.88562500	1.27652300
C	-3.14806100	-2.50042100	3.04093000
H	-3.87434000	-3.14696800	3.55898000
H	-2.24956200	-2.42298000	3.67373400
H	-3.59471400	-1.49604800	2.97070100
C	-2.82216400	-0.67018600	-0.78342100
O	-2.55198000	-1.36762500	-1.74340200
O	-3.78037300	0.27166800	-0.81273900
C	-4.39142700	0.52448000	-2.07965200
H	-4.85229400	-0.39153500	-2.47698200
H	-5.15712300	1.28846500	-1.90013500
H	-3.63900900	0.89863500	-2.78772700
C	2.38610400	0.68940100	0.03855900
C	3.26112600	2.72796500	0.08783700
C	1.75841600	2.77414000	0.47389300
N	1.33554600	1.38539100	0.24431700
H	3.46482800	3.16028200	-0.90131100
H	1.18976100	3.40450200	-0.22201800
C	1.16292200	-2.63029000	-0.72110600
C	2.69587900	-2.85868500	-0.70425100
C	2.21805100	-0.74774300	-0.21476400
N	1.03479800	-1.24753400	-0.21451700
H	0.66961000	-3.31099600	-0.01741700
H	3.10494200	-3.26434200	-1.63732500
H	3.93497500	3.17166100	0.82981400
H	3.03246700	-3.47218200	0.14259500
O	3.56696800	1.29634200	0.00518300
O	3.24972200	-1.51917600	-0.52175000
C	1.45237800	3.20602400	1.92231400
H	0.39523400	2.95287500	2.07926700
C	0.49174400	-2.75663700	-2.10629900
H	-0.56121500	-2.46998600	-1.95742200
C	1.08439100	-1.78360700	-3.12945900
H	0.56604100	-1.89137700	-4.09435600
H	0.96023500	-0.73818500	-2.80942400
H	2.15616200	-1.96761800	-3.31251400
C	0.51775100	-4.20735100	-2.61535300
H	1.56294400	-4.54535900	-2.73902200
H	0.08824200	-4.20737100	-3.63102100
C	-0.25298700	-5.20608600	-1.75132600
H	-1.29868300	-4.88506000	-1.61576800
H	-0.26721300	-6.20247700	-2.21959900
H	0.18961400	-5.32583000	-0.74975900
C	2.27600800	2.43769800	2.95769700
H	1.90760400	2.66747400	3.96758900
H	2.19369300	1.34973100	2.81876300
H	3.34285500	2.71277200	2.92407600
C	1.58857200	4.72509100	2.11084800
H	2.62417100	5.03905000	1.88375100
H	1.43812900	4.93473700	3.18250200
C	0.59596500	5.55838400	1.30007200
H	-0.44007400	5.24421500	1.50781100
H	0.68077400	6.62703700	1.55148300
H	0.75684900	5.46625000	0.21427700
C	-1.30765800	3.12462100	5.19037400
F	-2.34894200	3.97029000	5.28624300
F	-1.25585100	2.41783800	6.33572100
F	-0.18908900	3.89744200	5.17570600

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.688714 (Hartree/Particle)
Thermal correction to Energy= 0.733456
Thermal correction to Enthalpy= 0.734400
Thermal correction to Gibbs Free Energy= 0.607045
Sum of electronic and zero-point Energies= -5921.192079
Sum of electronic and thermal Energies= -5921.147337
Sum of electronic and thermal Enthalpies= -5921.146393
Sum of electronic and thermal Free Energies= -5921.273748
HF=-5921.880793

^{2}F'-TS-H^S-B^{CF3}-Conf4

Ni	-1.16203000	1.12868200	-0.45476700
C	-2.38953100	1.98314200	0.75763500
C	-3.34645500	4.25889400	2.09609200
C	-1.91449300	2.30600800	2.03770100
C	-3.37896500	2.79371400	0.17022900
C	-3.84397300	3.92909600	0.82754700
C	-2.38308700	3.44198500	2.69929600
H	-1.15125500	1.68999000	2.51539000
H	-3.78438500	2.52131000	-0.80599800
H	-4.59235900	4.56445900	0.35111900
H	-1.98193500	3.70248000	3.68025600
Br	-1.44628300	1.25920400	-2.91152500
C	1.52113300	2.34599400	-0.13132400
C	2.24423800	4.20188400	-1.11415400
C	0.74127600	3.96558200	-1.42910200
N	0.42746800	2.74711700	-0.65336700
H	2.88233900	4.22496200	-2.00620500
H	0.60344000	3.69705100	-2.48822300
C	0.96902200	-1.00413500	1.14007000
C	2.42639100	-0.72687600	1.58431800
C	1.57196500	1.05022700	0.56231900
N	0.52179700	0.31814000	0.65296500
H	0.36077600	-1.29901400	2.00353900
H	3.16303500	-1.44426600	1.20339700
H	2.42366900	5.10320800	-0.51117900
H	2.53341500	-0.63193900	2.67352400
O	2.63733400	3.04777600	-0.31440400
O	2.72964100	0.57556300	0.99956800
C	-0.16565000	5.16834900	-1.10937100
H	0.35758400	6.04960500	-1.52681900
C	0.79360700	-2.06189900	0.03079600
H	-0.26918800	-2.01926400	-0.25535600
C	-2.29924100	-0.86564100	1.63822900
H	-1.64983200	-0.26824000	2.29036200
C	-2.84968100	-0.02209200	0.50632800
H	-3.82462000	0.39314700	0.75615500
H	-1.67722200	-1.65847800	1.20684600
C	-3.37753700	-1.52758200	2.53594000
C	-4.34493200	-2.37466700	1.69316900
H	-5.06284600	-2.90136800	2.34211800
H	-4.92818200	-1.75559400	0.99345400

H	-3.80022800	-3.12733900	1.10226800
C	-4.16008000	-0.45639000	3.31245400
H	-3.48550700	0.15289100	3.93489100
H	-4.70177400	0.22716100	2.63980500
H	-4.90563900	-0.92441600	3.97500200
C	-2.64393300	-2.43857800	3.53311600
H	-3.35445100	-2.92758900	4.21878700
H	-2.08191600	-3.22753400	3.00712800
H	-1.92783000	-1.86282700	4.14214700
C	-3.04143000	-0.77081600	-0.77664900
O	-2.41126800	-1.74859300	-1.13451100
O	-4.08990700	-0.28569000	-1.46309200
C	-4.37076300	-0.90072200	-2.72231600
H	-4.56588900	-1.97524100	-2.59240500
H	-5.26248400	-0.39690100	-3.11369600
H	-3.52149100	-0.75729300	-3.40450000
C	1.60968000	-1.73752300	-1.22333600
H	1.40813100	-2.47145000	-2.01637900
H	1.33928900	-0.75076900	-1.62878300
H	2.69546200	-1.75116300	-1.03164600
C	1.06579400	-3.46514100	0.59593800
H	0.51145100	-3.56994500	1.54536200
H	2.13550400	-3.56575600	0.85546400
C	0.65666000	-4.60003700	-0.34252500
H	1.25177300	-4.60386800	-1.26867700
H	0.79305100	-5.58006000	0.14067400
H	-0.40399200	-4.50827100	-0.62834500
C	-1.50696600	5.03381900	-1.83172600
H	-2.17171500	5.88072300	-1.60802600
H	-1.36060300	4.99581200	-2.92203000
H	-2.01489600	4.10786800	-1.53512800
C	-0.30666800	5.37095800	0.40605700
H	0.69525800	5.34846400	0.86983800
H	-0.84787900	4.51045100	0.82365400
C	-1.00400800	6.66654700	0.81375700
H	-2.04575900	6.69840800	0.46254000
H	-1.03303600	6.76641000	1.90917200
H	-0.48317100	7.54920700	0.40599300
C	-3.87762900	5.45768700	2.82402500
F	-4.94507000	5.15674700	3.59666500
F	-4.28186000	6.42831200	1.97959000
F	-2.95711400	6.00352800	3.64567400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.689915 (Hartree/Particle)
Thermal correction to Energy= 0.734361
Thermal correction to Enthalpy= 0.735306
Thermal correction to Gibbs Free Energy= 0.609731
Sum of electronic and zero-point Energies= -5921.190218
Sum of electronic and thermal Energies= -5921.145771
Sum of electronic and thermal Enthalpies= -5921.144827
Sum of electronic and thermal Free Energies= -5921.270402
HF=-5921.8801328

Figure A3.10
F'^{R}-lac

Ni	-1.68577800	1.30158000	-0.41516100
C	-1.54801800	1.10075000	1.48047500
C	-1.16061700	1.16287900	4.24968000
C	-0.64275000	0.21909400	2.07338100
C	-2.28338700	1.99208600	2.26579300
C	-2.08016800	2.03007400	3.64851600
C	-0.44841400	0.25512600	3.46176500
H	-0.08236800	-0.49758500	1.47178300
H	-3.02180000	2.65121400	1.80448500
H	-2.65039000	2.73535600	4.25900100
H	0.26350000	-0.43417500	3.92368900
H	-1.00883600	1.18787500	5.33146600
Br	-3.07739600	3.07509700	-1.51462600
C	1.12478900	2.08431600	-0.76260100
C	1.60862100	4.24603900	-0.54579500
C	0.07886600	4.02355700	-0.41345000
N	-0.04192700	2.55270900	-0.52509300
H	1.89311100	4.91408600	-1.36787800
H	-0.46561000	4.44856600	-1.27004600
C	0.99242000	-1.51836700	-1.26245500
C	2.51996300	-1.22826600	-1.23463000
C	1.34942200	0.64461900	-0.97167300
N	0.38130600	-0.18583300	-1.04209700
H	0.71283100	-2.16611900	-0.41671500
H	3.02750800	-1.49207200	-2.17283000
H	2.07238700	4.58950400	0.39015800
H	3.04229100	-1.69455700	-0.38891900
O	2.14798300	2.92241000	-0.83967700
O	2.60535000	0.21383500	-1.07128800
C	-4.00229900	-1.54704800	-2.24737900
C	-5.25442800	-2.00117300	-1.48021100
H	-6.04291400	-2.30366900	-2.18736500
H	-5.04614200	-2.86158200	-0.82600800
H	-5.66392800	-1.19271300	-0.85554900
C	-3.50096300	-2.69550700	-3.14018500
H	-2.62160400	-2.38544600	-3.72721700
H	-3.22559900	-3.58895300	-2.55924300
H	-4.28639100	-2.99673000	-3.85111500
C	-4.35535100	-0.35703800	-3.15448200
H	-5.11267800	-0.65511400	-3.89682700
H	-4.75494600	0.49536500	-2.58727600
H	-3.46649600	-0.00097700	-3.69986200
C	-2.41723700	-2.19641500	-0.26493900
C	-2.85411400	-1.11828200	-1.27594700
C	-3.22140300	0.01845100	-0.32239200
C	-3.62935800	-0.66215300	0.93976900
O	-3.13284600	-1.92976900	0.94899800
H	-2.64783300	-3.22417700	-0.57219400
H	-1.99940100	-0.85342700	-1.91519000
H	-4.00461800	0.70584300	-0.64891900
O	-4.33357000	-0.26502800	1.83618100
H	-1.34234800	-2.12879300	-0.05027300
C	-0.51630300	4.57291000	0.87309000
H	-0.32881400	5.65634300	0.92973300
H	-1.60016600	4.40656400	0.88799000
H	-0.06968700	4.08817600	1.75371300
C	0.52316900	-2.15975200	-2.56344400
H	1.04712200	-3.11543700	-2.71686400
H	-0.55438200	-2.36405800	-2.54431200
H	0.73787000	-1.50162000	-3.41945500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.493978 (Hartree/Particle)
Thermal correction to Energy= 0.525909

Thermal correction to Enthalpy= 0.526853
Thermal correction to Gibbs Free Energy= 0.427734
Sum of electronic and zero-point Energies= -5347.637996
Sum of electronic and thermal Energies= -5347.606066
Sum of electronic and thermal Enthalpies= -5347.605122
Sum of electronic and thermal Free Energies= -5347.704241
HF=-5348.1319749

F'-TS-H$^{R\text{-lac}}$

Ni	-1.71375600	1.57770000	-0.22051200
C	-1.61539400	0.94554500	1.59196700
C	-0.43038200	1.02030200	4.14014300
C	-0.63159500	0.00865800	1.94269100
C	-2.04194800	1.88532100	2.54533700
C	-1.43900200	1.93148200	3.80364800
C	-0.03511800	0.05617700	3.20763300
H	-0.30803100	-0.74903300	1.22947000
H	-2.84937400	2.57485300	2.29668200
H	-1.76425100	2.68311900	4.52743100
H	0.74221900	-0.66903400	3.46141000
H	0.03361100	1.05247200	5.12852500
Br	-3.32978600	3.36933500	-0.93654000
C	1.04880400	2.33582500	-0.70103200
C	1.61581000	4.45978900	-0.35329500
C	0.08649500	4.26914700	-0.15173900
N	-0.09155500	2.82454300	-0.39366000
H	1.87533000	5.16000500	-1.15707400
H	-0.49106000	4.79677000	-0.92637300
C	0.65206100	-1.17897200	-1.53096100
C	2.17696500	-1.06019800	-1.27439000
C	1.17718700	0.90469500	-1.01708000
N	0.14355300	0.16337000	-1.15789300
H	0.20261100	-1.93035800	-0.86433800
H	2.79485400	-1.41867600	-2.10722700
H	2.13724300	4.74595500	0.57116600
H	2.50074200	-1.53654400	-0.33800700
O	2.10455700	3.13805700	-0.74044800
O	2.39250000	0.37327700	-1.13495100
C	-3.70935600	-1.80338000	-1.20363700
C	-5.21090300	-1.86701700	-0.87599200
H	-5.77187400	-2.21625000	-1.75709000
H	-5.42945600	-2.55990200	-0.04970700
H	-5.60957400	-0.87686600	-0.60575600
C	-3.20261600	-3.20700700	-1.57568600
H	-2.14212600	-3.18122200	-1.87291500
H	-3.29872100	-3.91310500	-0.73621900
H	-3.77925200	-3.61620200	-2.41987900
C	-3.50830000	-0.86339100	-2.40723000
H	-3.88152900	-1.33668200	-3.32854300
H	-4.04812200	0.08723300	-2.28608500
H	-2.44704400	-0.61644700	-2.55278400
C	-3.16033000	-2.00632600	1.34044400
C	-2.86851000	-1.28567800	0.00991900
C	-3.16878600	0.15975200	0.37329000
C	-4.11007000	0.08619400	1.53301700
O	-4.07874800	-1.16456800	2.05599900
H	-3.63391900	-2.98868500	1.21825600
H	-1.81326600	-1.42017900	-0.25672600
H	-3.65739500	0.75062200	-0.41241300
O	-4.84607800	0.93448600	1.97425600
H	-2.25426100	-2.12782700	1.95053000
C	-0.42310300	4.68833300	1.21914500
H	-0.22992300	5.76059500	1.37689400
H	-1.50466400	4.51297500	1.28220800
H	0.07610700	4.11568600	2.01510000
C	0.31434200	-1.51406700	-2.98122700
H	0.69915400	-2.51414300	-3.23232100
H	-0.76998000	-1.51074200	-3.14715000
H	0.77177600	-0.78112200	-3.66378500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.493840 (Hartree/Particle)
Thermal correction to Energy= 0.525002
Thermal correction to Enthalpy= 0.525946
Thermal correction to Gibbs Free Energy= 0.429437
Sum of electronic and zero-point Energies= -5347.630303
Sum of electronic and thermal Energies= -5347.599141
Sum of electronic and thermal Enthalpies= -5347.598196
Sum of electronic and thermal Free Energies= -5347.694705
HF=-5348.1241424

F'$^{S\text{-lac}}$

Ni	-0.93175100	0.98925000	0.27779800
C	-1.12577200	1.20947400	2.16683300
C	-1.28008200	1.72078500	4.91282400
C	-0.33012800	0.48053800	3.05335800
C	-1.99993800	2.19109400	2.64220100
C	-2.07317100	2.44593500	4.01656300
C	-0.40883200	0.74043600	4.42888100
H	0.34967500	-0.29283000	2.69054300
H	-2.62548300	2.75226600	1.94513300
H	-2.75738100	3.21434300	4.38635600
H	0.21627300	0.17019900	5.12132300
H	-1.34281500	1.91807800	5.98559000
Br	-1.94350400	2.85447600	-1.09751200
C	1.99970400	1.21294400	0.26769500
C	2.91326200	3.24141200	0.36280700
C	1.36337000	3.35285900	0.31249700
N	0.94640500	1.93955500	0.27175600
H	3.42091900	3.71276900	-0.48782800
H	1.02317400	3.81423000	-0.62724500
C	1.02447500	-2.27396000	-0.06324800
C	2.51180000	-2.38108900	0.36080600
C	1.89217900	-0.25641900	0.21151300
N	0.75388500	-0.82407100	0.07703000
H	0.37107000	-2.82705300	0.62476800
H	3.12579800	-2.98249200	-0.32084900
H	3.34050600	3.61380800	1.30444200
H	2.64771100	-2.73008000	1.39467600
O	3.18341700	1.80532100	0.29866000
O	2.99016700	-1.00226100	0.30016400
C	-4.73517300	-0.96837100	1.66833100
C	-5.32410700	0.44829200	1.78534100
H	-6.41711600	0.39927600	1.91290100
H	-4.90213100	0.97904500	2.65354600
H	-5.12269200	1.05669800	0.89100400

C	-5.12519700	-1.75310000	2.93293100
H	-4.76813400	-2.79404100	2.90389300
H	-4.70989000	-1.27685500	3.83592300
H	-6.22081800	-1.78611500	3.04164000
C	-5.31688100	-1.66880300	0.42980300
H	-6.41274400	-1.74377900	0.51410000
H	-5.09557500	-1.11321100	-0.49463000
H	-4.92183400	-2.68981600	0.31330100
C	-2.43473800	-2.19285400	1.45475900
C	-3.17695300	-0.85699300	1.60697200
C	-2.66066800	-0.10449200	0.38464600
C	-2.32541700	-1.17026900	-0.60076300
O	-2.18754900	-2.35680400	0.04498400
H	-1.46348300	-2.16620100	1.97342300
H	-2.87258200	-0.38494200	2.54699700
H	-3.31746800	0.66138500	-0.03346100
O	-2.14825600	-1.08743100	-1.79757800
H	-2.99296400	-3.07187900	1.79917600
C	0.74829800	4.10220900	1.48536400
H	1.12385300	5.13686900	1.50240700
H	-0.34365000	4.12521700	1.38166400
H	1.00116800	3.61520100	2.43912800
C	0.76686700	-2.73162500	-1.49721700
H	0.94901600	-3.81450700	-1.57785100
H	-0.26818600	-2.51907300	-1.79269400
H	1.44594900	-2.21280600	-2.19271800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.494551 (Hartree/Particle)
Thermal correction to Energy= 0.526241
Thermal correction to Enthalpy= 0.527185
Thermal correction to Gibbs Free Energy= 0.429690
Sum of electronic and zero-point Energies= -5347.642565
Sum of electronic and thermal Energies= -5347.610876
Sum of electronic and thermal Enthalpies= -5347.609932
Sum of electronic and thermal Free Energies= -5347.707427
HF=-5348.1371164

F'-TS-H$^{S\text{-lac}}$

Ni	-0.77053900	0.99055600	0.10588900
C	-1.33473500	0.98147000	1.95441000
C	-1.10383100	1.78655900	4.64248000
C	-0.52205000	0.25960400	2.84598900
C	-2.05778500	2.08789900	2.43016800
C	-1.93531400	2.48938200	3.76244700
C	-0.39789000	0.67181000	4.17644700
H	0.03024500	-0.61645100	2.50432700
H	-2.70444800	2.64202700	1.74805900
H	-2.49399100	3.36084600	4.11389200
H	0.25499500	0.11308600	4.85227900
H	-1.01287800	2.10012700	5.68492300
Br	-1.95727100	2.77461600	-1.18076500
C	2.10480900	1.26666900	0.27953200
C	2.99077700	3.29602400	0.50319300
C	1.45000000	3.39662500	0.31135100
N	1.05102000	1.98530800	0.18520400
H	3.57033600	3.78321100	-0.29097800
H	1.19679000	3.89420100	-0.63773200
C	1.06561200	-2.19394100	-0.10182600
C	2.55337300	-2.34259400	0.31483500
C	1.98488400	-0.19926800	0.20309600
N	0.83548800	-0.73802300	0.03650500
H	0.40009700	-2.72345000	0.59389200
H	3.15407300	-2.92769300	-0.39280600
H	3.32653200	3.65936400	1.48459000
H	2.68569400	-2.73682500	1.33238500
O	3.27780100	1.86243500	0.44545800
O	3.06056200	-0.97252800	0.30817900
C	-4.83448500	-1.01943600	1.74994200
C	-5.41350200	0.39859200	1.89606500
H	-6.51294900	0.35765400	1.94502500
H	-5.04838800	0.88179200	2.81623600
H	-5.14629900	1.04607800	1.04776900
C	-5.34541800	-1.86849400	2.92706800
H	-4.99317400	-2.90994600	2.87330200
H	-5.01526500	-1.44736600	3.89041300
H	-6.44638200	-1.89497600	2.92923800
C	-5.31266100	-1.63625500	0.42539300
H	-6.41252100	-1.69330800	0.40924800
H	-5.00260900	-1.03335100	-0.44195600
H	-4.92560100	-2.65710700	0.28396500
C	-2.54483000	-2.27859900	1.65498200
C	-3.27567600	-0.93776200	1.83695400
C	-2.65003700	-0.10835800	0.71432500
C	-2.27233500	-1.12067500	-0.31489700
O	-2.15842700	-2.33989700	0.26831500
H	-1.63476100	-2.33022800	2.27021100
H	-3.04633300	-0.53315300	2.82995500
H	-3.25278600	0.70000400	0.29866000
O	-2.07589400	-0.97828500	-1.50491000
H	-3.15992700	-3.16147000	1.86766900
C	0.71159900	4.08750000	1.44943200
H	1.06160100	5.12646400	1.54900400
H	-0.36581900	4.09373700	1.24026700
H	0.88026500	3.56133000	2.40136200
C	0.77641000	-2.65401700	-1.52817800
H	0.93676400	-3.74038900	-1.60811000
H	-0.26128600	-2.42183500	-1.79975200
H	1.45014700	-2.14914700	-2.23886400

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.494413 (Hartree/Particle)
Thermal correction to Energy= 0.525435
Thermal correction to Enthalpy= 0.526379
Thermal correction to Gibbs Free Energy= 0.430536
Sum of electronic and zero-point Energies= -5347.633252
Sum of electronic and thermal Energies= -5347.602230
Sum of electronic and thermal Enthalpies= -5347.601285
Sum of electronic and thermal Free Energies= -5347.697129
HF=-5348.1276648

F'$^{R\text{-amide}}$

Ni	-1.35427400	1.06602900	-0.24325800
C	-1.44692500	1.19709000	1.66613800
C	-1.43939900	1.70235600	4.43020200
C	-0.39797500	0.73341400	2.46281000

C	-2.50024100	1.90411700	2.25678100
C	-2.49857000	2.15258600	3.63430000
C	-0.38839800	0.99446300	3.83942800
H	0.41997300	0.15370500	2.02918600
H	-3.31911500	2.27722200	1.63687100
H	-3.32643900	2.70648200	4.08571500
H	0.44151000	0.63216300	4.45235100
H	-1.43558200	1.89818900	5.50518500
C	-2.74455800	-0.85881700	-1.50355000
H	-2.00720000	-1.66851500	-1.56618500
C	-2.73600500	-0.33914400	-0.07567200
H	-3.63208800	0.24117100	0.16800900
H	-2.42697800	-0.07141700	-2.20925100
C	-4.10594600	-1.40650400	-2.02549400
C	-5.16239100	-0.29380900	-2.08896000
H	-6.10164600	-0.68113400	-2.51681400
H	-5.39182000	0.10715800	-1.08997000
H	-4.81715300	0.54849200	-2.70710100
C	-4.61140300	-2.54641300	-1.12701400
H	-3.85930800	-3.34486900	-1.03514600
H	-4.84306300	-2.18926300	-0.11251100
H	-5.53186900	-2.98604400	-1.54472400
C	-3.86154300	-1.95020700	-3.44261100
H	-4.79141800	-2.35258000	-3.87662100
H	-3.49089900	-1.15716400	-4.11238800
H	-3.11441400	-2.76066800	-3.43222000
C	-2.49248200	-1.42760200	0.93794100
O	-1.72104600	-2.37160200	0.72588000
Br	-2.90052400	2.76261300	-1.31317000
C	1.35078200	1.95133100	-0.40485900
C	1.86225200	4.10417700	-0.19837900
C	0.31799600	3.91079300	-0.15716200
N	0.17816100	2.45181000	-0.30563600
H	2.21122400	4.70919300	-1.04462500
H	-0.16829500	4.37275700	-1.02980300
C	0.82794900	-1.59503400	-0.94100800
C	2.30555700	-1.55439300	-0.48428100
C	1.46540300	0.49395900	-0.55864300
N	0.39533200	-0.19311700	-0.72636500
H	0.20535800	-2.23782700	-0.30562600
H	2.99944900	-2.06842300	-1.16023200
H	2.27067200	4.50521900	0.73958000
H	2.45407500	-1.90717300	0.54666600
O	2.40321500	2.75398900	-0.36861800
O	2.63567600	-0.12656800	-0.50199800
N	-3.22277800	-1.32728000	2.07655800
H	-3.75984600	-0.47646200	2.19108300
C	-3.22119600	-2.26705900	3.21306200
C	-3.75570000	-3.63218300	2.75047900
C	-1.81001400	-2.41541700	3.80305300
C	-4.15792500	-1.66515200	4.26773200
H	-4.77747500	-3.53179700	2.35244400
H	-3.11252800	-4.04463700	1.96188300
H	-3.77934600	-4.33915800	3.59436700
H	-1.43837400	-1.44319000	4.15449900
H	-1.83111000	-3.11376800	4.65428100
H	-1.11695800	-2.79955800	3.04400100
H	-4.20973300	-2.32100900	5.14895700
H	-3.79298300	-0.67791500	4.59336400
H	-5.17810400	-1.54737600	3.86804700
C	-0.34436400	4.42716800	1.11227000
H	-0.17614200	5.51144900	1.20269800
H	-1.42395600	4.23717500	1.07118700
H	0.06615000	3.92582600	2.00147800
C	0.67412300	-1.98128500	-2.41143700
H	0.97804400	-3.02953800	-2.55471100
H	-0.36761000	-1.87501600	-2.73918500
H	1.30547600	-1.34488600	-3.05171200

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.610541 (Hartree/Particle)
Thermal correction to Energy= 0.648224
Thermal correction to Enthalpy= 0.649169
Thermal correction to Gibbs Free Energy= 0.539207
Sum of electronic and zero-point Energies= -5446.775954
Sum of electronic and thermal Energies= -5446.738271
Sum of electronic and thermal Enthalpies= -5446.737327
Sum of electronic and thermal Free Energies= -5446.847288
HF=-5447.3864951

F'-TS-H$^{R\text{-amide}}$

Ni	-1.30266500	1.18714200	-0.48527900
C	-1.68921800	0.95386600	1.39586600
C	-1.25676400	1.82735900	4.04563400
C	-0.62499400	0.43736100	2.15798300
C	-2.56609600	1.87260400	2.00220200
C	-2.34694100	2.30787900	3.31105500
C	-0.39894900	0.88904000	3.45941400
H	0.01885200	-0.33485500	1.73875800
H	-3.40324600	2.27153200	1.42629200
H	-3.03031100	3.03580500	3.75654500
H	0.44683400	0.49021200	4.02570900
H	-1.08509800	2.16942900	5.06881700
C	-2.66104200	-0.78092000	-1.24519100
H	-1.90699900	-1.57310000	-1.29051200
C	-2.73579100	-0.29013900	0.21098700
H	-3.68037900	0.22998800	0.38636200
H	-2.34639900	0.00859800	-1.95296100
C	-3.99330000	-1.34719600	-1.82284800
C	-5.09232400	-0.27489600	-1.85771400
H	-5.99139000	-0.66906600	-2.35866800
H	-5.39170300	0.03717000	-0.84506300
H	-4.75460100	0.62581200	-2.39086900
C	-4.48083100	-2.55824600	-1.01146800
H	-3.69990000	-3.33019900	-0.93644700
H	-4.76960200	-2.27423300	0.01078200
H	-5.36452600	-3.00759400	-1.49290100
C	-3.68782900	-1.79823000	-3.26152000
H	-4.58910100	-2.20945600	-3.74393400
H	-3.33084300	-0.95425700	-3.87376400
H	-2.91082700	-2.57988100	-3.27552800
C	-2.55648300	-1.45471700	1.16355300
O	-1.71425000	-2.33381200	0.96350900
Br	-2.91823500	2.85487400	-1.48097100
C	1.42515600	2.01274900	-0.44121300
C	1.98452000	4.13327500	-0.07590700
C	0.43842600	3.99134800	-0.19572600
N	0.26481500	2.55126700	-0.44320300
H	2.43317800	4.76331500	-0.85466000
H	0.05683300	4.52766500	-1.07846900

C	0.80368600	-1.50480400	-1.05088100
C	2.28958100	-1.51558300	-0.61054900
C	1.50448200	0.55910200	-0.62973800
N	0.41792100	-0.09317000	-0.82765400
H	0.17835200	-2.13229700	-0.40015400
H	2.96111500	-2.01622200	-1.31899800
H	2.30905300	4.48098800	0.91489700
H	2.44174000	-1.92232600	0.39955000
O	2.49707200	2.77492000	-0.25439200
O	2.65572800	-0.09978100	-0.56771700
N	-3.39160600	-1.45295100	2.22977800
H	-3.97838300	-0.63401800	2.33924500
C	-3.38299200	-2.41514700	3.34922200
C	-3.69216400	-3.82585700	2.82407500
C	-2.02325400	-2.38955600	4.06501300
C	-4.48623400	-1.96378600	4.31344500
H	-4.67358400	-3.84500700	2.32531900
H	-2.92744400	-4.14168600	2.10291900
H	-3.71264000	-4.54400200	3.65832300
H	-1.81203700	-1.38273600	4.45383800
H	-2.02596600	-3.09956900	4.90661200
H	-1.22010000	-2.66657300	3.36981200
H	-4.53756200	-2.64405100	5.17582800
H	-4.28564100	-0.94805500	4.69109700
H	-5.46918200	-1.96462400	3.81589200
C	-0.33664500	4.44173500	1.03526900
H	-0.15849000	5.51214100	1.22176900
H	-1.41010900	4.28059800	0.87306900
H	-0.02928500	3.86809200	1.92286400
C	0.61041700	-1.88985300	-2.51663900
H	0.88020900	-2.94658100	-2.66562000
H	-0.43405100	-1.75264300	-2.82545800
H	1.24740000	-1.27146600	-3.16854500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.610028 (Hartree/Particle)
Thermal correction to Energy= 0.647107
Thermal correction to Enthalpy= 0.648051
Thermal correction to Gibbs Free Energy= 0.539816
Sum of electronic and zero-point Energies= -5446.761502
Sum of electronic and thermal Energies= -5446.724423
Sum of electronic and thermal Enthalpies= -5446.723479
Sum of electronic and thermal Free Energies= -5446.831714
HF=-5447.3715297

F'*S*-amide

Ni	-1.18521400	0.93543900	-0.04971200
C	-1.39992600	1.31799100	1.82461100
C	-1.48687400	2.08963000	4.52123700
C	-0.47342800	0.79866900	2.73326400
C	-2.37644500	2.21467900	2.26527700
C	-2.41800700	2.60002300	3.61118500
C	-0.51403300	1.18763800	4.07877900
H	0.28688900	0.08429100	2.40892800
H	-3.10021800	2.62468700	1.55803500
H	-3.18603200	3.30194200	3.94768900
H	0.21976400	0.78178400	4.78059000
H	-1.52125000	2.39006500	5.57129900
Br	-2.35895400	2.88799100	-1.32081300
C	-2.48056100	-1.48572500	1.12801000
H	-1.74010600	-1.23746500	1.89841100
C	-2.76252500	-0.28727500	0.23236000
H	-3.54017000	0.36796000	0.63806900
H	-2.03946500	-2.27443200	0.50246000
C	-3.71691600	-2.07280900	1.86178600
C	-3.25512400	-3.33787200	2.60272700
H	-4.08542900	-3.79290000	3.16733600
H	-2.87227300	-4.09199600	1.89574200
H	-2.44836900	-3.10477700	3.31709100
C	-4.82874200	-2.44661200	0.86837000
H	-5.21758800	-1.56165800	0.34187000
H	-4.45810400	-3.14981700	0.10686900
H	-5.67428500	-2.92058000	1.39339800
C	-4.25506000	-1.06177200	2.88748900
H	-5.09858300	-1.49152300	3.45226500
H	-3.47169600	-0.77325600	3.60651500
H	-4.61409100	-0.14059900	2.40375000
C	-3.12763600	-0.71295700	-1.17998100
O	-2.66632900	-1.73664900	-1.69633200
C	1.72369100	1.35204300	-0.19633300
C	2.53894500	3.42069400	-0.28942900
C	0.98643900	3.45613800	-0.19972100
N	0.63589900	2.02463300	-0.18910200
H	2.93675600	3.82269000	-1.23021500
H	0.54060400	3.89756200	-1.10322000
C	0.83565300	-2.17371300	-0.11160200
C	2.37339700	-2.21430800	0.11937100
C	1.67416700	-0.11996200	-0.13887700
N	0.54820900	-0.72538800	-0.16604800
H	0.29848000	-2.59397300	0.75146300
H	2.91225300	-2.80868000	-0.63010800
H	3.03437400	3.90742500	0.56153100
H	2.65990500	-2.54031600	1.12857500
O	2.87918900	1.99847000	-0.24072700
O	2.79564600	-0.82339100	-0.02721400
N	-4.03357800	0.08269700	-1.80189100
H	-4.12868800	1.01037100	-1.39516700
C	-4.42989300	-0.01943200	-3.22035400
C	-3.19991800	0.13361000	-4.13244200
C	-5.13006800	-1.36319900	-3.47136100
C	-5.41107500	1.13201200	-3.47407900
H	-2.70403800	1.09629800	-3.93762800
H	-2.48149900	-0.67560000	-3.94466700
H	-3.50212500	0.09784100	-5.19093000
H	-6.01097800	-1.46470300	-2.81816400
H	-5.46630300	-1.42279500	-4.51826300
H	-4.44683400	-2.19724800	-3.26814500
H	-5.75014500	1.11885500	-4.52037900
H	-6.29499200	1.04292500	-2.82274400
H	-4.92991700	2.10306900	-3.27806600
C	0.44281300	4.17571100	1.02783400
H	0.75409300	5.23156400	1.00792400
H	-0.65330400	4.12826100	1.03140800
H	0.81661900	3.71060400	1.95268700
C	0.37713600	-2.87123000	-1.38718500
H	0.56717900	-3.95328600	-1.31130400
H	-0.69601100	-2.69653400	-1.54447200
H	0.93123400	-2.48136300	-2.25636700

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)

Zero-point correction= 0.611076 (Hartree/Particle)
Thermal correction to Energy= 0.648751
Thermal correction to Enthalpy= 0.649695
Thermal correction to Gibbs Free Energy= 0.538585
Sum of electronic and zero-point Energies= -5446.771331
Sum of electronic and thermal Energies= -5446.733656
Sum of electronic and thermal Enthalpies= -5446.732712
Sum of electronic and thermal Free Energies= -5446.843823
HF=-5447.3824072

F'-TS-H$^{S\text{-amide}}$

Ni	-0.89698600	0.90882500	-0.28613000
C	-1.81341300	1.27561500	1.37786100
C	-1.92849500	2.84976800	3.71766100
C	-1.06321100	0.92810900	2.51229600
C	-2.65158300	2.40585300	1.44325600
C	-2.70128300	3.18632200	2.59766700
C	-1.10834400	1.71971000	3.66618900
H	-0.41007400	0.05380400	2.49389000
H	-3.24583900	2.68446200	0.57110900
H	-3.34995800	4.06593000	2.62357700
H	-0.49403100	1.44590900	4.52810000
H	-1.97142700	3.46082400	4.62216000
Br	-1.58111200	2.64805800	-1.97606300
C	-2.29592700	-1.56720400	1.03777200
H	-1.52302300	-1.41072900	1.80005900
C	-2.69484100	-0.25531200	0.37933100
H	-3.59329500	0.15191100	0.84203500
H	-1.85303400	-2.20642700	0.26452000
C	-3.45762400	-2.34054800	1.71253700
C	-2.88553600	-3.67257200	2.22390000
H	-3.66136800	-4.26867700	2.73119900
H	-2.48497800	-4.27471700	1.39212000
H	-2.06659600	-3.50195600	2.94189800
C	-4.58232100	-2.62948700	0.70521700
H	-5.04816200	-1.70436300	0.33380700
H	-4.19837800	-3.18065100	-0.16735600
H	-5.37501400	-3.23627700	1.17215900
C	-4.01372300	-1.54390100	2.90404200
H	-4.81145200	-2.10936600	3.41225000
H	-3.22249900	-1.33170400	3.64086900
H	-4.44341900	-0.57942000	2.59048500
C	-3.00966500	-0.44970300	-1.10178600
O	-2.40382800	-1.26675700	-1.80358700
C	1.97390400	1.16826400	0.18848400
C	2.88676700	3.18827500	0.37421700
C	1.37585500	3.30429400	0.02146800
N	0.95086100	1.89679700	-0.04190200
H	3.55464600	3.62425400	-0.37949900
H	1.22880300	3.73007100	-0.98316800
C	0.86869000	-2.27931600	-0.07421600
C	2.36446000	-2.44654400	0.31098800
C	1.82264000	-0.29491500	0.17878500
N	0.66643900	-0.81555200	-0.00023700
H	0.22317300	-2.75939000	0.67391700
H	2.94647000	-3.01603900	-0.42553500
H	3.12850700	3.59847600	1.36520600
H	2.51469900	-2.87291500	1.31247200
O	3.14651500	1.74981000	0.41957400
O	2.88246000	-1.08266300	0.33177600
N	-4.07372500	0.25794100	-1.54701700
H	-4.48759800	0.91547500	-0.89846000
C	-4.71654300	0.15016100	-2.87252500
C	-3.70797300	0.35061500	-4.01347800
C	-5.38786300	-1.22862500	-2.99146400
C	-5.77297500	1.26063100	-2.92262900
H	-3.19819000	1.31766400	-3.90777800
H	-2.94806400	-0.44010000	-3.99913000
H	-4.23772300	0.32087600	-4.97855900
H	-6.14365200	-1.36345800	-2.20199200
H	-5.88400400	-1.33106900	-3.96919900
H	-4.63655300	-2.02476600	-2.89541100
H	-6.31535000	1.22651600	-3.87853800
H	-6.50830900	1.14523400	-2.10945300
H	-5.29766800	2.24962800	-2.82885000
C	0.54800500	4.09694700	1.02297800
H	0.90882500	5.13594400	1.07237300
H	-0.50418500	4.10000300	0.71204500
H	0.60979800	3.64895500	2.02618500
C	0.51311900	-2.79687500	-1.46393300
H	0.61610700	-3.89270300	-1.49748400
H	-0.51948700	-2.51486700	-1.71102500
H	1.18669100	-2.35989200	-2.21867200

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.610694 (Hartree/Particle)
Thermal correction to Energy= 0.647891
Thermal correction to Enthalpy= 0.648835
Thermal correction to Gibbs Free Energy= 0.539282
Sum of electronic and zero-point Energies= -5446.757133
Sum of electronic and thermal Energies= -5446.719936
Sum of electronic and thermal Enthalpies= -5446.718991
Sum of electronic and thermal Free Energies= -5446.828545
HF=-5447.3678264

Figure A3.11
Styrene

C	-4.38102900	-3.76073900	-0.90984900
H	-3.49745700	-3.63618700	-1.54203700
C	-4.33613000	-4.37463900	0.28219400
H	-5.26602100	-4.45840500	0.85649000
H	-5.32021200	-3.35704700	-1.29571800
C	-3.15779700	-4.96773900	0.93771400
C	-3.30956400	-5.56196800	2.20475500
C	-1.87455400	-4.96947000	0.35433300
C	-2.22334300	-6.13698300	2.86869600
H	-4.29764200	-5.57012500	2.67266700
C	-0.78980500	-5.54300200	1.01552000
H	-1.72253100	-4.51773600	-0.62798500
C	-0.95777500	-6.12993100	2.27648100
H	-2.36659200	-6.59189000	3.85181900
H	0.19647400	-5.53363600	0.54505800
H	-0.10533200	-6.57856300	2.79192300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)

Zero-point correction= 0.133407 (Hartree/Particle)
Thermal correction to Energy= 0.140095
Thermal correction to Enthalpy= 0.141039
Thermal correction to Gibbs Free Energy= 0.102310
Sum of electronic and zero-point Energies= -309.325631
Sum of electronic and thermal Energies= -309.318943
Sum of electronic and thermal Enthalpies= -309.317999
Sum of electronic and thermal Free Energies= -309.356729
HF=-309.4590384

TS-Giese Addition[sty]

C	-2.21402700	-1.39806100	0.87653700
H	-1.79611000	-1.22371300	1.86890500
C	-2.66357400	-0.35345200	0.13036100
H	-2.73148100	0.62998900	0.60813100
H	-2.03052100	-2.38253900	0.44230100
C	-4.12243600	-2.42245300	2.02664600
C	-3.39227400	-3.50097800	2.76463500
H	-4.09347300	-4.10719400	3.37723600
H	-2.88739200	-4.19923100	2.07711700
H	-2.64082600	-3.08872700	3.45770100
C	-4.95639000	-2.82770600	0.85186000
H	-5.19893500	-1.96472300	0.21179400
H	-4.45571000	-3.58827400	0.23201300
H	-5.92132000	-3.26530800	1.18606000
C	-4.59976600	-1.24297500	2.81489000
H	-5.51166600	-1.49772900	3.39534800
H	-3.84377100	-0.89702400	3.53823500
H	-4.86281800	-0.39974000	2.15581800
C	-3.14047500	-0.40484700	-1.24942700
C	-3.64879900	0.76749800	-1.85071000
C	-3.12002200	-1.58394400	-2.02937900
C	-4.11830500	0.76502300	-3.16473600
H	-3.67418700	1.69194700	-1.26722100
C	-3.58880900	-1.58570300	-3.34113300
H	-2.73402800	-2.51039800	-1.60043900
C	-4.09257500	-0.41250200	-3.91929600
H	-4.50751900	1.68764100	-3.60283000
H	-3.56269400	-2.51145400	-3.92172400
H	-4.46014000	-0.41828400	-4.94805500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.250915 (Hartree/Particle)
Thermal correction to Energy= 0.264257
Thermal correction to Enthalpy= 0.265201
Thermal correction to Gibbs Free Energy= 0.209273
Sum of electronic and zero-point Energies= -466.911500
Sum of electronic and thermal Energies= -466.898158
Sum of electronic and thermal Enthalpies= -466.897214
Sum of electronic and thermal Free Energies= -466.953142
HF=-467.162415

Int-Giese Addition[sty]

C	-2.47691900	-1.50670300	0.84804800
H	-1.67085900	-1.18085700	1.52989800
C	-2.90454600	-0.33920500	0.02361800
H	-3.01019700	0.62172800	0.53686500
H	-2.04654600	-2.29817400	0.21398300
C	-3.59049300	-2.15414000	1.73373100
C	-2.94876300	-3.28540900	2.55062500
H	-3.69814100	-3.78414800	3.18649400
H	-2.50402100	-4.04821300	1.89085400
H	-2.15150300	-2.89935600	3.20651500
C	-4.70385400	-2.73108700	0.84695900
H	-5.17074800	-1.94831600	0.22965500
H	-4.31197000	-3.50643100	0.16899100
H	-5.49139400	-3.19182800	1.46516900
C	-4.18315900	-1.10697000	2.68915300
H	-4.92283600	-1.57086100	3.36151700
H	-3.39857900	-0.64966900	3.31432900
H	-4.69127300	-0.30050200	2.13800100
C	-3.21979400	-0.35243800	-1.35766300
C	-3.63360500	0.85411500	-2.00335100
C	-3.15108900	-1.52745300	-2.16724800
C	-3.95478600	0.88076200	-3.35336300
H	-3.69589800	1.76964800	-1.40899700
C	-3.47480000	-1.48895900	-3.51819200
H	-2.84250800	-2.47257600	-1.71902800
C	-3.87928400	-0.29010600	-4.12608700
H	-4.26873900	1.81951500	-3.81700600
H	-3.41385700	-2.40468300	-4.11202400
H	-4.13283000	-0.26805400	-5.18826500

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.255459 (Hartree/Particle)
Thermal correction to Energy= 0.267758
Thermal correction to Enthalpy= 0.268702
Thermal correction to Gibbs Free Energy= 0.216395
Sum of electronic and zero-point Energies= -466.953351
Sum of electronic and thermal Energies= -466.941052
Sum of electronic and thermal Enthalpies= -466.940108
Sum of electronic and thermal Free Energies= -466.992415
HF=-467.2088102

F'*R*-sty

Ni	-1.88038400	0.87120700	0.05444400
C	-1.92580400	0.96817000	1.96984800
C	-1.86389600	1.27249600	4.76246500
C	-1.09893700	0.15323700	2.74944200
C	-2.72687900	1.93189200	2.59162900
C	-2.69592400	2.08344000	3.98352200
C	-1.06392700	0.30768800	4.14080000
H	-0.49114900	-0.62568000	2.28376800
H	-3.38103000	2.56650600	1.98832600
H	-3.32769300	2.83837700	4.46043500
H	-0.41343900	-0.33478300	4.74113800
C	-3.48741700	-0.79641500	-1.26633200
H	-2.80054200	-1.64662400	-1.37154200
C	-3.51427800	-0.31405000	0.17663500
H	-4.27391800	0.45837500	0.33461000
H	-3.08603500	0.00377800	-1.91311700

C	-4.85696200	-1.19861000	-1.89711500
C	-5.84063000	-0.01931800	-1.86014200
H	-6.76091700	-0.27149900	-2.41165500
H	-6.13069200	0.23342100	-0.82884300
H	-5.39787200	0.88268000	-2.30933900
C	-5.47156600	-2.40486100	-1.17157700
H	-4.78175500	-3.26375500	-1.16681700
H	-5.71664300	-2.16890000	-0.12611700
H	-6.40083400	-2.71782900	-1.67557300
C	-4.57924200	-1.57941200	-3.36084000
H	-5.50685000	-1.88906500	-3.86896000
H	-4.15498200	-0.72850300	-3.91809600
H	-3.86363000	-2.41569800	-3.42394900
Br	-3.15427000	2.81652500	-1.05272100
C	1.01753200	1.33580400	-0.23125000
C	1.78063600	3.42678800	-0.25319100
C	0.23321400	3.41676600	-0.09979400
N	-0.08340900	1.97691500	-0.13467600
H	2.13061200	3.89452500	-1.18256600
H	-0.26306500	3.88076000	-0.96501200
C	0.31026200	-2.23074900	-0.33593200
C	1.85435600	-2.19628500	-0.15495400
C	1.02263900	-0.13645900	-0.26073200
N	-0.06876300	-0.80087200	-0.31412600
H	-0.16893800	-2.72177600	0.52371600
H	2.40033700	-2.69751000	-0.96551000
H	2.29760300	3.87644000	0.60567400
H	2.19215500	-2.58644800	0.81460100
O	2.15516700	2.01501200	-0.30191700
O	2.18631800	-0.77941100	-0.20162400
C	-0.27327300	4.07553100	1.17602400
H	0.01492900	5.13812900	1.18508400
H	-1.36683800	4.00408000	1.22218200
H	0.14966800	3.58452400	2.06565700
C	-0.13152500	-2.91063200	-1.62772900
H	0.17887800	-3.96650500	-1.62185700
H	-1.22328500	-2.87516400	-1.74340300
H	0.32243600	-2.41597300	-2.50031600
H	-1.84249500	1.38804100	5.84909000
C	-3.56970400	-1.33394600	1.25113900
C	-4.29776300	-1.06933100	2.42855000
C	-2.90603900	-2.57087100	1.16423200
C	-4.34088400	-1.98470300	3.47827800
H	-4.82375200	-0.11696700	2.51864000
C	-2.94281200	-3.49095000	2.21410800
H	-2.35899600	-2.82577400	0.25855500
C	-3.65560600	-3.20191700	3.38161000
H	-4.91053500	-1.74731800	4.38035800
H	-2.41347800	-4.44240600	2.11653100
H	-3.68424900	-3.92002100	4.20457800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.552457 (Hartree/Particle)
Thermal correction to Energy= 0.586504
Thermal correction to Enthalpy= 0.587449
Thermal correction to Gibbs Free Energy= 0.483440
Sum of electronic and zero-point Energies= -5351.980912
Sum of electronic and thermal Energies= -5351.946865
Sum of electronic and thermal Enthalpies= -5351.945921
Sum of electronic and thermal Free Energies= -5352.049930
HF=-5352.5333692

F'-TS-H$^{R\text{-sty}}$

Ni	-1.25306700	1.26683100	-0.46626300
C	-1.67101600	1.07101200	1.40824500
C	-1.27838200	1.91985300	4.07031800
C	-0.65877500	0.50008300	2.20153800
C	-2.51072100	2.04066400	1.98275200
C	-2.31110400	2.46476100	3.29943900
C	-0.45255600	0.93509200	3.51210100
H	-0.03216300	-0.29624800	1.79677200
H	-3.31018000	2.48048300	1.38274500
H	-2.96677200	3.23001400	3.72407000
H	0.35242900	0.49347400	4.10613400
H	-1.12484500	2.24906100	5.10080500
C	-2.62063500	-0.83894700	-1.15185200
H	-1.84026100	-1.60877100	-1.10535100
C	-2.83647800	-0.22426600	0.23608600
H	-3.69271100	0.45350800	0.22620800
H	-2.26064800	-0.08270400	-1.87379000
C	-3.88078800	-1.46579300	-1.82921600
C	-5.03112500	-0.44961500	-1.89898700
H	-5.85574100	-0.85003400	-2.51058700
H	-5.43916300	-0.23111500	-0.90004200
H	-4.69640300	0.50293100	-2.33711000
C	-4.35735300	-2.73155700	-1.09943900
H	-3.54655700	-3.47193200	-1.00988000
H	-4.71938400	-2.50917400	-0.08636300
H	-5.18427900	-3.19892600	-1.65915300
C	-3.46015400	-1.84829600	-3.25917200
H	-4.29949800	-2.30769500	-3.80541400
H	-3.12961100	-0.96283600	-3.82583900
H	-2.62979100	-2.57339900	-3.24822500
Br	-2.85740000	2.84402000	-1.62005300
C	1.52538300	2.05640400	-0.51830100
C	2.05571800	4.19796600	-0.22847500
C	0.51232000	4.03037400	-0.33418400
N	0.35719200	2.57745500	-0.51516100
H	2.49032300	4.81973000	-1.02146000
H	0.11957600	4.51674400	-1.24085000
C	1.07938100	-1.50439800	-1.04825800
C	2.59905100	-1.40928600	-0.74660900
C	1.65707300	0.60027000	-0.67427100
N	0.60861200	-0.12647200	-0.79387300
H	0.58519000	-2.18713500	-0.34174400
H	3.23414800	-1.84115100	-1.53036800
H	2.38050300	4.56920500	0.75387000
H	2.87563500	-1.82877100	0.23102200
O	2.58646300	2.84467900	-0.38366400
O	2.85684700	0.02564900	-0.69749000
C	-0.26463800	4.53115200	0.87531700
H	-0.09644500	5.61092500	1.00941800
H	-1.33708000	4.35314000	0.72484300
H	0.05021600	4.00412400	1.78867400
C	0.76655700	-1.92562100	-2.48218300
H	1.10652700	-2.95799300	-2.65543200
H	-0.31267200	-1.87681800	-2.67783800
H	1.27776100	-1.26321900	-3.19797700
C	-2.95202100	-1.21196100	1.34611500
C	-3.93081200	-1.03366500	2.34014200

C	-2.09828500	-2.32264900	1.45748700
C	-4.05444300	-1.92935500	3.40278900
H	-4.59897400	-0.17182500	2.27485900
C	-2.21573100	-3.21973500	2.52024600
H	-1.32538100	-2.48973700	0.70672900
C	-3.19522000	-3.02946300	3.50019400
H	-4.82634700	-1.76867600	4.15968000
H	-1.53712500	-4.07417300	2.58324900
H	-3.28878100	-3.73191900	4.33171900

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.552764 (Hartree/Particle)
Thermal correction to Energy= 0.585950
Thermal correction to Enthalpy= 0.586894
Thermal correction to Gibbs Free Energy= 0.485231
Sum of electronic and zero-point Energies= -5351.966081
Sum of electronic and thermal Energies= -5351.932895
Sum of electronic and thermal Enthalpies= -5351.931951
Sum of electronic and thermal Free Energies= -5352.033614
HF=-5352.5188452

G-TS-F'*S*-sty

Ni	-1.39228000	1.64295300	-0.98849200
C	-1.93741600	2.18239200	0.83819000
C	-2.76687600	3.03241900	3.42572700
C	-1.10457300	2.04449900	1.96241300
C	-3.19537400	2.77654100	1.05088200
C	-3.61010400	3.19565900	2.32140400
C	-1.50590000	2.45588400	3.24040600
H	-0.11002700	1.59590400	1.86279300
H	-3.87573900	2.91094400	0.20405900
H	-4.59691700	3.65036300	2.45125800
H	-0.83369500	2.32463100	4.09390400
Br	-3.01401800	2.27009600	-2.68168700
C	1.32246200	2.29853700	-0.68139100
C	2.03431500	4.40013200	-0.83752800
C	0.54760500	4.29871500	-1.29117400
N	0.26769500	2.86183400	-1.14385400
H	2.71769000	4.72089400	-1.63381700
H	0.44651900	4.55477900	-2.35770000
C	0.32284100	-1.15752600	-0.24058600
C	1.71805000	-1.14822000	0.44024900
C	1.24385000	0.86418300	-0.36895100
N	0.12322800	0.26793800	-0.56371600
H	-0.46387700	-1.47343600	0.45910100
H	2.41157200	-1.89719800	0.03841900
H	2.17389300	5.03183200	0.05041500
H	1.67034000	-1.22963200	1.53498700
O	2.40303400	3.03241400	-0.46404000
O	2.26079300	0.17652400	0.12821100
C	-3.41186100	-0.87840100	1.66024200
H	-2.96440500	0.05745500	2.02793400
C	-3.51267000	-0.78807000	0.17627500
H	-3.84271400	0.16586300	-0.24220800
H	-2.73160800	-1.69196100	1.96229500
C	-4.76268700	-1.07796100	2.42026900
C	-5.35878800	-2.45558800	2.09777600
H	-6.31384400	-2.59958900	2.62917500
H	-5.55123700	-2.56545100	1.01935800
H	-4.67831700	-3.26694700	2.40372900
C	-5.76240800	0.02008300	2.02635500
H	-5.33895700	1.01979300	2.20490700
H	-6.03353500	-0.04702600	0.96117200
H	-6.68931700	-0.07284100	2.61556500
C	-4.47012100	-0.98147400	3.92511400
H	-5.38824500	-1.13440400	4.51568800
H	-3.73724000	-1.74407800	4.23650400
H	-4.05928400	0.00806300	4.18276300
C	-0.42943400	5.13663400	-0.47596600
H	-0.20920000	6.20705200	-0.60637800
H	-1.45800500	4.94159000	-0.81029900
H	-0.36302100	4.88140100	0.59189700
C	0.25689000	-2.00146800	-1.50858800
H	0.36764700	-3.06677800	-1.25939400
H	-0.71065500	-1.86599400	-2.00815900
H	1.06067700	-1.71419700	-2.20467000
H	-3.08763900	3.35406900	4.42011900
C	-3.26899200	-1.83382200	-0.74940000
C	-3.42007200	-1.58894000	-2.14965600
C	-2.87430800	-3.14924600	-0.35908000
C	-3.19934400	-2.59111800	-3.08455100
H	-3.69411000	-0.58240300	-2.47435300
C	-2.65732400	-4.14411500	-1.30531200
H	-2.74503700	-3.38033200	0.69871100
C	-2.81798200	-3.87976600	-2.67402100
H	-3.31953500	-2.37256600	-4.14885100
H	-2.35726200	-5.14268800	-0.97699100
H	-2.64476200	-4.66625600	-3.41189800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.549596 (Hartree/Particle)
Thermal correction to Energy= 0.583574
Thermal correction to Enthalpy= 0.584518
Thermal correction to Gibbs Free Energy= 0.480175
Sum of electronic and zero-point Energies= -5351.971676
Sum of electronic and thermal Energies= -5351.937698
Sum of electronic and thermal Enthalpies= -5351.936754
Sum of electronic and thermal Free Energies= -5352.041097
HF=-5352.5212715

F'*S*-sty

Ni	-1.15616300	1.11368300	-0.02849100
C	-1.31931900	1.38005600	1.87442600
C	-1.37959900	1.94970700	4.63430600
C	-0.44611900	0.73001000	2.75510100
C	-2.22821500	2.31344100	2.38810500
C	-2.25852900	2.59673500	3.75910100
C	-0.47154400	1.01550400	4.12716100
H	0.26519900	-0.01271800	2.38726800
H	-2.91113700	2.83106900	1.71093400
H	-2.97597700	3.32695600	4.14434700
H	0.22269200	0.50277000	4.79900000
H	-1.40410000	2.17006100	5.70447300
Br	-2.20401600	3.19925500	-1.12233000
C	-2.51746700	-1.33901900	0.89004200
H	-1.77010400	-1.19409600	1.68097000

C	-2.79291600	-0.02718800	0.16207200
H	-3.54458700	0.58017900	0.67461100
H	-2.08287100	-2.05947200	0.18361400
C	-3.75025500	-2.00626200	1.55684400
C	-3.28337900	-3.35546200	2.12803200
H	-4.10719300	-3.87314600	2.64589700
H	-2.91677600	-4.01859500	1.32728400
H	-2.46358600	-3.21551600	2.85170100
C	-4.87233000	-2.25064000	0.53689400
H	-5.27654000	-1.30701300	0.14234000
H	-4.50789700	-2.84011700	-0.32003200
H	-5.70457100	-2.80413900	1.00200900
C	-4.27099000	-1.13023700	2.70788800
H	-5.11586500	-1.62082200	3.21807800
H	-3.48038600	-0.94764300	3.45340600
H	-4.62261700	-0.15062500	2.35005600
C	1.78994400	1.23293800	-0.21845700
C	2.71932800	3.23461300	-0.50411700
C	1.18794700	3.37549300	-0.29996800
N	0.74347600	1.96798500	-0.25394500
H	3.05109900	3.48562600	-1.52105100
H	0.70259800	3.85492600	-1.16106900
C	0.84324700	-2.25517700	0.21893800
C	2.38430100	-2.28571100	0.43421000
C	1.69005300	-0.22654600	-0.04311100
N	0.56531500	-0.83135300	-0.07590500
H	0.31316000	-2.50826400	1.15077200
H	2.90899100	-2.91215100	-0.30090500
H	3.31491200	3.79266900	0.22976300
H	2.68473800	-2.57860000	1.44872700
O	2.98158900	1.81137600	-0.29875300
O	2.80318600	-0.90882300	0.22486400
C	0.78787700	4.10809500	0.97564100
H	1.14673300	5.14819600	0.93506700
H	-0.30517900	4.11045600	1.07145700
H	1.21981300	3.61699600	1.86132100
C	0.37864400	-3.19393700	-0.88909000
H	0.68614000	-4.22437600	-0.65364300
H	-0.71435900	-3.18581400	-0.99068900
H	0.82507000	-2.90920300	-1.85417800
C	-3.09463100	-0.12207000	-1.28998200
C	-4.22872100	0.52208600	-1.83024200
C	-2.24463000	-0.81134400	-2.17983800
C	-4.51646700	0.45427200	-3.18926400
H	-4.88476500	1.08107300	-1.16031200
C	-2.52054000	-0.86134100	-3.54974700
H	-1.35037300	-1.29885100	-1.79625800
C	-3.65982100	-0.23564600	-4.05974400
H	-5.40929200	0.94833700	-3.58042800
H	-1.84159300	-1.39630100	-4.21836600
H	-3.88245100	-0.28101900	-5.12846300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.552686 (Hartree/Particle)
Thermal correction to Energy= 0.586666
Thermal correction to Enthalpy= 0.587610
Thermal correction to Gibbs Free Energy= 0.483678
Sum of electronic and zero-point Energies= -5351.978924
Sum of electronic and thermal Energies= -5351.944944
Sum of electronic and thermal Enthalpies= -5351.944000
Sum of electronic and thermal Free Energies= -5352.047933
HF=-5352.5316103

F'-TS-H$^{S\text{-sty}}$

Ni	-1.02293600	1.12110600	-0.27746900
C	-1.80637500	1.32593100	1.49513500
C	-1.75565400	2.66635600	3.98020800
C	-0.98316200	0.87352500	2.53791100
C	-2.63476500	2.43982600	1.72861000
C	-2.60336400	3.10602500	2.95384300
C	-0.94630500	1.54799900	3.76472300
H	-0.33696800	0.00540500	2.39319700
H	-3.28945200	2.79592200	0.93070000
H	-3.24705300	3.97591100	3.11029900
H	-0.27739300	1.19255200	4.55323900
H	-1.73399600	3.18767600	4.94011500
Br	-1.75609900	3.08264700	-1.70273200
C	-2.35737900	-1.47072300	0.91599700
H	-1.55916300	-1.37558700	1.66172200
C	-2.76949000	-0.10644800	0.37626800
H	-3.63920400	0.27037400	0.91217900
H	-1.94254400	-2.07408600	0.09950400
C	-3.50250200	-2.28001600	1.57709200
C	-2.92785800	-3.65430200	1.95828100
H	-3.68914500	-4.27824100	2.45376400
H	-2.57399800	-4.19626400	1.06603200
H	-2.07544500	-3.54896400	2.64942600
C	-4.67350300	-2.47569700	0.60161300
H	-5.14531100	-1.51925800	0.33131200
H	-4.33506500	-2.95405800	-0.33157600
H	-5.44924400	-3.11618700	1.05189700
C	-3.99300800	-1.57242800	2.85091100
H	-4.77728500	-2.16640800	3.34714300
H	-3.16731300	-1.43030600	3.56641200
H	-4.41952700	-0.58070900	2.63369300
C	1.88154300	1.14767700	0.05868900
C	2.84858700	3.15279700	0.08462700
C	1.30940400	3.29664600	-0.05636300
N	0.86185300	1.89216500	-0.14550000
H	3.40325900	3.47622700	-0.80686400
H	1.02928200	3.79306000	-0.99593100
C	0.85588700	-2.34050900	0.08221600
C	2.37079300	-2.42652500	0.42384500
C	1.74306900	-0.31406500	0.11828800
N	0.61416900	-0.88594400	-0.06436800
H	0.24984300	-2.69956800	0.92762400
H	2.95162200	-2.98389600	-0.32475300
H	3.25469000	3.65203000	0.97445800
H	2.57542600	-2.83223200	1.42351300
O	3.06874100	1.71792800	0.24201500
O	2.82208000	-1.04571300	0.39995600
C	0.63111700	4.00940100	1.10706700
H	0.99754300	5.04545000	1.17502400
H	-0.45413400	4.02487500	0.94797000
H	0.83683700	3.49498400	2.05815200
C	0.47782600	-3.12448500	-1.16998100
H	0.75603100	-4.18223000	-1.04459400
H	-0.60325500	-3.08355700	-1.35871000
H	1.00349100	-2.72683500	-2.05175300

C	-3.08565600	-0.04554800	-1.08516600
C	-4.24709700	0.62797700	-1.51850300
C	-2.27219800	-0.65075700	-2.06793400
C	-4.58649900	0.68669800	-2.86656500
H	-4.88901700	1.10599800	-0.77466900
C	-2.60815600	-0.58123500	-3.42249200
H	-1.36820500	-1.17902300	-1.77140400
C	-3.76645900	0.08410000	-3.82948000
H	-5.49714400	1.20738000	-3.17302700
H	-1.95854000	-1.05578600	-4.16213600
H	-4.03277600	0.13209800	-4.88793300

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.552549 (Hartree/Particle)
Thermal correction to Energy= 0.585845
Thermal correction to Enthalpy= 0.586790
Thermal correction to Gibbs Free Energy= 0.485042
Sum of electronic and zero-point Energies= -5351.965523
Sum of electronic and thermal Energies= -5351.932227
Sum of electronic and thermal Enthalpies= -5351.931283
Sum of electronic and thermal Free Energies= -5352.033030
HF=-5352.5180721

Figure A3.12
G-TS-F'^{R}-Conf2

Ni	-0.58740300	1.03748700	-1.05976800
C	-0.35275200	1.03331200	-3.01235300
C	-0.03316300	1.07393300	-5.83778200
C	-1.16690900	1.83607600	-3.83411600
C	0.64644200	0.27594900	-3.65033000
C	0.80559400	0.28531800	-5.04168900
C	-1.01762600	1.85817900	-5.22687100
H	-1.95918300	2.44799600	-3.38759500
H	1.31228400	-0.35421500	-3.05252400
H	1.58469400	-0.32527100	-5.50825200
H	-1.67566400	2.48308300	-5.83806900
H	0.08161800	1.07947400	-6.92494100
C	-2.56117900	-1.42328900	-3.49279000
H	-2.17020100	-2.36408000	-3.07897100
C	-3.06303000	-0.58626000	-2.37733900
H	-3.42215000	0.42706700	-2.56101600
H	-1.73450700	-0.90725000	-4.00230600
C	-3.63495000	-1.77538600	-4.57249900
C	-4.13767100	-0.49883200	-5.26331000
H	-4.84582900	-0.75050100	-6.06935400
H	-4.66005200	0.16649900	-4.55839200
H	-3.30137600	0.06633300	-5.70354200
C	-4.81133900	-2.51851700	-3.92200800
H	-4.46718500	-3.42245700	-3.39391000
H	-5.33309900	-1.87987000	-3.19101400
H	-5.54679400	-2.82734400	-4.68243800
C	-2.95780700	-2.68168300	-5.61088500
H	-3.66549700	-2.96185400	-6.40794700
H	-2.10129700	-2.17079500	-6.07975700
H	-2.58585800	-3.60888200	-5.14549300
C	-3.37622300	-1.17429000	-1.08440100
O	-2.91255900	-2.22578700	-0.65943800
O	-4.26774700	-0.43928100	-0.39382000
C	-4.57353300	-0.88172600	0.92626200
H	-3.68357500	-0.80006900	1.56745800
H	-5.35970800	-0.21402500	1.29852100
H	-4.92771700	-1.92321300	0.91963900
Br	-1.85415300	1.63867200	0.93517500
C	2.01746900	1.11453400	0.04549600
C	3.18343700	3.00065000	0.20901000
C	1.84469800	3.25667500	-0.54369200
N	1.21359300	1.92906500	-0.52750800
H	4.07738600	3.22319000	-0.38623300
H	2.03292000	3.52126800	-1.59711800
C	0.30333500	-2.07514300	-0.12783000
C	1.44263500	-2.38745500	0.87860800
C	1.58928300	-0.28553400	0.18175300
N	0.47254600	-0.62615400	-0.34728800
H	-0.69152200	-2.24701900	0.30477600
H	2.06032200	-3.24910000	0.59674000
H	3.23844000	3.52378700	1.17424200
H	1.09108800	-2.50002000	1.91362200
O	3.18249100	1.56379500	0.48958200
O	2.29429000	-1.19492300	0.83881200
C	0.95039000	4.31238800	0.09218100
H	1.45524100	5.29037100	0.08591100
H	0.00826600	4.40012800	-0.46735600
H	0.70659700	4.03877100	1.12941000
C	0.41764200	-2.82961600	-1.44792900
H	0.21858600	-3.89999800	-1.28802000
H	-0.31215100	-2.44213500	-2.16813500
H	1.42583100	-2.71867000	-1.87678800

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511160 (Hartree/Particle)
Thermal correction to Energy= 0.545252
Thermal correction to Enthalpy= 0.546196
Thermal correction to Gibbs Free Energy= 0.440485
Sum of electronic and zero-point Energies= -5348.803524
Sum of electronic and thermal Energies= -5348.769432
Sum of electronic and thermal Enthalpies= -5348.768488
Sum of electronic and thermal Free Energies= -5348.874199
HF=-5349.3146838

G-TS-F'^{S}-Conf2

Ni	-0.27584700	-0.36460900	0.61566700
C	-1.12223700	-1.76981200	-0.48789100
C	-2.39857600	-3.81892800	-1.99393600
C	-0.42164300	-2.52615900	-1.44368100
C	-2.48776100	-2.06652500	-0.31811300
C	-3.12154600	-3.07775300	-1.05289400
C	-1.04243800	-3.53615800	-2.19105700
H	0.64385200	-2.33814700	-1.62196700
H	-3.07475800	-1.49367100	0.40679800
H	-4.18389700	-3.28631200	-0.89202400
H	-0.46665100	-4.10601500	-2.92695300
Br	-1.88816800	1.24590500	1.45358100
H	-2.88801500	-4.60810700	-2.57112800
C	2.46112200	-0.89506100	0.12140200
C	3.63809900	-2.42595100	1.22290900
C	2.19754800	-2.33088900	1.80411800

N	1.59797500	-1.24353800	1.00515100
H	4.41945000	-2.11329900	1.92778300
H	2.22700900	-2.00591200	2.85539800
C	0.68858200	1.50399800	-1.93866900
C	2.08159500	1.47202300	-2.63331300
C	2.06583100	0.11051900	-0.87568000
N	0.87857500	0.58767200	-0.80294400
H	-0.08311300	1.06021300	-2.58857300
H	2.61148000	2.43311700	-2.57357700
H	3.87779800	-3.41786300	0.81724300
H	2.05310600	1.12691600	-3.67406200
O	3.64849800	-1.47960300	0.10728400
O	2.85710900	0.49609400	-1.86480200
C	1.38474500	-3.61460700	1.69388800
H	1.87194900	-4.41072700	2.27840900
H	0.37330800	-3.45459800	2.08900800
H	1.31334700	-3.93790800	0.64436900
C	0.23725000	2.88541100	-1.48506400
H	0.08942200	3.54122800	-2.35655700
H	-0.70847500	2.80863000	-0.93005400
H	0.99211200	3.34112500	-0.82542200
C	-0.19905200	-0.32541300	4.31756300
H	-0.00465000	0.71868400	4.02036600
C	-1.65058200	-0.59188400	4.17364600
H	-2.39217800	0.12763200	4.52183000
H	0.34578400	-0.97482000	3.61803800
C	0.39445200	-0.53967600	5.74473300
C	1.89454300	-0.21748000	5.67927900
H	2.36751000	-0.34842000	6.66591500
H	2.41221400	-0.88144200	4.96774500
H	2.06459200	0.82212900	5.35569700
C	0.20158500	-1.99917900	6.18260100
H	-0.86649500	-2.25646300	6.25828800
H	0.66153600	-2.69402800	5.46261900
H	0.66139100	-2.17164800	7.16922800
C	-0.28868300	0.40098200	6.74858500
H	0.15908300	0.29198900	7.74962600
H	-0.18053900	1.45431300	6.44227400
H	-1.36433500	0.18246200	6.83779500
C	-2.13744800	-1.82139800	3.58869600
O	-1.43325400	-2.74973000	3.21017800
O	-3.48683600	-1.86136000	3.50765700
C	-4.05219000	-3.06227100	2.98571700
H	-3.79084700	-3.92475600	3.61831600
H	-5.13880700	-2.91364500	2.98278700
H	-3.69272900	-3.25403700	1.96444100

UB3LYP-D3(BJ)/def2-SVP-CPCM(THF)
Zero-point correction= 0.511052 (Hartree/Particle)
Thermal correction to Energy= 0.545183
Thermal correction to Enthalpy= 0.546127
Thermal correction to Gibbs Free Energy= 0.440113
Sum of electronic and zero-point Energies= -5348.804773
Sum of electronic and thermal Energies= -5348.770642
Sum of electronic and thermal Enthalpies= -5348.769698
Sum of electronic and thermal Free Energies= -5348.875711
HF=-5349.3158248

Appendix 4: Computational Methods, Results, Coordinates and Energies from Chapter 5 (Mechanistic Study of Enantioselective Three-Component Alkenylation of Organophosphonates via Nickel Metallaphotoredox Catalysis)

A4.1 Methods

All optimizations were carried out without constraints with B3LYP functional using def2-SVP as basis set with "opt=noeigen" keyword as implemented in Gaussian16. Grimme's empirical dispersion correction (with Becke-Johnson dampling) was added to address the non-local correlation [noted as (U)B3LYP-D3(BJ)/def2-SVP]. For Ir-involved system, pseudo potential LANL2DZ was employed for structural optimization and SDD was applied for single point energy calculations. Vibrational frequencies were computed at the same level to obtain thermal corrections (at 298 K; enthalpic correction H_{corr} and free energy G_{corr}) and to characterize the stationary points as transition states (one and only one imaginary frequency) or minima (zero imaginary frequencies). To include the solvent effect, solvent correction $E_{sol\text{-}corr}$ was calculated by equation $E_{sol\text{-}corr} = E_{sol} - E_{gas}$, where E_{sol} and E_{gas} are the electronic energy values obtained at the mixed solution phase (ethyl acetate/DMA = 3/1, same as experiment; noted as EA/DMA) with SMD implicit solvent model and gas phase at the M062X-6-31G(d) level of theory, correspondingly. Mixed solution phase was modeled based on the corresponding solvent descriptors.

To refine energetics, single point energy calculations were carried out in gas phase with a larger basis set def2-TZVP followed by adding the previously obtained solvent correction values, E_{sol}(def2-TZVP) = E_{gas}(def2-TZVP) + $E_{sol\text{-}corr}$ [noted as (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)]. For comparison, single point energies with M06 functional were also calculated.

Exhaustive conformational searches were performed for all intermediates to map out the lowest energy profile, and intrinsic reaction coordinate (IRCs) calculations were undertaken for selected transition state structures to ensure they connected the illustrated ground states. All structural figures were generated using CYLview.

A4.2 Supplementary Figures

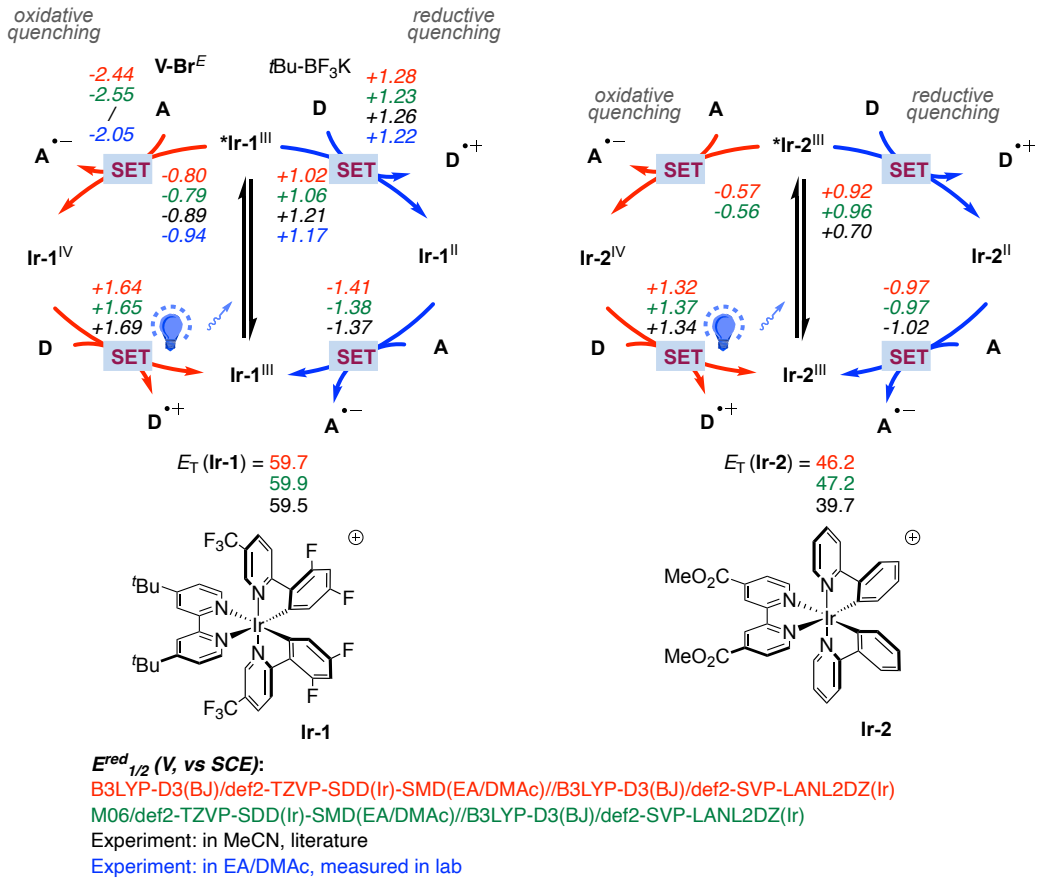


Figure A4.1 Benchmark of properties of photocatalysts with computational methods against experimental values. **A** = electron acceptor, **D** = electron donor.

Reduction potential values (V, vs SCE) of corresponding species were calculating based on the equation:

$$E_{1/2}^{red} = -\frac{\Delta G}{nF} - E_{1/2}^{SHE} + E_{1/2}^{SCE}$$

Where n is the number of electrons transferred (in calculations of this system, n = 1), F is the Faraday constant (value 23.061 kcal•mol^{-1}•V^{-1}), $E_{1/2}^{SHE}$ is the absolute value for the standard hydrogen electrode (SHE, value = 4.281 V) and $E_{1/2}^{SCE}$ is the potential of the saturated calomel electrode (SCE) relative to SHE (value - 0.141V).

Free energy difference ΔG = [E_{gas}(reduced) + G_{corr}(reduced) + $E_{sol\text{-}corr}$(reduced)] – [E_{gas}(original) + G_{corr}(original) + $E_{sol\text{-}corr}$(original)]

Based on the experimental values of the redox potential of *t*Bu-BF_3K and the triplet state energy of photocatalysts, (U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)-SMD(EA/DMA) was chosen as the method to compute the single point energy values in the system.

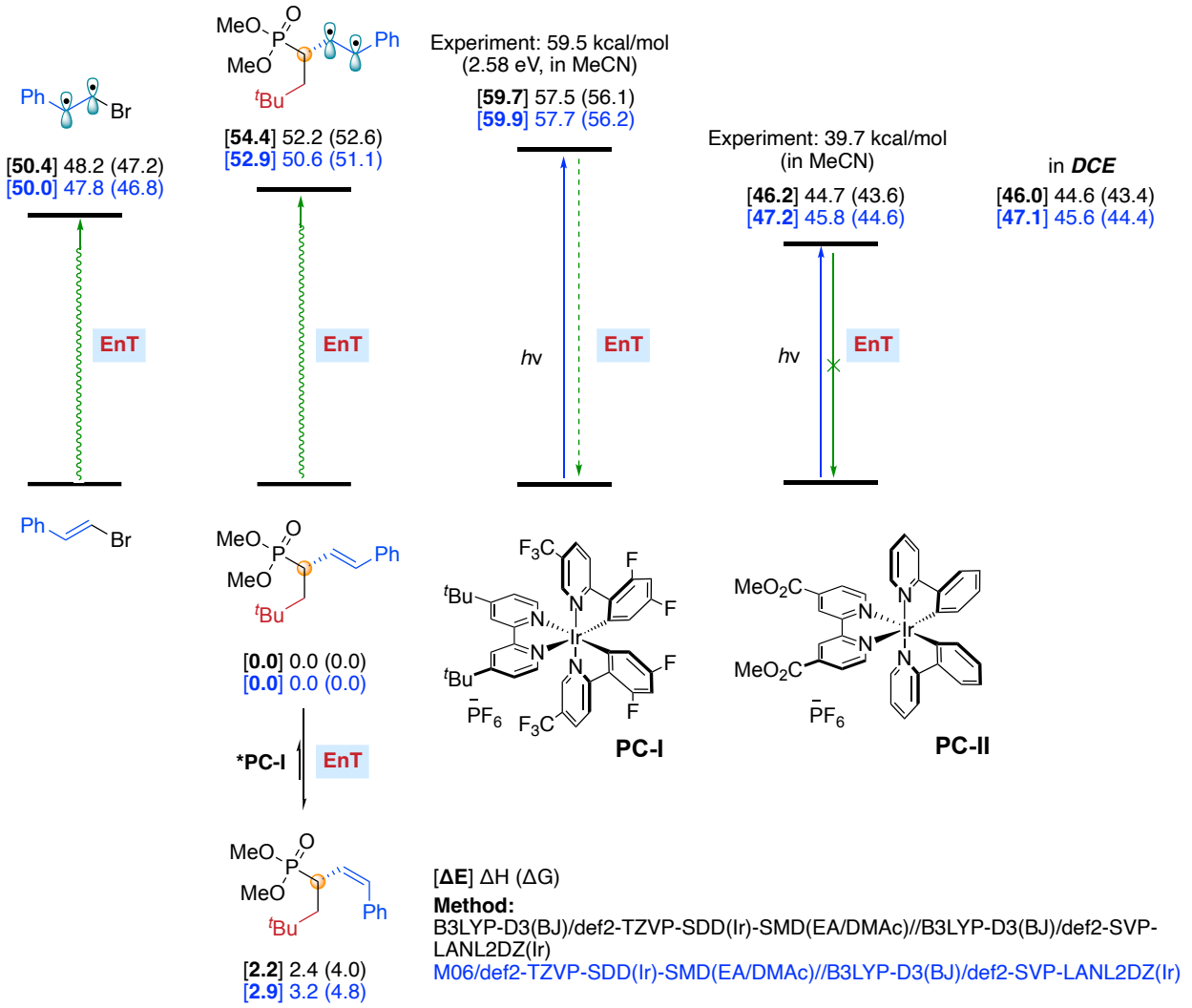


Figure A4.2 Energy transfer between reagents and products with photocatalysts. Electronic energy (in bracket), enthalpy, and free energy values (in parenthesis) were calculated at the (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (black) and M06/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (blue) levels of method.

Since the redox potential of vinyl bromide substrates (**V-Br**^{E}) and photocatalysts are unmatched (**Figure A4.1**), while the triplet state energy of both are lose, the strong quenching of photocatalyst by vinyl bromide was attributed to the energy transfer event rather than electron transfer between these two species. Similarly, the triplet state energy of product is higher than that of **PC-II** while smaller than **PC-I**, thus energy transfer is only viable between product and **PC-I**. As a result, *E*/*Z* isomerization of the final product is applicable when **PC-I** is employed.

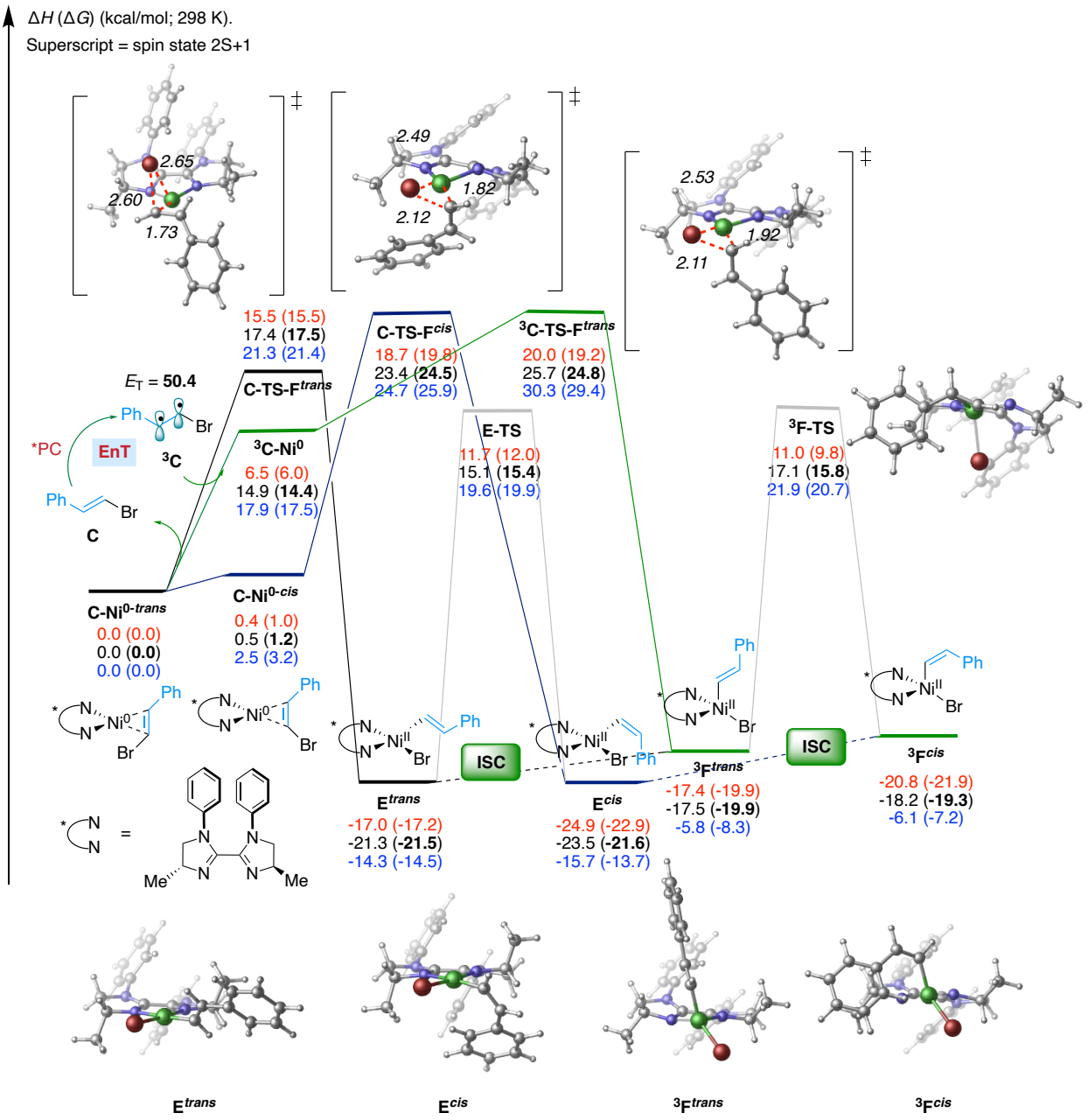


Figure A4.3 Energy profile of quenching of photocatalysts by vinyl bromide and the generation of Ni(II) species with truncated model ligand. Enthalpy and free energy values (in parenthesis) were calculated at the (U)B3LYP-D3(BJ)/def2-SVP (red), (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (black) and M06/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (blue) levels of method.

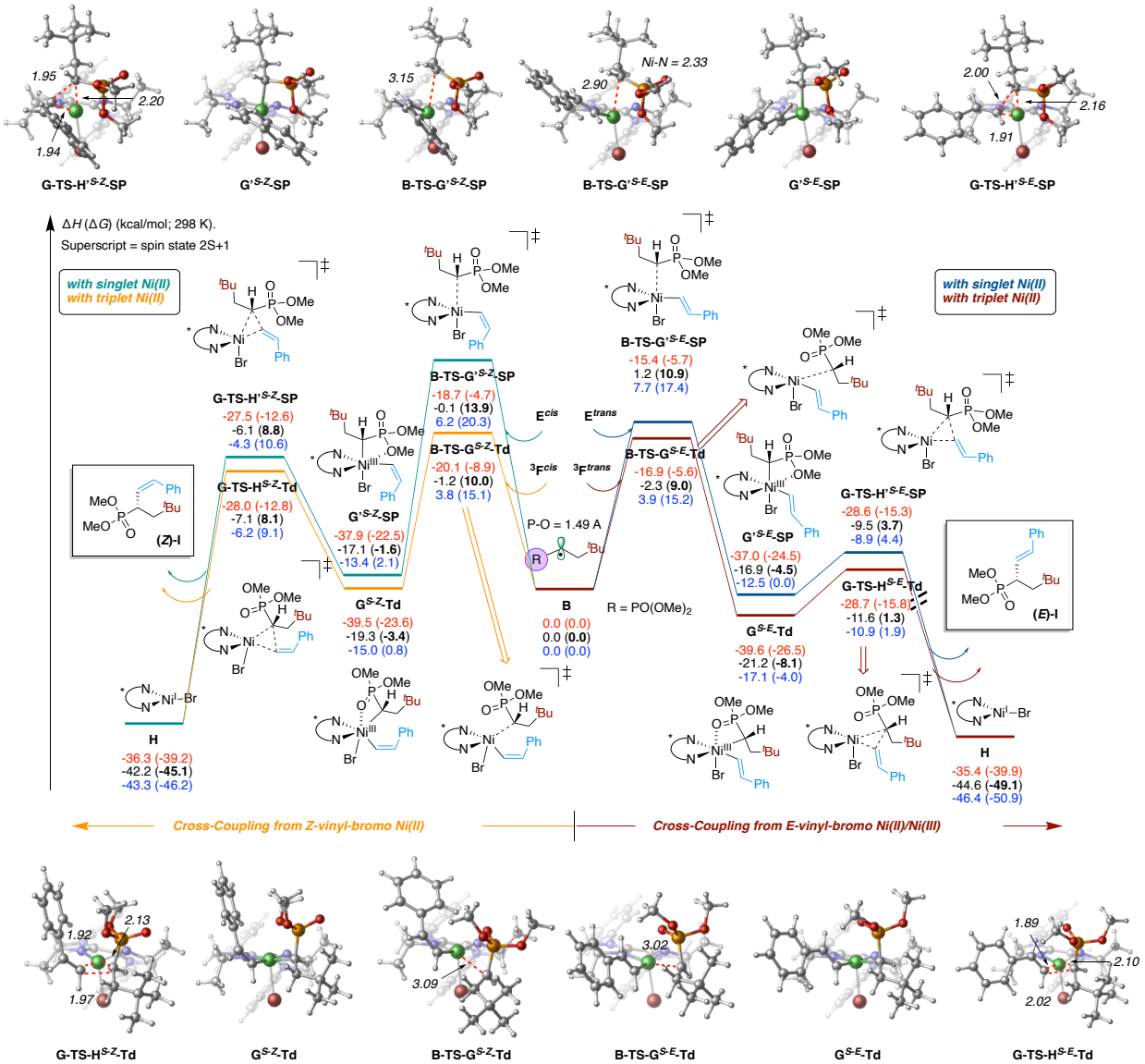


Figure A4.4 Energy profile of potential interaction pathways between α-phosphonate radical and different Ni(II) intermediates. Enthalpy and free energy values (in parenthesis) were calculated at the (U)B3LYP-D3(BJ)/def2-SVP (red), (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (black) and M06/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (blue) levels of method.

Upon evaluating the interaction of α-phosphonate radical and different Ni(II) intermediates, we found that the interaction with triplet state, tetrahedral, *trans*-vinyl Ni(II) intermediate $^{3}\mathbf{F}^{trans}$ is the most favorable pathway (red), while other pathways are close in energy. Overall, the radical addition transition state is higher in energy than the reductive elimination transition state, thus the

former is the enantiodetermining step for all pathways. The radical is favorable to approach from the equatorial position of the Ni center due to the coordination effect between Ni and O. Moreover, the barrier for reductive elimination was found higher for *cis*-vinyl-alkyl-bromo Ni(III) intermediates (green and orange pathways).

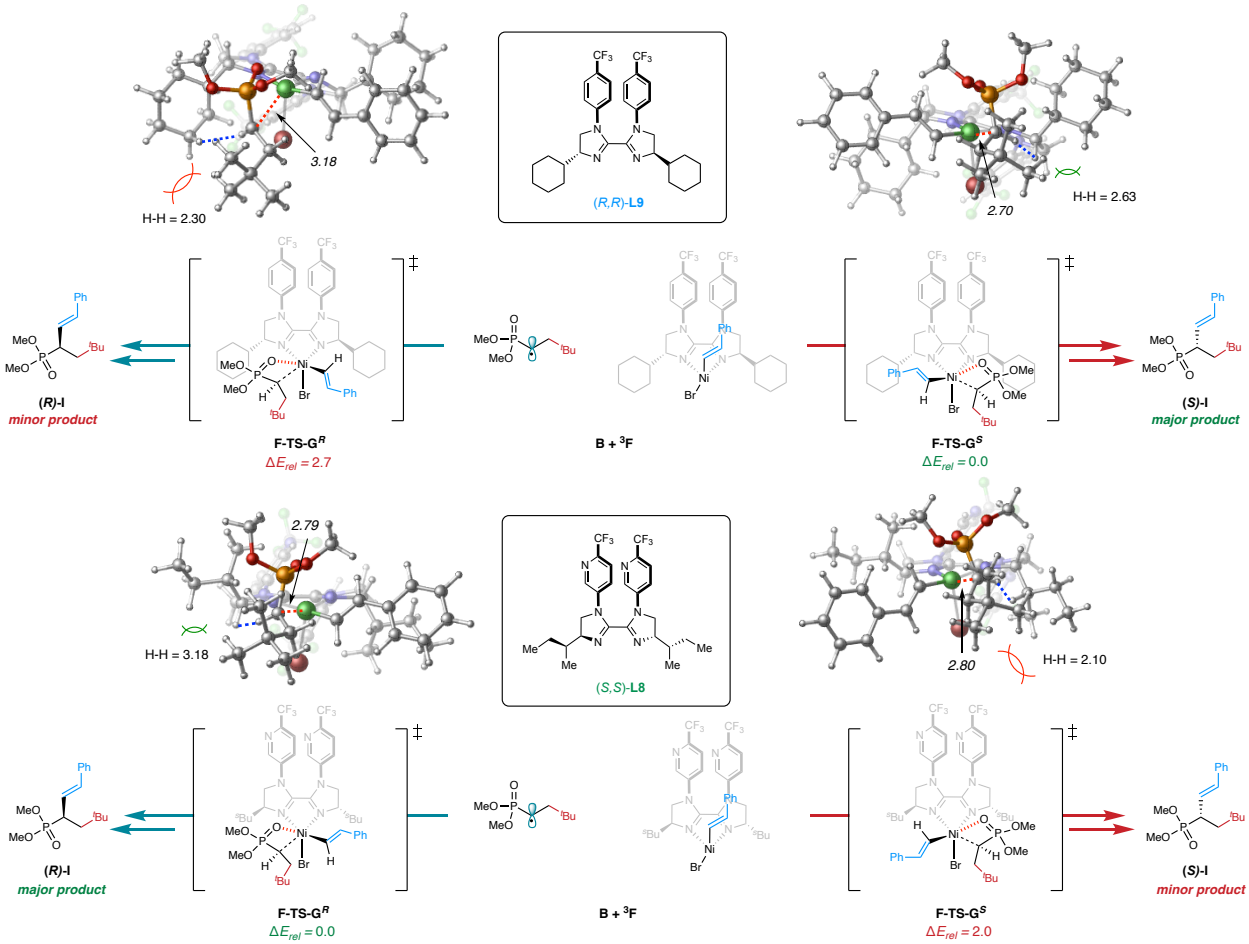


Figure A4.5 Models for the divergent enantioselectivity of full ligand (*R*,*R*)-**L2** and (*S*,*S*)-**L1** systems. Electronic energy values were calculated at the (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP levels of method.

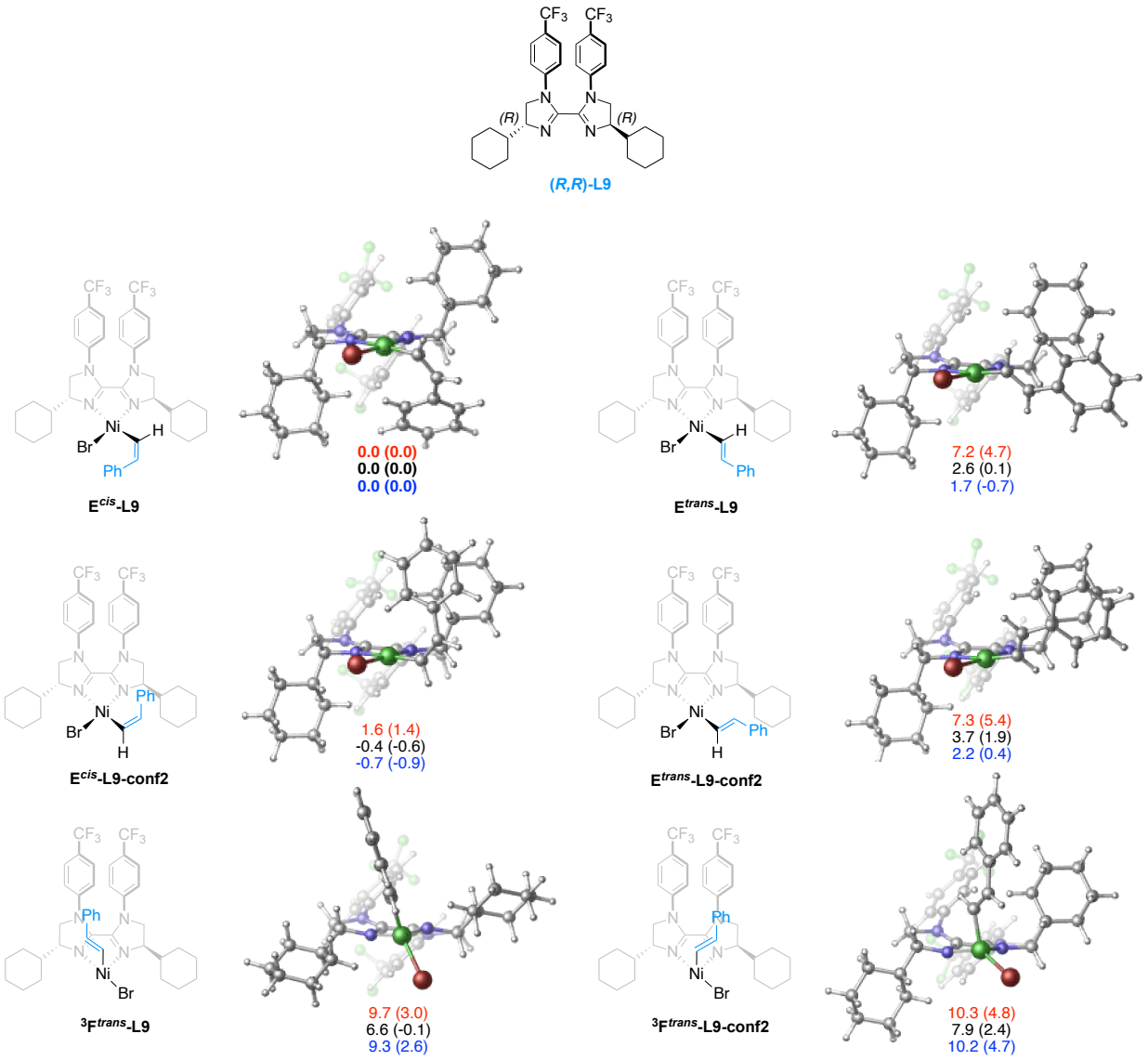


Figure A4.6 Comparison of singlet and triplet *trans*/*cis*-vinyl-bromo-Ni(II) intermediates with full ligand (*R*,*R*)-**L2** system. Enthalpy and free energy values (in parenthesis) were calculated at the (U)B3LYP-D3(BJ)/def2-SVP (red), (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (black) and M06/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (blue) levels of method.

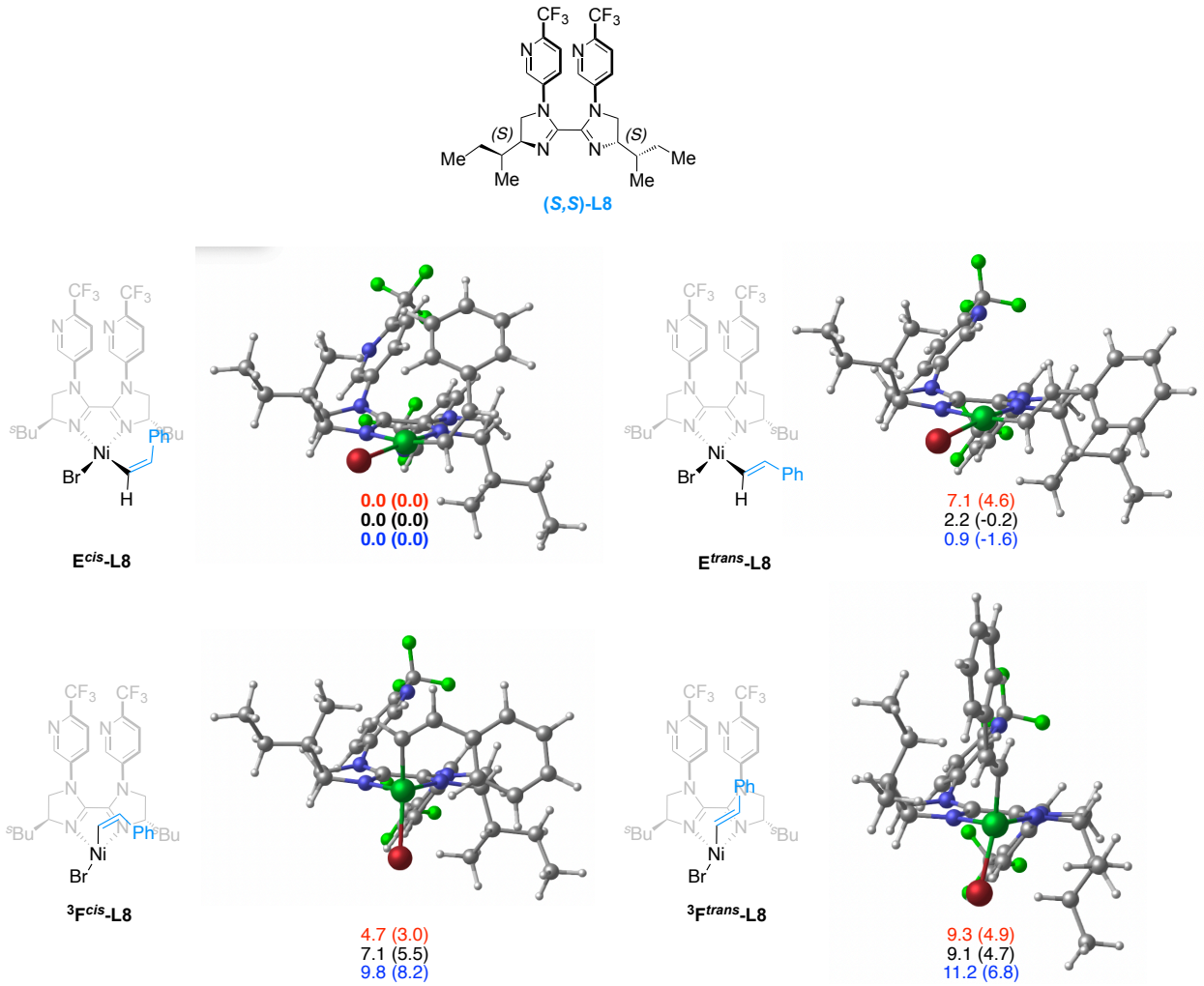


Figure A4.7 Comparison of singlet and triplet *trans*/*cis*-vinyl-bromo-Ni(II) intermediates with full ligand (*S*,*S*)-**L1** system. Enthalpy and free energy values (in parenthesis) were calculated at the (U)B3LYP-D3(BJ)/def2-SVP (red), (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (black) and M06/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (blue) levels of method.

Upon evaluating the structural properties and energetics of Ni(II) intermediates in full ligand systems (*R*,*R*)-**L2** and (*S*,*S*)-**L1**, we found that the *trans*- and *cis*-vinyl Ni(II) intermediates are close in energy in both systems. Moreover, the triplet state Ni(II) intermediates are higher in energy compared to the singlet state intermediates but only for 7–9 kcal/mol in enthalpy values.

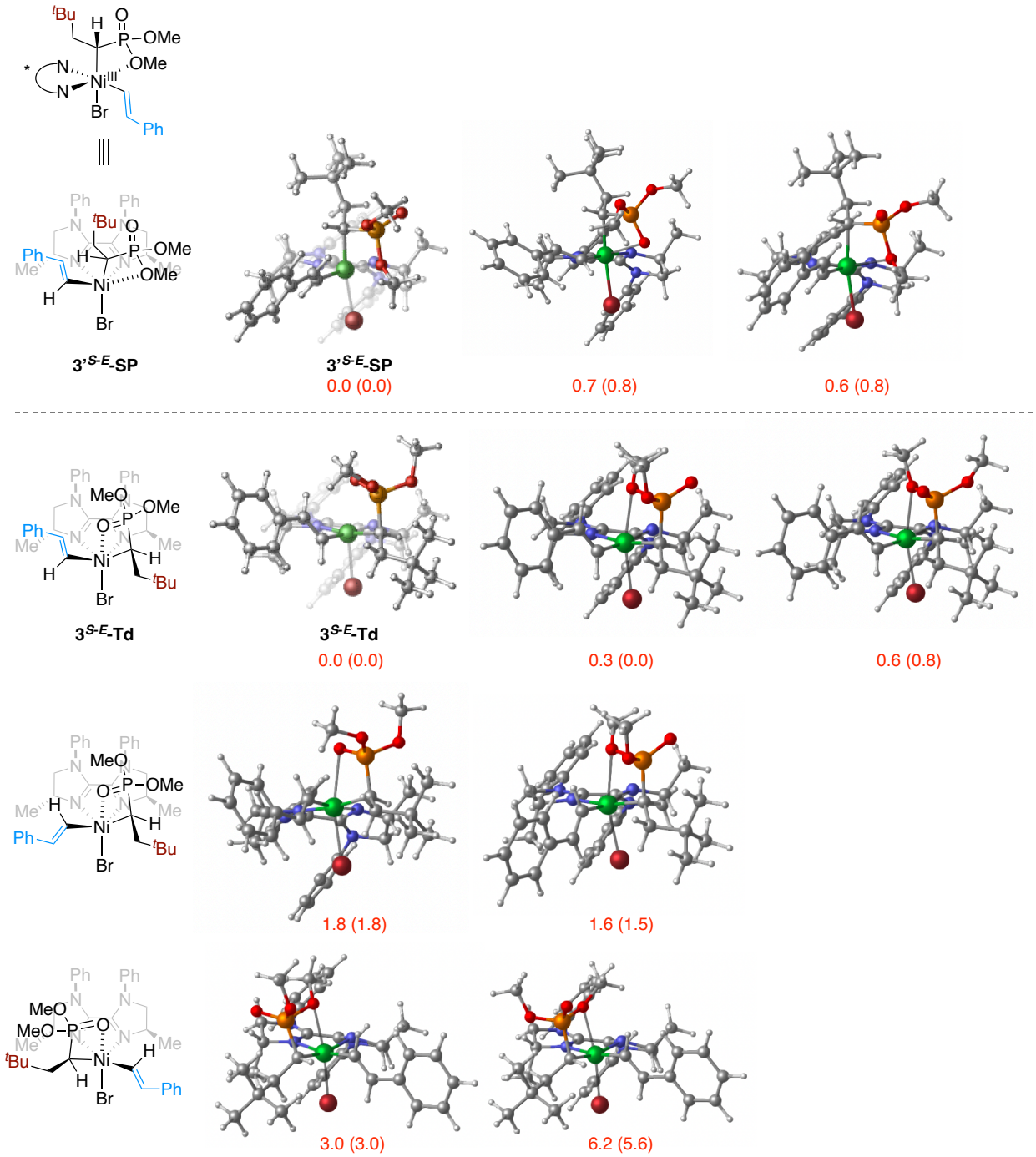


Figure A4.8 Conformational search of Ni(III) intermediates (**3'$^{S\text{-}E}$-SP** and **3$^{S\text{-}E}$-Td**) revealing the effect of coordination between directing group P=O and Ni center. Enthalpy and free energy values (in parenthesis) were calculated at the (U)B3LYP-D3(BJ)/def2-SVP (red), (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (black) and M06/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (blue) levels of method.

With manual conformational search of Ni(III) intermediates, we found that (1) coordination between O and Ni is more favorable when O occupies the axial position (**Figure A4.4**, **G$^{S\text{-}E}$-Td** and **G'$^{S\text{-}E}$-SP**); (2) coordination of OMe and Ni is also favorable but slightly higher in energy than the coordination of O and Ni; (3) Ph substituent of the vinyl group is favorable to avoid steric repulsion with the alkyl chain of the chiral ligand.

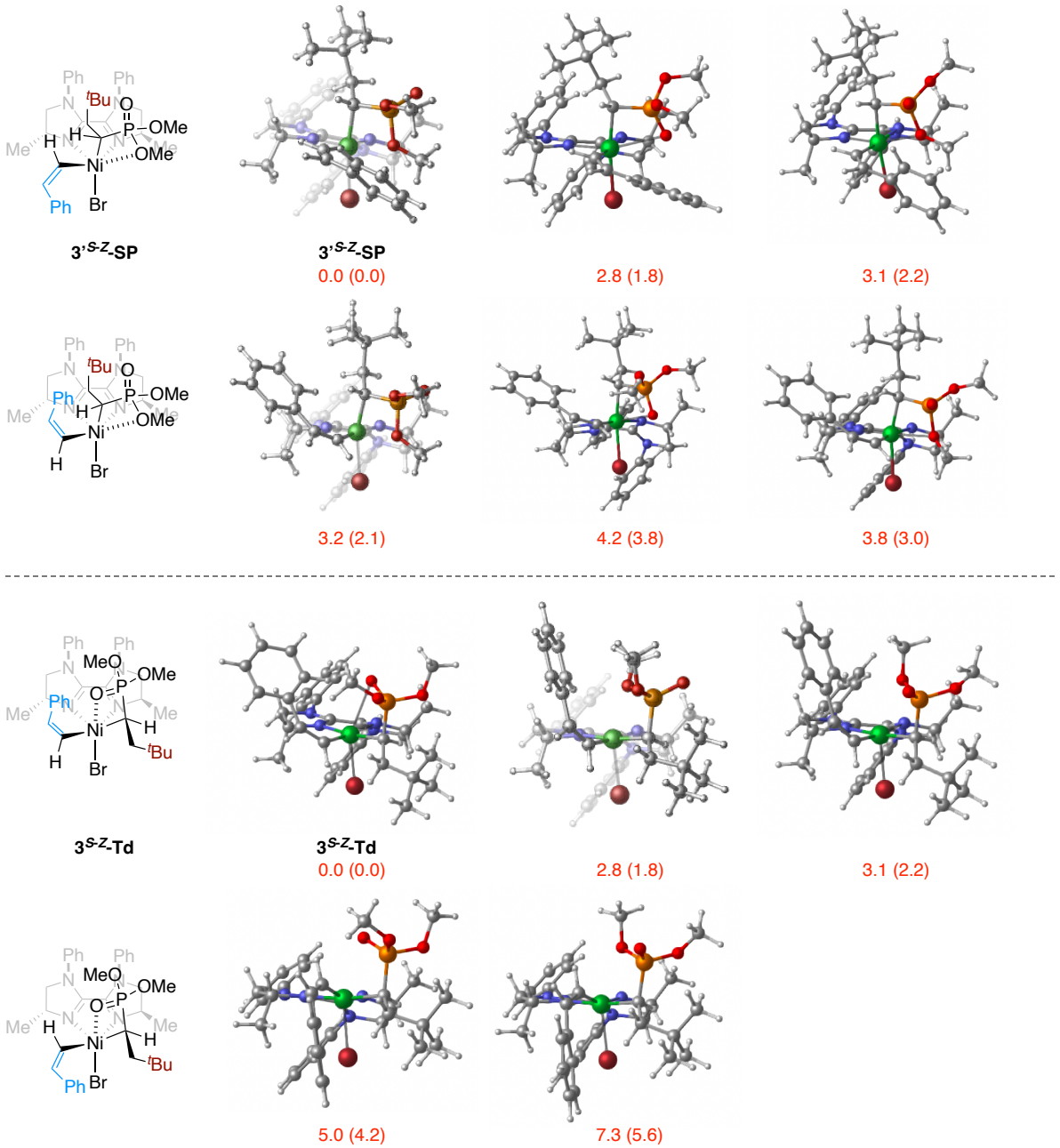


Figure A4.9 Conformational search of Ni(III) intermediates (**3'$^{S\text{-}Z}$-SP** and **3$^{S\text{-}Z}$-Td**) revealing the effect of coordination between directing group P=O and Ni center. Enthalpy and free energy values (in parenthesis) were calculated at the (U)B3LYP-D3(BJ)/def2-SVP (red), (U)B3LYP-D3(BJ)/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (black) and M06/def2-TZVP-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (blue) levels of method.

A4.3 Coordinates and Energies

Figure A4.1

Ir-1

Ir	-0.36515100	0.77492400	0.38784600
C	-0.78190500	3.28591600	1.86569000
C	-1.11443100	3.59956500	-0.41877300
C	-1.06798300	4.62913100	2.09860300
C	-0.45223200	2.32444200	2.93793800
C	-1.41001800	4.94546400	-0.23515300
H	-1.13200100	3.14594300	-1.40933000
C	-1.39354600	5.50317000	1.05062600
H	-1.03132000	5.00308300	3.11959600
C	-0.51311100	2.62797600	4.29608800
H	-1.65451300	5.54228600	-1.11170700
C	0.20769400	0.15569200	3.41998100
C	-0.19985900	1.66373500	5.26722900
H	-0.82060700	3.62437400	4.60697400
C	0.16623900	0.39802500	4.79024100
H	0.48812500	-0.82391300	3.03109400
H	0.41986500	-0.41374500	5.46917200
C	-1.06305500	-2.03847100	0.77605600
C	1.14005500	-1.79953100	-0.02520200
C	-0.90799900	-3.43702100	0.78103200
C	-2.25375800	-1.28368600	1.15041500
C	1.34077400	-3.17222300	-0.03418600
H	1.91912800	-1.11265200	-0.34686600
C	0.29218000	-4.00479200	0.37680300
H	-1.73824700	-4.06321300	1.09477800
C	-2.15841100	0.13173700	1.00988600
C	-3.46655200	-1.83607700	1.60283100
H	0.41430200	-5.08949800	0.36959800
C	-3.26411300	0.92643100	1.32023800
C	-4.56959900	-1.05463900	1.91384100
C	-4.44220400	0.32584400	1.76268000
H	-3.24725800	2.01150500	1.21587600
H	-5.49798500	-1.50817700	2.25931100
C	-0.84230300	0.63940600	-1.56844600
C	0.15766200	1.03445000	-2.50395300
C	-2.08432700	0.20027100	-2.04395300
C	-0.15641100	0.96994000	-3.88093400
C	1.45085100	1.46636900	-1.96477900
C	-2.33735800	0.15746800	-3.41177600
H	-2.88040800	-0.10879200	-1.36820200
C	-1.38530200	0.53928900	-4.35392200
C	2.51259600	1.94696500	-2.76377300
H	-1.58722900	0.50002500	-5.42379100
C	2.79597800	1.69433200	-0.06756800
C	3.72003800	2.29614900	-2.18669000
H	2.37392300	2.03431500	-3.83546300
C	3.87810500	2.15465500	-0.80666600
H	4.54069700	2.66548100	-2.80462400
H	4.81809300	2.39034800	-0.31210200
N	-0.80569700	2.78187500	0.60007200
N	-0.08274400	1.09319000	2.51612200
N	-0.01667400	-1.25208800	0.37442100
N	1.60154400	1.37500500	-0.60906400
C	2.67790900	-3.74062300	-0.43852800
C	2.98507200	1.53485800	1.42942500
F	2.61189300	0.31009600	1.84393100
F	2.27471400	2.44589400	2.11792700
F	4.26439500	1.69355000	1.77771200
F	3.40994500	-4.06262700	0.63997000
F	3.38753000	-2.85467900	-1.15751200
F	2.52993500	-4.85093100	-1.17090200
F	-3.58870500	-3.16310300	1.74934800
F	-5.48914500	1.09688300	2.05462700
F	0.74419500	1.32499600	-4.81280300
F	-3.52711500	-0.26005300	-3.83994100
C	-0.27488900	2.01504300	6.75458200
C	0.69809200	3.17977400	7.03986900
C	-1.71917500	2.44507500	7.09211400
C	0.10688300	0.82273000	7.64408200
H	1.73373500	2.90110800	6.79162500
H	0.44162500	4.08289200	6.46563400
H	0.66232100	3.44448800	8.10753400
H	-2.43379100	1.63495800	6.88035500
H	-1.79466500	2.69610000	8.16101600
H	-2.03146200	3.33216700	6.52057100
H	0.04280100	1.11685200	8.70172400
H	-0.57166700	-0.03175200	7.49860400
H	1.13808300	0.48542700	7.45800100
C	-1.70866800	6.97177500	1.33887200
C	-2.92761400	7.04055100	2.28493500
C	-0.48255800	7.62031100	2.01786400
C	-2.03340400	7.74929200	0.05496400
H	-3.81149300	6.56933100	1.82834000
H	-2.73367400	6.54139000	3.24634700
H	-3.17441700	8.09113500	2.50060800
H	0.40414700	7.56997800	1.36737300
H	-0.69021200	8.68008600	2.22970800
H	-0.23246100	7.13442200	2.97308400
H	-2.25269300	8.79742900	0.30482100
H	-1.18794600	7.74897700	-0.65005300
H	-2.91733400	7.34204400	-0.45929300

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.685068 (Hartree/Particle)
Thermal correction to Energy= 0.735592
Thermal correction to Enthalpy= 0.736536
Thermal correction to Gibbs Free Energy= 0.597190
Sum of electronic and zero-point Energies= -2940.546001
Sum of electronic and thermal Energies= -2940.495477
Sum of electronic and thermal Enthalpies= -2940.494532
Sum of electronic and thermal Free Energies= -2940.633879
HF = -2941.2310683
M06-2X/6-31G(d)-SDD(Ir)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2941.5682497

M06-2X/6-31G(d)-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2941.4876949
Solvent correction = -0.0805548
(U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2944.0947415
M06/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2942.1004359

***Ir-1 (*triplet*)**

Ir	-0.35734600	0.78731400	0.36727600
C	-0.78681200	3.29364700	1.86652800
C	-1.07473400	3.63820900	-0.42053600
C	-1.08103500	4.63322200	2.11124200
C	-0.45738800	2.32402900	2.93366700
C	-1.37346300	4.98175700	-0.22595200
H	-1.07307300	3.19646100	-1.41705900
C	-1.38669200	5.52055400	1.06828100
H	-1.06476700	4.99480400	3.13714000
C	-0.52619500	2.61718800	4.29386600
H	-1.59849900	5.59129400	-1.09893400
C	0.23608700	0.16017300	3.40343400
C	-0.20410800	1.64916500	5.25895300
H	-0.84512700	3.60769000	4.61179100
C	0.18410100	0.39242000	4.77541500
H	0.53436500	-0.81036100	3.00491500
H	0.44813600	-0.41960900	5.45003200
C	-1.06650400	-2.01577700	0.84447500
C	1.15159600	-1.77182800	-0.01959200
C	-0.86829100	-3.43849700	0.90280700
C	-2.22291700	-1.28614100	1.15393300
C	1.35627300	-3.14667600	0.01453300
H	1.93385000	-1.10847300	-0.38322900
C	0.31005700	-4.00349000	0.50562400
H	-1.68415600	-4.05830200	1.26611700
C	-2.14722000	0.17495200	0.98170300
C	-3.47603900	-1.82535000	1.62113500
H	0.45900300	-5.08265300	0.54747300
C	-3.25257400	0.96210800	1.26871300
C	-4.55778100	-1.03238700	1.89530800
C	-4.43652300	0.36754900	1.71549300
H	-3.23756600	2.04505100	1.14250000
H	-5.49394900	-1.47033600	2.24274300
C	-0.84942900	0.63924800	-1.58048100
C	0.15381600	0.99842000	-2.52718600
C	-2.10016700	0.20792500	-2.03926200
C	-0.16458000	0.89545800	-3.90009900
C	1.45406800	1.43187800	-2.00453900
C	-2.35706800	0.12611300	-3.40446800
H	-2.89986100	-0.06220100	-1.35116300
C	-1.40086500	0.46661500	-4.35760700
C	2.51791900	1.87730100	-2.82017400
H	-1.60538900	0.40016100	-5.42572700
C	2.79907400	1.72152200	-0.11593200
C	3.72675900	2.24173000	-2.25486600
H	2.38084500	1.92621700	-3.89448400
C	3.88247900	2.15291700	-0.87033800
H	4.54981800	2.58335800	-2.88538900
H	4.82220700	2.40524100	-0.38349200
N	-0.78938100	2.80790100	0.59409100
N	-0.06973900	1.10020600	2.50769600
N	0.02363700	-1.19792400	0.39438500
N	1.60619500	1.38297800	-0.64788000
C	2.65851900	-3.73432700	-0.44071700
C	2.98330200	1.61420100	1.38623700
F	2.63348700	0.39636400	1.83585200
F	2.24644200	2.53096300	2.03979600
F	4.25573500	1.81412100	1.73636300
F	3.27304300	-4.38569200	0.56219500
F	3.50467700	-2.78949900	-0.89087600
F	2.47248000	-4.62206200	-1.43044400
F	-3.59017300	-3.14943000	1.79238700
F	-5.49513300	1.12802300	1.98650300
F	0.73720300	1.21009100	-4.84374600
F	-3.55307900	-0.28641200	-3.81708000
C	-0.29084500	1.98857400	6.74842400
C	0.66589800	3.16350900	7.04681100
C	-1.74217500	2.39792200	7.08163700
C	0.10156500	0.79480200	7.63130800
H	1.70618000	2.89982700	6.80167400
H	0.40068900	4.06771200	6.47825700
H	0.62165300	3.41954600	8.11625500
H	-2.44540300	1.58026300	6.86082900
H	-1.82594600	2.64016700	8.15192300
H	-2.06298000	3.28518500	6.51505300
H	0.02735100	1.08024500	8.69065100
H	-0.56460300	-0.06754800	7.47548600
H	1.13823400	0.47262200	7.44904300
C	-1.71131700	6.98437600	1.36994900
C	-2.94921000	7.03730400	2.29216300
C	-0.50057100	7.62628200	2.08213400
C	-2.01220400	7.77861700	0.09045400
H	-3.82267600	6.57069900	1.81138900
H	-2.77351300	6.52551900	3.25043200
H	-3.20276900	8.08430200	2.51711200
H	0.39921500	7.58633900	1.44914600
H	-0.71502500	8.68274000	2.30344000
H	-0.26878200	7.12856000	3.03586700
H	-2.23971700	8.82254700	0.35027500
H	-1.15256400	7.79068700	-0.59710000
H	-2.88430400	7.37619000	-0.44730600

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.680971 (Hartree/Particle)
Thermal correction to Energy= 0.732130
Thermal correction to Enthalpy= 0.733074
Thermal correction to Gibbs Free Energy= 0.591379
Sum of electronic and zero-point Energies= -2940.451133
Sum of electronic and thermal Energies= -2940.399973
Sum of electronic and thermal Enthalpies= -2940.399029
Sum of electronic and thermal Free Energies= -2940.540724
HF = -2941.1321035
M06-2X/6-31G(d)-SDD(Ir)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2941.4278747
M06-2X/6-31G(d)-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2941.3436126

Solvent correction = -0.0842621
(U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2943.9959011
M06/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2942.001305

Ir-1 (1e-reduced)

Ir	-0.42722000	0.70895400	0.37693100
C	-0.79761100	3.22223200	1.85055500
C	-1.14316800	3.55040000	-0.46292400
C	-1.11746600	4.58987500	2.06040700
C	-0.45553300	2.30127400	2.88366200
C	-1.44967300	4.88608800	-0.29013400
H	-1.16386400	3.10107800	-1.45578000
C	-1.44271200	5.44394600	1.02462000
H	-1.10121100	4.96278700	3.08379700
C	-0.40447500	2.61250000	4.26841800
H	-1.70009100	5.47785600	-1.16723300
C	0.15333300	0.09131400	3.39198600
C	-0.07672400	1.66234500	5.21940000
H	-0.63711700	3.63061900	4.57764800
C	0.20456000	0.34773200	4.75261900
H	0.37103200	-0.90785000	3.00875600
H	0.45861300	-0.46404000	5.42976200
C	-1.21557500	-2.07425900	0.80730100
C	1.00732000	-1.92382700	0.04081600
C	-1.09943400	-3.47705200	0.86572200
C	-2.39427900	-1.27547900	1.10989400
C	1.16773500	-3.30181300	0.07654500
H	1.80999300	-1.26326800	-0.27974400
C	0.08934000	-4.09115400	0.50351900
H	-1.95320800	-4.06634700	1.18754500
C	-2.24915400	0.13348900	0.91766100
C	-3.64028800	-1.77379000	1.53269500
H	0.18235100	-5.17816100	0.53950500
C	-3.34744400	0.97134700	1.14470700
C	-4.73131600	-0.95116400	1.76031100
C	-4.55549900	0.42017200	1.55642700
H	-3.27715000	2.05058000	1.01105600
H	-5.68595400	-1.36193200	2.08631400
C	-0.77381900	0.58218100	-1.60934800
C	0.23329100	1.10995400	-2.46958100
C	-1.92296200	0.01899900	-2.18740700
C	0.03315200	1.04335200	-3.86350800
C	1.43328700	1.66719100	-1.83528000
C	-2.07017700	-0.01664200	-3.56800900
H	-2.72450200	-0.38966800	-1.57172800
C	-1.10196300	0.48999400	-4.43446800
C	2.37802100	2.46647100	-2.51243900
H	-1.22011300	0.44789300	-5.51643900
C	2.73199700	1.77335000	0.09896100
C	3.50609200	2.92151600	-1.84951800
H	2.20919900	2.72240000	-3.55332000
C	3.70973100	2.54522700	-0.52181500
H	4.23427200	3.54992500	-2.36631400
H	4.60698300	2.83167800	0.02345900
N	-0.82060000	2.72235800	0.54746900
N	-0.14244300	1.01845100	2.47654500
N	-0.13687000	-1.33049800	0.40674800
N	1.59936600	1.38155400	-0.51074600
C	2.48165100	-3.93035300	-0.29459100
C	2.99453600	1.33541700	1.53175900
F	2.58889100	0.07475400	1.74832000
F	2.40589800	2.13598000	2.42510500
F	4.31498100	1.36753200	1.79218300
F	3.14926600	-4.35568900	0.79427300
F	3.28310800	-3.06980100	-0.94368800
F	2.30444600	-5.00311800	-1.08537400
F	-3.80954600	-3.09548700	1.73197900
F	-5.60156400	1.22605000	1.77289700
F	0.96817900	1.50667800	-4.71911800
F	-3.17495500	-0.55529900	-4.09843400
C	-0.02460000	2.04202300	6.70639600
C	1.04107200	3.13941400	6.91038400
C	-1.40418100	2.57296600	7.14851400
C	0.33933800	0.84199000	7.59447900
H	2.03294200	2.78605200	6.58812200
H	0.80514400	4.04616800	6.33374900
H	1.10463900	3.42223700	7.97392800
H	-2.18342700	1.80915400	7.00081900
H	-1.38732300	2.84552300	8.21641800
H	-1.69883600	3.46650600	6.57845400
H	0.36538900	1.15396800	8.65001300
H	-0.39874600	0.03032900	7.50471000
H	1.33039100	0.43449700	7.34290100
C	-1.78610900	6.91360500	1.30560000
C	-3.02730000	6.97968800	2.22041000
C	-0.59233900	7.59424900	2.00755500
C	-2.09357000	7.68799800	0.01436900
H	-3.89115800	6.49066700	1.74395200
H	-2.84827100	6.47881900	3.18351700
H	-3.29740400	8.02773500	2.42998200
H	0.30895500	7.55251800	1.37616300
H	-0.81901200	8.65310400	2.21387000
H	-0.35309600	7.10933700	2.96569300
H	-2.32879300	8.73625500	0.25518400
H	-1.23490000	7.68827400	-0.67449400
H	-2.96002600	7.26622200	-0.51737900

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.681059 (Hartree/Particle)
Thermal correction to Energy= 0.731974
Thermal correction to Enthalpy= 0.732919
Thermal correction to Gibbs Free Energy= 0.591254
Sum of electronic and zero-point Energies= -2940.697266
Sum of electronic and thermal Energies= -2940.646351
Sum of electronic and thermal Enthalpies= -2940.645407
Sum of electronic and thermal Free Energies= -2940.787071
HF = -2941.3783253
M06-2X/6-31G(d)-SDD(Ir)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2941.661248
M06-2X/6-31G(d)-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2941.626597
Solvent correction = -0.0346506
(U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)

HF = -2944.245431
M06/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2942.252106

Ir-1 (1e-oxidized)

Ir	-0.41807100	0.73132200	0.36886500
C	-0.80296200	3.26235500	1.85342900
C	-1.13526800	3.58932200	-0.43302800
C	-1.06760000	4.60854200	2.08793400
C	-0.48030300	2.29792500	2.92393600
C	-1.40772600	4.93793500	-0.24585100
H	-1.16531400	3.14584000	-1.42724500
C	-1.38005500	5.49352000	1.04251200
H	-1.02588500	4.98083900	3.10910400
C	-0.48898200	2.61173000	4.27940300
H	-1.64609700	5.54228900	-1.11913500
C	0.12755800	0.10715800	3.40710800
C	-0.17209500	1.64606200	5.25113600
H	-0.75068900	3.61989100	4.59328000
C	0.13991200	0.36383400	4.77324700
H	0.37091100	-0.88391900	3.02285400
H	0.39618600	-0.44655700	5.45300900
C	-1.11605500	-2.06920200	0.78030600
C	1.11731300	-1.82410800	0.04076400
C	-0.94820800	-3.46682900	0.82680100
C	-2.32037700	-1.32025700	1.08641600
C	1.32364800	-3.19326500	0.06987100
H	1.90288400	-1.13975900	-0.26988300
C	0.26927600	-4.02852000	0.47220400
H	-1.77942900	-4.09611700	1.13355600
C	-2.22337500	0.10358100	0.94085800
C	-3.55271800	-1.87054600	1.50094800
H	0.40363100	-5.11209800	0.49692400
C	-3.32968100	0.90931500	1.20280400
C	-4.65766900	-1.07738800	1.75969100
C	-4.52362400	0.31063200	1.60434700
H	-3.30337700	1.99331300	1.09495100
H	-5.60336000	-1.52085400	2.07360100
C	-0.86810700	0.61661900	-1.57112600
C	0.13686300	1.08253400	-2.48653000
C	-2.07494200	0.09333100	-2.07232600
C	-0.12558900	0.96161100	-3.86342800
C	1.39921600	1.58105200	-1.92429400
C	-2.28513800	0.01056400	-3.44210100
H	-2.87590000	-0.23370800	-1.41127600
C	-1.31838800	0.43893800	-4.35795400
C	2.40570200	2.20086400	-2.69163400
H	-1.48529200	0.37039900	-5.43401000
C	2.72724100	1.77888600	-0.01486100
C	3.58660500	2.60879200	-2.08862100
H	2.25671400	2.35435800	-3.75542600
C	3.76490700	2.37576200	-0.72515900
H	4.37013500	3.08910000	-2.67793400
H	4.69135000	2.64086700	-0.21767400
N	-0.83777800	2.76266300	0.58451600
N	-0.16229500	1.04968100	2.50362100
N	-0.05885100	-1.27861800	0.39636500
N	1.56137500	1.40952200	-0.57985100
C	2.67705000	-3.76773000	-0.29841800
C	2.93904700	1.51807400	1.46724800
F	2.53153800	0.27603400	1.79823800
F	2.24966500	2.39422900	2.21753700
F	4.21970500	1.62345900	1.79829300
F	3.32610000	-4.16599100	0.79954000
F	3.43124500	-2.84691100	-0.91843000
F	2.53698300	-4.81816400	-1.10685900
F	-3.67686000	-3.18697700	1.65029100
F	-5.57308700	1.07241500	1.85030800
F	0.77494200	1.33742600	-4.76993900
F	-3.42325600	-0.47700700	-3.90066200
C	-0.17898000	2.01195300	6.73389600
C	0.85037900	3.14190200	6.96409400
C	-1.59329700	2.50426900	7.11562500
C	0.18866000	0.81349300	7.62090900
H	1.86449700	2.82137700	6.68065100
H	0.60502500	4.05110000	6.39438300
H	0.86593900	3.41476100	8.02961700
H	-2.34817900	1.72196400	6.94280100
H	-1.61617000	2.76712600	8.18349000
H	-1.89030900	3.40048400	6.54995300
H	0.17268900	1.12025700	8.67621200
H	-0.52734300	-0.01555200	7.51118700
H	1.20040200	0.43651200	7.40612800
C	-1.67047100	6.96383100	1.33321100
C	-2.88843500	7.04526500	2.28164100
C	-0.43106600	7.58536600	2.01626400
C	-1.98169200	7.74919100	0.05086100
H	-3.78153900	6.59240700	1.82458900
H	-2.70162000	6.54431100	3.24366500
H	-3.11635700	8.09934900	2.49816800
H	0.45572300	7.52362400	1.36704300
H	-0.62219600	8.64759000	2.22848000
H	-0.19237700	7.09646600	2.97298700
H	-2.18245800	8.79962300	0.30428100
H	-1.13592500	7.73953300	-0.65390300
H	-2.87447500	7.36184600	-0.46374200

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.684084 (Hartree/Particle)
Thermal correction to Energy= 0.734890
Thermal correction to Enthalpy= 0.735834
Thermal correction to Gibbs Free Energy= 0.595050
Sum of electronic and zero-point Energies= -2940.189982
Sum of electronic and thermal Energies= -2940.139176
Sum of electronic and thermal Enthalpies= -2940.138232
Sum of electronic and thermal Free Energies= -2940.279016
HF = -2940.874066
M06-2X/6-31G(d)-SDD(Ir)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2941.333999
M06-2X/6-31G(d)-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2941.118847
Solvent correction = -0.2151511
(U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2943.735436
M06/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)

HF = -2941.74077

Ir-2

Ir	-0.55272700	0.79617900	0.34612100
C	-0.83103500	3.28850500	1.86554800
C	-1.38726800	3.60325100	-0.38786600
C	-1.10199600	4.62895200	2.13861000
C	-0.39269100	2.32437300	2.89284200
C	-1.67413800	4.94699800	-0.17484300
H	-1.49008300	3.14001800	-1.36902600
C	-1.52872700	5.47296800	1.11271400
H	-0.99204700	5.04343700	3.14018800
C	-0.23370300	2.64579500	4.24206500
H	-2.00833900	5.57549800	-0.99951700
C	0.21627200	0.10828100	3.30593000
C	0.16400400	1.65375300	5.14020300
H	-0.41676100	3.64933900	4.62508300
C	0.39058600	0.35729400	4.66427200
H	0.37209800	-0.88533300	2.88170100
H	0.69273300	-0.43931700	5.34322400
C	-1.33264000	-2.01377100	0.53964900
C	0.92469500	-1.81319500	-0.10127400
C	-1.22356600	-3.41196900	0.47790300
C	-2.53675700	-1.26049700	0.88532100
C	1.08182300	-3.18999900	-0.17585800
H	1.74272700	-1.13133600	-0.33236500
C	-0.01793500	-4.00366000	0.12151600
H	-2.09440000	-4.02607500	0.70448400
C	-2.39837100	0.15199600	0.84450800
C	-3.76251800	-1.86083500	1.22235900
H	0.06633700	-5.09111000	0.06928700
C	-3.52524300	0.92633900	1.15455100
C	-4.86593900	-1.06763500	1.52399200
C	-4.74349800	0.32748200	1.48933700
H	-3.46572100	2.01730800	1.12892000
H	-5.81949900	-1.53111200	1.78397800
C	-0.86344400	0.74946400	-1.65474800
C	0.25996900	1.09698200	-2.45648900
C	-2.05565000	0.41364700	-2.31444400
C	0.16695100	1.10753200	-3.86083100
C	1.49445000	1.44827100	-1.74360700
C	-2.14124400	0.42697700	-3.70979100
H	-2.93529900	0.13899300	-1.72933500
C	-1.02986100	0.77427000	-4.48760300
C	2.70148000	1.84341300	-2.34681900
H	-1.09826100	0.78246500	-5.57718200
C	2.47978600	1.67993900	0.37601600
C	3.80274400	2.15669000	-1.55842900
H	2.76901500	1.90530900	-3.43222800
C	3.69665100	2.07658900	-0.16438700
H	4.74105900	2.46381800	-2.02534000
H	4.53640500	2.31619200	0.48898300
N	-0.97601600	2.79224200	0.60404000
N	-0.15597100	1.06638200	2.44649900
N	-0.24092300	-1.24253900	0.25438700
N	1.41948600	1.37283700	-0.38688100
H	2.04410500	-3.61132800	-0.46843500
H	-3.86204600	-2.94805500	1.24847300
H	-5.60868000	0.95307900	1.72355200
H	1.03069600	1.37486800	-4.47285100
H	-3.08336800	0.16194700	-4.19649200
H	2.33627800	1.59713700	1.45585000
C	0.32087400	2.03829800	6.58408400
O	0.12882900	3.15840500	6.98887300
O	0.69129500	1.00410200	7.33873300
C	-1.81083300	6.90776900	1.45520500
O	-1.67553700	7.35498000	2.56766000
O	-2.21992400	7.60256400	0.39437700
C	-2.52099200	8.98875100	0.61526200
H	-1.63030200	9.51805200	0.98283600
H	-2.83601800	9.38767000	-0.35509100
H	-3.32610700	9.08986200	1.35698100
C	0.86405600	1.26529700	8.73986000
H	1.16342900	0.31256700	9.19005300
H	1.64052800	2.02850800	8.89217300
H	-0.07780800	1.62373700	9.17911400

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.569675 (Hartree/Particle)
Thermal correction to Energy= 0.607464
Thermal correction to Enthalpy= 0.608408
Thermal correction to Gibbs Free Energy= 0.497022
Sum of electronic and zero-point Energies= -2011.543529
Sum of electronic and thermal Energies= -2011.505740
Sum of electronic and thermal Enthalpies= -2011.504796
Sum of electronic and thermal Free Energies= -2011.616182
HF = -2012.113204
M06-2X/6-31G(d)-SDD(Ir)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.105145
M06-2X/6-31G(d)-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.015642
Solvent correction = -0.0895029
M06-2X/6-31G(d)-SDD(Ir)-SMD(DCE)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.09781
Solvent correction (DCE) = -0.0821674
(U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2013.86835
M06/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.25954

***Ir-2 (*triplet*)**

Ir	-0.76561400	0.72851100	0.38094900
C	-0.87418800	3.24080100	1.85238300
C	-1.60473900	3.54798500	-0.38718600
C	-1.08269000	4.61268000	2.09673300
C	-0.40114700	2.30362500	2.83089100
C	-1.82302300	4.89399600	-0.18864000
H	-1.79589400	3.07230600	-1.34950500
C	-1.55186300	5.44351500	1.09501500
H	-0.87766200	5.04488300	3.07601000
C	-0.13794500	2.61648000	4.17678500
H	-2.19451700	5.52144400	-0.99641900
C	0.19476700	0.03649000	3.26371000
C	0.29761800	1.64068700	5.05749400
H	-0.27402600	3.62977700	4.55520700

C	0.46293000	0.29958600	4.58326900
H	0.30239200	-0.96844200	2.85124700
H	0.79172400	-0.48919700	5.25697400
C	-1.54394700	-2.08472500	0.52455400
C	0.74987200	-1.89194200	0.04645300
C	-1.44576600	-3.48132300	0.48766600
C	-2.76158200	-1.30952600	0.77000500
C	0.90249700	-3.27326200	-0.00462000
H	1.58388900	-1.21116700	-0.12766600
C	-0.21686400	-4.07984400	0.22336400
H	-2.33180800	-4.09108000	0.66212000
C	-2.59238500	0.11622900	0.74482000
C	-4.01652600	-1.87039700	1.01536500
H	-0.13183400	-5.16785600	0.19091700
C	-3.72392900	0.93142700	0.98378200
C	-5.11756500	-1.03647300	1.23898800
C	-4.96922300	0.36147700	1.22412000
H	-3.61611600	2.01697200	0.97662300
H	-6.09818500	-1.47739500	1.42954500
C	-0.81540900	0.67245900	-1.65906500
C	0.33370500	1.14627200	-2.34017500
C	-1.89368200	0.19685400	-2.42271800
C	0.36852900	1.16953200	-3.74492400
C	1.46298500	1.58163900	-1.50807900
C	-1.85225500	0.22971300	-3.81937800
H	-2.78952100	-0.17984500	-1.92664900
C	-0.72178800	0.71753300	-4.48381600
C	2.65797000	2.13720600	-1.99113000
H	-0.68924600	0.73902200	-5.57474900
C	2.24470800	1.78289600	0.69324000
C	3.65377700	2.51765000	-1.09732200
H	2.79882800	2.27633000	-3.06216200
C	3.44868700	2.33747900	0.27420700
H	4.58390100	2.95489100	-1.46651000
H	4.20255200	2.62272000	1.00885200
N	-1.14823200	2.73309200	0.59243500
N	-0.21166400	0.99512500	2.39083200
N	-0.43462900	-1.32162400	0.31386000
N	1.28860200	1.41335400	-0.17199900
H	1.88089100	-3.70269900	-0.22280700
H	-4.15384900	-2.95299900	1.03687500
H	-5.83720900	0.99938900	1.40428800
H	1.25256500	1.53451500	-4.27048200
H	-2.71138600	-0.12704900	-4.39281300
H	2.02904900	1.62223400	1.74987600
C	0.56614000	2.04153700	6.46529800
O	0.43297100	3.16850500	6.88503500
O	0.97506900	1.00513700	7.21356100
C	-1.74893400	6.88681100	1.42031800
O	-1.51700300	7.37086200	2.50349100
O	-2.21234500	7.57873500	0.37041500
C	1.25684500	1.29194000	8.58661400
H	0.36054800	1.68096000	9.09136500
H	1.57113800	0.34363200	9.03736100
H	2.05686400	2.04217400	8.66817100
C	-2.43594200	8.97630500	0.58394000
H	-2.80928400	9.37310700	-0.36694400
H	-3.17472700	9.13045200	1.38377300
H	-1.49974000	9.47685300	0.87081800

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.566929 (Hartree/Particle)
Thermal correction to Energy= 0.605157
Thermal correction to Enthalpy= 0.606101
Thermal correction to Gibbs Free Energy= 0.492845
Sum of electronic and zero-point Energies= -2011.471723
Sum of electronic and thermal Energies= -2011.433495
Sum of electronic and thermal Enthalpies= -2011.432551
Sum of electronic and thermal Free Energies= -2011.545807
HF = -2012.038652
M06-2X/6-31G(d)-SDD(Ir)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.017946
M06-2X/6-31G(d)-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2011.927692
Solvent correction = -0.0902535
M06-2X/6-31G(d)-SDD(Ir)-SMD(DCE)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.010854
Solvent correction = -0.0831623
(U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2013.794021
M06/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.183535

Ir-2 (1e-reduced)

Ir	-0.63931400	0.75677900	0.34069800
C	-0.86060900	3.25629200	1.86431500
C	-1.48985500	3.58306600	-0.39436200
C	-1.11017800	4.61524600	2.12119200
C	-0.41890000	2.31499300	2.86083400
C	-1.75127500	4.92055400	-0.18955100
H	-1.62786700	3.12005300	-1.37158400
C	-1.55269800	5.46077700	1.11517300
H	-0.96331200	5.02911000	3.11848600
C	-0.17673700	2.63642800	4.20866200
H	-2.10103100	5.54792200	-1.00681100
C	0.14161400	0.06555600	3.30242700
C	0.23050000	1.65875500	5.10501300
H	-0.30732900	3.65387200	4.57671800
C	0.38878700	0.32029200	4.63591300
H	0.24336900	-0.94222700	2.89264000
H	0.69128300	-0.47616400	5.31271000
C	-1.43450500	-2.05016900	0.54149400
C	0.84141000	-1.86637200	-0.02739100
C	-1.32471700	-3.45078000	0.51563900
C	-2.64495000	-1.28679700	0.82919000
C	1.00094600	-3.24508000	-0.06628800
H	1.66673100	-1.18677900	-0.24201300
C	-0.10907000	-4.05141200	0.21411100
H	-2.20357500	-4.05797600	0.73059500
C	-2.49078200	0.12664300	0.77458600
C	-3.88668300	-1.87660400	1.12952200
H	-0.02396100	-5.14015000	0.19287300
C	-3.62823900	0.91022900	1.03595900
C	-4.99439200	-1.07412300	1.38029600
C	-4.85844300	0.32209600	1.33300100

H	-3.55016000	1.99927000	1.00663800
H	-5.96025900	-1.52745600	1.61365400
C	-0.84995000	0.72870900	-1.67414900
C	0.30268000	1.11742400	-2.41696400
C	-1.99263500	0.36370800	-2.40856500
C	0.28587800	1.14063800	-3.82427300
C	1.48813100	1.49772700	-1.63689400
C	-2.00428000	0.38840100	-3.80472800
H	-2.89442600	0.06051800	-1.87191000
C	-0.86341900	0.77820900	-4.51960700
C	2.70289900	1.96384800	-2.17038100
H	-0.87338600	0.79740300	-5.61171100
C	2.35750700	1.71332900	0.53371500
C	3.74931600	2.30465300	-1.32041300
H	2.81670600	2.06476400	-3.24919700
C	3.57999500	2.18059400	0.06332800
H	4.69240300	2.67095800	-1.73263300
H	4.37254800	2.44474200	0.76468600
N	-1.05535000	2.75630500	0.58393400
N	-0.23209600	1.01700100	2.42494800
N	-0.33235100	-1.28618300	0.27532400
N	1.35424700	1.37894500	-0.28857300
H	1.97288900	-3.67279000	-0.31503400
H	-3.99165800	-2.96366200	1.16772800
H	-5.72678500	0.95635600	1.53253000
H	1.17391300	1.44125400	-4.38507100
H	-2.91119500	0.10173600	-4.34473200
H	2.15675700	1.59801400	1.60123900
C	0.47207600	2.05746800	6.51038300
O	0.35313800	3.18282500	6.94593400
O	0.84996400	1.01161200	7.27915800
C	-1.79757600	6.88104100	1.45223300
O	-1.63490400	7.37540600	2.54763400
O	-2.23185700	7.58994400	0.38654600
C	-2.49527800	8.96824800	0.62334100
H	-1.58810400	9.48830000	0.96767000
H	-2.83392900	9.38576300	-0.33304200
H	-3.27369800	9.09310300	1.39171100
C	1.09701300	1.30636600	8.64943800
H	0.19513400	1.71265800	9.13252500
H	1.38738300	0.35912900	9.12074600
H	1.90403400	2.04799700	8.75280300

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.566259 (Hartree/Particle)
Thermal correction to Energy= 0.604214
Thermal correction to Enthalpy= 0.605158
Thermal correction to Gibbs Free Energy= 0.493009
Sum of electronic and zero-point Energies= -2011.708859
Sum of electronic and thermal Energies= -2011.670904
Sum of electronic and thermal Enthalpies= -2011.669959
Sum of electronic and thermal Free Energies= -2011.782109
HF = -2012.275118
M06-2X/6-31G(d)-SDD(Ir)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.215966
M06-2X/6-31G(d)-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.168551
Solvent correction = -0.0474149
M06-2X/6-31G(d)-SDD(Ir)-SMD(DCE)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.210782
Solvent correction = -0.0422306
(U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2014.033219
M06/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2012.424332

Ir-2 (1e-oxidized)

Ir	-0.68978700	0.73038400	0.35526600
C	-0.87345800	3.24755500	1.85973100
C	-1.50867300	3.55990000	-0.37782700
C	-1.09021000	4.59838600	2.12616700
C	-0.41683700	2.28435600	2.88413500
C	-1.74220700	4.91622900	-0.16907400
H	-1.66132000	3.09399600	-1.35149000
C	-1.52878500	5.44585700	1.10618500
H	-0.92863800	5.02599300	3.11575200
C	-0.18418700	2.62876600	4.21580600
H	-2.08640700	5.55046900	-0.98587700
C	0.16565500	0.05851600	3.32250600
C	0.23744400	1.64716000	5.11640600
H	-0.32217400	3.64357400	4.58941200
C	0.41562500	0.33541700	4.66408200
H	0.28421200	-0.94777700	2.91624200
H	0.73921600	-0.44933500	5.34770700
C	-1.44776900	-2.08252100	0.48933200
C	0.83680100	-1.85843700	-0.03346900
C	-1.33589900	-3.47801200	0.42814200
C	-2.66855400	-1.33001100	0.76326500
C	0.99812800	-3.23768700	-0.11114000
H	1.66346200	-1.17242000	-0.21915100
C	-0.10809000	-4.06065000	0.12714000
H	-2.21196900	-4.10017100	0.60944500
C	-2.51250300	0.10503200	0.75705500
C	-3.91384500	-1.91035800	1.01564900
H	-0.01329100	-5.14700900	0.07217600
C	-3.65307300	0.90127100	1.02638000
C	-5.01881100	-1.09193100	1.26613700
C	-4.88504500	0.31424700	1.27214300
H	-3.56856900	1.98911300	1.03094800
H	-5.99364200	-1.54393700	1.46066000
C	-0.86883100	0.67304500	-1.65531000
C	0.26406800	1.13391000	-2.38732800
C	-1.98222700	0.20498900	-2.37326100
C	0.24061600	1.14597000	-3.79111200
C	1.43829800	1.54470600	-1.60691300
C	-1.99697400	0.22922700	-3.76874500
H	-2.86555800	-0.14882000	-1.83900800
C	-0.88532400	0.69976800	-4.48080300
C	2.62959700	2.05739700	-2.14384400
H	-0.89755600	0.71509900	-5.57214400
C	2.31736700	1.75100000	0.56098500
C	3.67234400	2.41880100	-1.29656400
H	2.73473600	2.17503000	-3.22160000
C	3.51818400	2.26393200	0.08595300
H	4.60079800	2.81906800	-1.70923100

H	4.31294400	2.53214900	0.78317600
N	-1.08747100	2.74985900	0.60905800
N	-0.23330400	1.00667000	2.46294600
N	-0.34757600	-1.30091000	0.27069000
N	1.31420800	1.39740800	-0.25971000
H	1.97495100	-3.65430200	-0.36039800
H	-4.04121100	-2.99399700	1.01961200
H	-5.76070800	0.93611300	1.47039100
H	1.10576200	1.49310100	-4.35792500
H	-2.88377600	-0.11259200	-4.30740400
H	2.14949000	1.60719800	1.62967000
C	0.47474000	2.07076000	6.54599000
O	0.31807000	3.20971700	6.90692700
O	0.86084900	1.05379900	7.30270300
C	-1.74792500	6.89822100	1.45234400
O	-1.54990800	7.32553800	2.56172400
O	-2.16888500	7.59486700	0.40675800
C	-2.41506200	9.00078400	0.61985000
H	-2.75044000	9.39521300	-0.34478400
H	-3.18916400	9.13334100	1.38827300
H	-1.49132900	9.49761400	0.94718400
C	1.11442100	1.34030400	8.69445600
H	0.20219500	1.72707100	9.16932300
H	1.41678500	0.38954900	9.14521800
H	1.91400000	2.08865200	8.78333500

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.569091 (Hartree/Particle)
Thermal correction to Energy= 0.607200
Thermal correction to Enthalpy= 0.608144
Thermal correction to Gibbs Free Energy= 0.495373
Sum of electronic and zero-point Energies= -2011.202411
Sum of electronic and thermal Energies= -2011.164302
Sum of electronic and thermal Enthalpies= -2011.163358
Sum of electronic and thermal Free Energies= -2011.276129
HF = -2011.7715018
M06-2X/6-31G(d)-SDD(Ir)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2011.885229
M06-2X/6-31G(d)-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2011.664709
Solvent correction = -0.2205195
M06-2X/6-31G(d)-SDD(Ir)-SMD(DCE)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2011.870046
Solvent correction = -0.2053372
(U)B3LYP-D3(BJ)/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2013.524587
M06/def2-TZVP-SDD(Ir)//(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
HF = -2011.914038

***trans*-styrenyl bromide**

C	-1.10729500	1.86773600	1.23199600
C	-0.49219600	2.23837900	2.36293400
H	0.06790700	1.48044600	2.91917100
Br	-1.04705200	0.09899500	0.56158300
C	-0.49055700	3.58611300	2.94873900
C	0.20974200	3.79606100	4.15139200
C	-1.15579500	4.68450800	2.36804500
C	0.24652500	5.05404000	4.75473500
H	0.73170100	2.95550400	4.61603900
C	-1.11913900	5.93975800	2.96994300
H	-1.70846500	4.55763000	1.43512000
C	-0.41805400	6.13216900	4.16656900
H	0.79700700	5.19184800	5.68841400
H	-1.64184900	6.77791200	2.50281300
H	-0.39169300	7.11842900	4.63556200
H	-1.69201100	2.53541700	0.59853300

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.123877 (Hartree/Particle)
Thermal correction to Energy= 0.131941
Thermal correction to Enthalpy= 0.132886
Thermal correction to Gibbs Free Energy= 0.088863
Sum of electronic and zero-point Energies= -2882.605180
Sum of electronic and thermal Energies= -2882.597115
Sum of electronic and thermal Enthalpies= -2882.596171
Sum of electronic and thermal Free Energies= -2882.640194
HF = -2882.7290566
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.694109
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.680742
Solvent correction = -0.0133668
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2883.376714
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2882.970137

***trans*-styrenyl bromide (*triplet*)**

C	-0.90070700	1.93184900	1.06072200
C	-0.21872600	2.30445500	2.28147800
H	0.40582000	1.54903700	2.78067400
Br	-2.62024200	1.12056800	1.14662900
C	-0.35401100	3.56500100	2.92440100
C	0.34989500	3.83754500	4.13269600
C	-1.18654900	4.59347900	2.39571200
C	0.23133400	5.06625900	4.76702900
H	0.99016200	3.05954100	4.55650200
C	-1.29836500	5.81823500	3.03958900
H	-1.74248400	4.39839700	1.47643600
C	-0.59208700	6.06623200	4.22660900
H	0.78068200	5.25485400	5.69264800
H	-1.94364300	6.59362200	2.61935600
H	-0.68492900	7.03158500	4.72923900
H	-0.42737600	1.82428700	0.08186900

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.120051 (Hartree/Particle)
Thermal correction to Energy= 0.128516
Thermal correction to Enthalpy= 0.129460

Thermal correction to Gibbs Free Energy= 0.083789
Sum of electronic and zero-point Energies= -2882.530042
Sum of electronic and thermal Energies= -2882.521577
Sum of electronic and thermal Enthalpies= -2882.520633
Sum of electronic and thermal Free Energies= -2882.566304
HF = -2882.6500929
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.606203
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.593482
Solvent correction = -0.0127212
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2883.297099
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2882.891168

***trans*-styrenyl bromide (1e-reduced)**

C	-1.37380500	1.76157400	1.39800900
C	-0.57371000	2.20898200	2.43823600
H	0.03470400	1.45909500	2.96278300
Br	-0.62273900	0.29361500	0.15750100
C	-0.51177700	3.53481800	2.97177500
C	0.19083700	3.79996500	4.19277400
C	-1.14417500	4.67419000	2.36987100
C	0.25538800	5.06757600	4.75276900
H	0.69185000	2.96269000	4.69094000
C	-1.07258900	5.93794700	2.93912500
H	-1.68385900	4.53988500	1.42880700
C	-0.37835000	6.16817100	4.14209900
H	0.81196100	5.21168100	5.68639700
H	-1.56798400	6.77577200	2.43394300
H	-0.33462200	7.16551000	4.58807600
H	-1.93235400	2.45347400	0.75848400

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.119480 (Hartree/Particle)
Thermal correction to Energy= 0.128032
Thermal correction to Enthalpy= 0.128976
Thermal correction to Gibbs Free Energy= 0.083354
Sum of electronic and zero-point Energies= -2882.605198
Sum of electronic and thermal Energies= -2882.596646
Sum of electronic and thermal Enthalpies= -2882.595701
Sum of electronic and thermal Free Energies= -2882.641324
HF = -2882.7246777
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.742689
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.666274
Solvent correction = -0.0764144
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2883.380784
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2882.97026

***cis*-styrenyl bromide**

C	-1.21958500	2.20174900	1.20072100
C	-0.49539000	2.12528500	2.32868500
H	-0.42195800	3.09129900	2.84302400
Br	-1.63501100	0.82125300	-0.03149700
C	0.21346800	1.04308900	3.01912100
C	0.87814400	1.37383500	4.21932000
C	0.28031100	-0.29429200	2.57646700
C	1.57978000	0.41660000	4.94933400
H	0.83861200	2.40514600	4.57986800
C	0.98316800	-1.25066900	3.30874800
H	-0.21894200	-0.58819700	1.65588900
C	1.63550900	-0.90410400	4.49572300
H	2.08480700	0.70195900	5.87526700
H	1.02117400	-2.28080300	2.94614500
H	2.18408400	-1.65925300	5.06370800
H	-1.65974300	3.14801900	0.88460500

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.124343 (Hartree/Particle)
Thermal correction to Energy= 0.132134
Thermal correction to Enthalpy= 0.133078
Thermal correction to Gibbs Free Energy= 0.089156
Sum of electronic and zero-point Energies= -2882.603601
Sum of electronic and thermal Energies= -2882.595810
Sum of electronic and thermal Enthalpies= -2882.594866
Sum of electronic and thermal Free Energies= -2882.638787
HF = -2882.7279435
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.692656
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.6801998
Solvent correction = -0.0124557
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2883.375185
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2882.96816

***cis*-styrenyl bromide (1e-reduced)**

C	-0.89828900	2.18764700	1.10691800
C	-0.37614000	2.24928600	2.34397000
H	-0.43357700	3.19463000	2.91831800
Br	-2.41255600	0.27664400	0.15657300
C	0.29541800	1.16080500	3.05893800
C	0.90456200	1.39276900	4.31078900
C	0.35275300	-0.15333600	2.53695200
C	1.55401900	0.37244200	5.00882500
H	0.86359200	2.40109200	4.73631800
C	0.99743000	-1.16897000	3.23891300
H	-0.15110500	-0.35131100	1.58719000
C	1.60780600	-0.91986600	4.47719200
H	2.02044600	0.58747100	5.97601600

H	1.02023500	-2.17882400	2.81665600
H	2.11335400	-1.72372500	5.02072000
H	-1.40952100	3.02416400	0.62083900

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.120000 (Hartree/Particle)
Thermal correction to Energy= 0.128608
Thermal correction to Enthalpy= 0.129553
Thermal correction to Gibbs Free Energy= 0.083407
Sum of electronic and zero-point Energies= -2882.607165
Sum of electronic and thermal Energies= -2882.598556
Sum of electronic and thermal Enthalpies= -2882.597612
Sum of electronic and thermal Free Energies= -2882.643757
HF = -2882.7271643
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.748997
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2880.670694
Solvent correction = -0.078303
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -2883.386207

***tert*-Bu-BF$_3$K**

C	-2.54437600	0.45507500	-0.04489900
C	-1.01060700	0.56097200	-0.04194800
H	-3.01122400	1.45327500	-0.06779900
H	-2.90241900	-0.09996800	-0.92728900
H	-2.91388500	-0.06911700	0.85558800
C	-0.39450400	-0.84745000	-0.01995900
C	-0.54842100	1.34740300	1.19565800
H	0.70664700	-0.79932200	-0.02453500
H	-0.70347900	-1.40842700	0.88117100
H	-0.70560300	-1.43089700	-0.90183100
H	-0.86179700	0.84779600	2.13074000
H	0.54936700	1.44358100	1.21787700
H	-0.97166400	2.36510900	1.20047800
B	-0.53123000	1.32689700	-1.36418800
F	0.90123000	1.48682800	-1.47255700
F	-0.91068100	0.67764300	-2.59848500
F	-1.04969200	2.66970700	-1.49513700
K	0.30050200	2.65357300	-3.65517100

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.133547 (Hartree/Particle)
Thermal correction to Energy= 0.144811
Thermal correction to Enthalpy= 0.145756
Thermal correction to Gibbs Free Energy= 0.096812
Sum of electronic and zero-point Energies= -1081.880763
Sum of electronic and thermal Energies= -1081.869498
Sum of electronic and thermal Enthalpies= -1081.868554
Sum of electronic and thermal Free Energies= -1081.917498
HF = -1082.0143098
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1082.186388
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1082.165355
Solvent correction = -0.0210331
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1082.658096
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1082.349045

***tert*-Bu-BF$_3$K (1e-oxidized)**

C	-2.44388300	0.61887200	-0.33360200
C	-1.02627500	0.45383300	0.14337800
H	-2.73864100	1.67659400	-0.40713500
H	-2.62552600	0.10236500	-1.28819800
H	-3.12007200	0.15393700	0.41047900
C	-0.45049000	-0.93160000	0.06549000
C	-0.61097500	1.29872300	1.31418700
H	0.62888100	-0.94616400	0.26983100
H	-0.93970300	-1.55113700	0.84405400
H	-0.64609300	-1.41513600	-0.90234100
H	-1.11503000	0.90333900	2.21911900
H	0.47105800	1.25166400	1.49865200
H	-0.91820300	2.34876200	1.20578500
B	0.05937600	1.40321300	-1.41164300
F	1.30556900	1.25834400	-0.99672200
F	-0.35000400	0.69353800	-2.50898700
F	-0.48876200	2.65815100	-1.40581700
K	-1.59306000	2.65538200	-3.84881200

(U)B3LYP-D3(BJ)/def2-SVP-LANL2DZ(Ir)
Zero-point correction= 0.131964 (Hartree/Particle)
Thermal correction to Energy= 0.144427
Thermal correction to Enthalpy= 0.145371
Thermal correction to Gibbs Free Energy= 0.091751
Sum of electronic and zero-point Energies= -1081.612349
Sum of electronic and thermal Energies= -1081.599886
Sum of electronic and thermal Enthalpies= -1081.598942
Sum of electronic and thermal Free Energies= -1081.652561
HF = -1081.7443129
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1081.971002
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1081.893911
Solvent correction = -0.0770909
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1082.387386
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1082.080342

Figure A4.2
***E*-product**

C	-1.31750800	1.50693100	2.99463800
C	-1.10086000	0.19023400	3.14332700

H	-1.24307000	-0.45531400	2.26837200
H	-1.20500600	2.18790300	3.84320800
C	-0.68013000	-0.50694200	4.36471200
C	-0.50894200	-1.90346500	4.33048200
C	-0.43008000	0.15872700	5.58161700
C	-0.10648800	-2.61178500	5.46378700
H	-0.69718500	-2.43774000	3.39525600
C	-0.02698000	-0.54665600	6.71290200
H	-0.55254100	1.24172600	5.64282300
C	0.13701200	-1.93618400	6.66160100
H	0.01815800	-3.69611300	5.41054000
H	0.16158000	-0.00923400	7.64560100
H	0.45299900	-2.48623000	7.55106200
C	-1.03605200	3.43501300	1.30949000
H	-1.14116300	4.17219200	2.12329500
C	-1.77507700	2.14404000	1.71847800
H	-1.71100700	1.41040400	0.89709000
H	-1.57756800	3.85323100	0.44604900
O	-4.15431300	3.11866400	0.55685800
O	-3.65839300	3.38114400	3.14532600
O	-4.30152000	1.13045000	2.24241300
P	-3.56723100	2.50976200	1.78382800
C	0.46139100	3.31255400	0.93148000
C	0.67441100	2.18687200	-0.09257100
H	1.71650100	2.18139200	-0.45016400
H	0.47395200	1.19631300	0.34460700
H	0.01868800	2.31462100	-0.96972700
C	1.34164000	3.05732000	2.16713700
H	1.18475900	3.83635600	2.93104200
H	1.13030700	2.08296800	2.62856000
H	2.40788500	3.07200900	1.88802400
C	0.87589200	4.65395000	0.30123100
H	1.94450900	4.64959900	0.03271500
H	0.29604000	4.86089500	-0.61261100
H	0.70798000	5.48833900	1.00163300
C	-4.91261300	0.27864100	1.27831000
H	-5.27084600	0.85899700	0.41445700
H	-4.19691600	-0.48670600	0.93303900
H	-5.76031200	-0.22413300	1.76515900
C	-4.91818200	3.91556900	3.54907900
H	-4.72213000	4.65200700	4.33967700
H	-5.42156400	4.40767700	2.70198100
H	-5.56578500	3.11629700	3.94400500

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.383740 (Hartree/Particle)
Thermal correction to Energy= 0.407064
Thermal correction to Enthalpy= 0.408008
Thermal correction to Gibbs Free Energy= 0.327558
Sum of electronic and zero-point Energies= -1190.826926
Sum of electronic and thermal Energies= -1190.803603
Sum of electronic and thermal Enthalpies= -1190.802659
Sum of electronic and thermal Free Energies= -1190.883109
HF= -1191.2106669
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.436593
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.414445
Solvent correction = -0.0221476
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1192.313084
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.579052

***E*-product (*triplet*)**

C	-0.29812900	1.73260600	2.98067900
C	-0.08549900	0.35056100	3.40554800
H	0.71359900	-0.22350300	2.91330000
H	0.11614700	2.55516300	3.57644300
C	-0.81693800	-0.31649500	4.42239800
C	-0.56105100	-1.68866100	4.71439700
C	-1.82179900	0.34497000	5.18998800
C	-1.27453800	-2.35882700	5.69841800
H	0.20828200	-2.21344400	4.14160600
C	-2.52744200	-0.33743500	6.17182900
H	-2.04998600	1.39317300	4.98770600
C	-2.26564600	-1.69107700	6.43536000
H	-1.06278800	-3.41204000	5.90007600
H	-3.29519900	0.18963400	6.74421300
H	-2.82456800	-2.22007700	7.21073800
C	-0.75636700	3.48826300	1.18719700
H	-0.68891900	4.21960800	2.01025500
C	-1.12149800	2.11838500	1.78706100
H	-1.06465400	1.32978900	1.01754300
H	-1.58604000	3.81996100	0.54386100
O	-3.29210000	2.88418400	3.46745500
O	-3.16085500	0.51079000	2.31325600
O	-3.70402700	2.55599000	0.91184300
P	-2.89738700	2.10445300	2.25645900
C	0.53328000	3.55566400	0.33153200
C	0.42016500	2.61326000	-0.87804300
H	1.29252500	2.72740800	-1.54108900
H	0.37905400	1.55631400	-0.57193400
H	-0.48474400	2.82933700	-1.46905700
C	1.78724500	3.19637300	1.14377600
H	1.88477600	3.83733400	2.03432000
H	1.76857800	2.15053200	1.48485400
H	2.69254600	3.33227300	0.52975000
C	0.66513400	5.00337800	-0.17289100
H	1.56219900	5.12176500	-0.80141200
H	-0.21027000	5.29616200	-0.77510100
H	0.74678200	5.71034900	0.66858000
C	-4.53668800	3.71424000	0.88983800
H	-4.68646900	4.10540800	1.90691600
H	-4.07033600	4.49171300	0.26330900
H	-5.50713400	3.43648000	0.45190300
C	-4.32381900	-0.01466500	2.95140300
H	-4.05820500	-0.99979400	3.35659100
H	-4.64448500	0.63991900	3.77550800
H	-5.14110500	-0.11832500	2.21920400

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.380031 (Hartree/Particle)
Thermal correction to Energy= 0.403443
Thermal correction to Enthalpy= 0.404387
Thermal correction to Gibbs Free Energy= 0.324701
Sum of electronic and zero-point Energies= -1190.749978

Sum of electronic and thermal Energies= -1190.726566
Sum of electronic and thermal Enthalpies= -1190.725622
Sum of electronic and thermal Free Energies= -1190.805308
HF= -1191.1300092
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.345786
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.326315
Solvent correction = -0.0194716
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1192.229021
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.497468

***Z*-product**

C	-1.09627200	1.65548600	2.94942400
C	-0.72476700	0.39552100	3.23553900
H	-0.19508500	0.23728500	4.18232800
H	-0.88871500	2.43191600	3.69358000
C	-0.86168400	-0.79842000	2.37945600
C	-2.05001300	-1.09750000	1.68584400
C	0.23052400	-1.67912200	2.25833100
C	-2.11989100	-2.22626400	0.86526000
H	-2.93006100	-0.46576500	1.82406600
C	0.15720100	-2.80138800	1.43367800
H	1.15112900	-1.46766900	2.80920000
C	-1.01919900	-3.07593100	0.72842100
H	-3.05092100	-2.44800700	0.33761800
H	1.01944700	-3.46663100	1.34244500
H	-1.08031400	-3.95723600	0.08522500
C	-1.05733400	3.42364800	1.10381500
H	-1.08494300	4.21744700	1.86952500
C	-1.72344300	2.15471500	1.67405600
H	-1.71168900	1.35583000	0.91712600
H	-1.68810400	3.77698600	0.27547300
O	-4.30043700	1.19206100	2.32926500
O	-3.98516800	3.21502000	0.67976400
O	-3.57511600	3.55957300	3.15005400
P	-3.50160700	2.40906100	1.99821800
C	0.39194500	3.28023000	0.56843100
C	0.51509700	2.05409400	-0.35059800
H	1.50769900	2.02898600	-0.82816900
H	0.39379600	1.11117800	0.20447400
H	-0.24147700	2.07767300	-1.15237400
C	1.42166000	3.17265600	1.70631000
H	1.33200200	4.02246000	2.40277900
H	1.29948200	2.24640200	2.28281500
H	2.44521500	3.18147300	1.29721900
C	0.69475100	4.55326200	-0.24219500
H	1.72640800	4.53792900	-0.62885800
H	0.01161100	4.65076300	-1.10139900
H	0.58212500	5.45561500	0.38096300
C	-3.99284400	3.25030300	4.47927900
H	-4.56045200	2.30837700	4.49840000
H	-3.11385900	3.15790900	5.13729400
H	-4.62580700	4.07526400	4.83739400
C	-5.36769600	3.53612900	0.53217500
H	-5.51943400	3.85360600	-0.50794100
H	-5.99545000	2.65745400	0.74790500
H	-5.64592700	4.35911800	1.21053800

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.384519 (Hartree/Particle)
Thermal correction to Energy= 0.407434
Thermal correction to Enthalpy= 0.408378
Thermal correction to Gibbs Free Energy= 0.330493
Sum of electronic and zero-point Energies= -1190.828086
Sum of electronic and thermal Energies= -1190.805171
Sum of electronic and thermal Enthalpies= -1190.804227
Sum of electronic and thermal Free Energies= -1190.882112
HF= -1191.2126052
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.434467
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.415459
Solvent correction = -0.0190075
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1192.312715
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -1191.577513

Figure 5.3
A

C	-4.78993100	-5.15180100	-2.55805300
C	-6.18141300	-5.46719800	-2.11258400
H	-6.69530500	-6.15714500	-2.81915900
H	-6.19546300	-5.96478400	-1.12832100
H	-6.80896100	-4.56220300	-2.05166000
C	-3.70896600	-6.15288300	-2.30612900
H	-2.70535200	-5.70032300	-2.37313300
H	-3.80947500	-6.62627200	-1.31498200
H	-3.72954400	-6.97983100	-3.05117300
C	-4.59176000	-4.13348000	-3.63411800
H	-4.78760200	-4.55673400	-4.64499200
H	-5.27545100	-3.27557800	-3.51961400
H	-3.55730800	-3.75123700	-3.65336800

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.115666 (Hartree/Particle)
Thermal correction to Energy= 0.122060
Thermal correction to Enthalpy= 0.123004
Thermal correction to Gibbs Free Energy= 0.086166
Sum of electronic and zero-point Energies= -157.582625
Sum of electronic and thermal Energies= -157.576231
Sum of electronic and thermal Enthalpies= -157.575287
Sum of electronic and thermal Free Energies= -157.612125
HF= -157.6982909
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP

HF = -157.7003821
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -157.6972035
Solvent correction = -0.0031786
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -157.8740734
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -157.7164404

sub

C	-4.20603900	-4.32638700	-1.42516500
H	-3.49007200	-4.93187800	-1.98976200
C	-4.19841800	-4.34202700	-0.08901500
H	-4.90100600	-3.75186400	0.50805300
H	-4.92069200	-3.72002400	-1.98977100
O	-2.08334500	-6.14709200	-0.06416200
O	-3.89787400	-6.08082900	1.87551900
O	-2.18923600	-4.27388600	1.75772100
P	-2.98059200	-5.32000100	0.78809400
C	-3.28499100	-6.98747100	2.79293200
H	-2.71979700	-6.43531800	3.56089200
H	-4.09067800	-7.56013000	3.27099000
H	-2.60602200	-7.67606200	2.26561900
C	-0.98193000	-3.66766800	1.30461200
H	-0.44438900	-3.30239400	2.19066200
H	-0.35846100	-4.39507400	0.76272000
H	-1.19823900	-2.81365700	0.63979900

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.133410 (Hartree/Particle)
Thermal correction to Energy= 0.144025
Thermal correction to Enthalpy= 0.144970
Thermal correction to Gibbs Free Energy= 0.096558
Sum of electronic and zero-point Energies= -724.405256
Sum of electronic and thermal Energies= -724.394640
Sum of electronic and thermal Enthalpies= -724.393696
Sum of electronic and thermal Free Energies= -724.442107
HF= -724.5386654
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -724.6983986
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -724.6885797
Solvent correction = -0.0098189
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -725.1445433
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -724.8491054

TS-Giese Addition

Imaginary Frequency (cm^{-1}) = -272.57

C	-4.15738200	-4.19010400	-1.33412700
H	-3.50013500	-4.86971500	-1.87964900
C	-3.99898500	-4.03042300	0.01281800
H	-4.54974400	-3.26895500	0.57220600
H	-4.68732800	-3.43368300	-1.91699800
O	-2.38211900	-6.27290900	0.15488700
O	-4.01284400	-5.61566500	2.13644600
O	-1.93566600	-4.29931900	1.81000500
P	-3.01044200	-5.16967600	0.94169700
C	-5.86281300	-5.73879200	-1.70621600
C	-6.65237400	-5.62962400	-0.43685600
H	-7.50769000	-6.33552000	-0.45966000
H	-6.04307000	-5.87714300	0.44497400
H	-7.06715700	-4.61906100	-0.29610600
C	-5.05001800	-6.98875100	-1.87637000
H	-4.46498800	-6.97323300	-2.80961600
H	-4.34975000	-7.14298200	-1.04124400
H	-5.71898600	-7.87279900	-1.92551600
C	-6.48062400	-5.15789200	-2.94328600
H	-7.28428800	-5.82348300	-3.32201100
H	-6.94143800	-4.17491500	-2.75522700
H	-5.74674700	-5.05311200	-3.75899500
C	-0.68248200	-3.96403700	1.22441800
H	-0.79839300	-3.15750300	0.47950600
H	-0.02591000	-3.61171500	2.03205200
H	-0.23170100	-4.84090600	0.73406600
C	-3.54961700	-6.54596100	3.11480900
H	-4.42829300	-6.89818400	3.67148600
H	-3.05046500	-7.40188500	2.63331700
H	-2.84538400	-6.05774400	3.80723000

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.252084 (Hartree/Particle)
Thermal correction to Energy= 0.268913
Thermal correction to Enthalpy= 0.269857
Thermal correction to Gibbs Free Energy= 0.206612
Sum of electronic and zero-point Energies= -881.994762
Sum of electronic and thermal Energies= -881.977933
Sum of electronic and thermal Enthalpies= -881.976989
Sum of electronic and thermal Free Energies= -882.040234
HF= -882.2468465
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -882.4025838
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -882.3909483
Solvent correction = -0.0116355
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -883.022813
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -882.5689618

B

C	-4.58628800	-4.42887900	-1.24779800
H	-3.70959600	-4.76881900	-1.82190200
C	-4.21412600	-4.32814500	0.18804600
H	-4.78539200	-3.69765500	0.87624200
H	-4.87756800	-3.43257700	-1.62456200
O	-2.14862700	-6.12552400	-0.12993100
O	-3.68461400	-6.15466100	2.03382100
O	-1.99388300	-4.35094000	1.78816400
P	-2.92074000	-5.33021000	0.86779200

C	-5.76579800	-5.41430800	-1.55999900
C	-7.05035100	-4.92845900	-0.87353700
H	-7.89461800	-5.59351100	-1.11685500
H	-6.94123600	-4.91767500	0.22225900
H	-7.31992900	-3.91061600	-1.20093500
C	-5.41543200	-6.82853300	-1.07142200
H	-4.44800400	-7.16309300	-1.47518700
H	-5.34340600	-6.86697000	0.02614600
H	-6.19289000	-7.54450400	-1.38344800
C	-5.96510100	-5.42743100	-3.08201800
H	-6.79593400	-6.09588200	-3.35985900
H	-6.19980100	-4.42071600	-3.46491300
H	-5.05851400	-5.78383400	-3.59669400
C	-0.84650900	-3.72595200	1.22041000
H	-1.12964700	-2.81010000	0.67360100
H	-0.17608400	-3.45322200	2.04739000
H	-0.32844300	-4.41071000	0.53161500
C	-2.95075100	-7.10731400	2.80455800
H	-3.68254900	-7.71115700	3.35730400
H	-2.35260200	-7.75992600	2.14924500
H	-2.28340000	-6.59436500	3.51550400

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.255683 (Hartree/Particle)
Thermal correction to Energy= 0.272057
Thermal correction to Enthalpy= 0.273001
Thermal correction to Gibbs Free Energy= 0.210695
Sum of electronic and zero-point Energies= -882.025954
Sum of electronic and thermal Energies= -882.009580
Sum of electronic and thermal Enthalpies= -882.008636
Sum of electronic and thermal Free Energies= -882.070942
HF= -882.2816367
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -882.4472641
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -882.4355134
Solvent correction = -0.0117507
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -883.0552792
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -882.607327

Figure 5.4
C-Ni^{0}-*trans*

Ni	-1.05362300	2.04658100	-0.46052800
C	-2.22515100	2.60624000	-1.80726600
C	-2.52641800	1.24779100	-1.43116900
H	-3.42738900	1.06601400	-0.83251300
Br	-3.53549600	4.00623400	-1.33159100
C	1.35738400	2.68063300	0.68519300
C	2.00207900	4.87297800	0.75458800
C	0.52812200	4.73266400	0.27648600
N	0.34869000	3.27917500	0.12063900
H	2.66265300	5.18450200	-0.07529100
C	0.24084900	-0.74362700	0.32454100
C	1.70418000	-1.03202800	0.77776600
C	1.29845600	1.21720500	0.64502700
N	0.11725000	0.72287400	0.41108900
H	2.24888000	-1.69046200	0.08681800
H	2.12845900	5.58090400	1.58536700
H	1.73293500	-1.48214700	1.78580000
C	0.19630300	5.48167000	-1.00311800
H	0.83873800	5.13580800	-1.82841600
H	-0.85264400	5.29968600	-1.27759800
H	0.34484200	6.56517500	-0.87020100
C	-0.82321900	-1.43626600	1.16001400
H	-0.71134400	-1.17946300	2.22575300
H	-1.81816400	-1.11425400	0.82476400
H	-0.75618000	-2.52960500	1.04767200
H	-0.16586100	5.06128000	1.07229800
H	0.09573700	-1.01802300	-0.73375100
N	2.32952100	3.50391700	1.19139500
N	2.31919600	0.31076600	0.79024900
C	3.29321100	3.17204100	2.15996300
C	4.57407900	3.74061400	2.09816700
C	2.98453800	2.27137500	3.19236300
C	5.53772900	3.39302700	3.04413000
H	4.81834300	4.43119400	1.28950900
C	3.96024600	1.91697800	4.12300500
H	1.97764400	1.85720400	3.26353200
C	5.24060400	2.47321900	4.05403500
H	6.53553500	3.83305200	2.98050600
H	3.71170900	1.21079100	4.91884800
H	6.00121100	2.19664000	4.78715200
C	3.67063600	0.56305100	0.47448600
C	4.00788000	1.43965200	-0.56925000
C	4.68817000	-0.05925400	1.21136300
C	5.34725300	1.71805400	-0.84103900
H	3.21693500	1.89174900	-1.17064600
C	6.02487900	0.21008000	0.92047200
H	4.42271400	-0.72891200	2.03093800
C	6.36106500	1.10715900	-0.09805200
H	5.60002500	2.40557000	-1.65178500
H	6.81048200	-0.27114700	1.50739400
H	7.40908000	1.32420800	-0.31522900
H	-1.83965800	2.85218200	-2.80298900
C	-2.04297700	0.07673300	-2.18050400
C	-0.95172000	0.13658000	-3.07790100
C	-2.60471500	-1.19491900	-1.94078500
C	-0.44291800	-1.01319200	-3.67929300
H	-0.48154600	1.09972900	-3.28613500
C	-2.09045100	-2.34773400	-2.53618200
H	-3.45824600	-1.27209700	-1.26163500
C	-0.99962600	-2.26933600	-3.40729800
H	0.40492500	-0.93030100	-4.36515900
H	-2.54930600	-3.31669900	-2.32049800
H	-0.59451400	-3.16985400	-3.87472300

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.512405 (Hartree/Particle)
Thermal correction to Energy= 0.543996
Thermal correction to Enthalpy= 0.544940
Thermal correction to Gibbs Free Energy= 0.445616
Sum of electronic and zero-point Energies= -5384.233272
Sum of electronic and thermal Energies= -5384.201681

Sum of electronic and thermal Enthalpies= -5384.200737
Sum of electronic and thermal Free Energies= -5384.300061
HF= -5384.7456769
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.770013
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.723651
Solvent correction = -0.0463616
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.67076
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.312054

C-TS-F*trans*
Imaginary Frequency (cm^{-1}) = -124.85

Ni	-0.44341800	1.41812700	-0.70138300
C	-2.05367500	1.97196000	-0.99998700
C	-2.28778600	0.58481600	-0.95970800
H	-2.43058600	0.11702100	0.02109800
Br	-1.46959800	2.50889500	1.48107800
C	1.97040700	2.50594600	-0.04001600
C	2.10054300	4.77553900	0.19653900
C	0.83800400	4.35531600	-0.61315900
N	0.97495900	2.89852400	-0.77289100
H	2.82489700	5.32106600	-0.43296500
C	1.44349900	-1.08413700	-0.01449600
C	2.76358800	-1.02831000	0.80319300
C	2.15910400	1.05116300	0.07057300
N	1.12620800	0.33151800	-0.25591800
H	3.51987400	-1.75209400	0.46934800
H	1.86203100	5.39331300	1.07301000
H	2.57251000	-1.18915600	1.88009800
C	0.69306100	5.05539000	-1.95532600
H	1.57908400	4.88042400	-2.58679600
H	-0.18892700	4.66974800	-2.48710700
H	0.56957700	6.14141900	-1.81800000
C	0.29244700	-1.79246400	0.68149300
H	0.04447900	-1.28081000	1.62435900
H	-0.59994000	-1.77233600	0.04010100
H	0.54951200	-2.84157200	0.89749900
H	-0.07462600	4.50861900	-0.01210800
H	1.62272900	-1.55892500	-0.99696500
N	2.66844200	3.48012600	0.63206600
N	3.22593100	0.34839000	0.56350900
C	3.16991400	3.27509700	1.94629800
C	4.39243800	3.84312400	2.32262000
C	2.44234600	2.49901800	2.86131300
C	4.89951200	3.61437100	3.60142900
H	4.95322100	4.43314800	1.59648400
C	2.96751600	2.25795400	4.13199500
H	1.45642600	2.11812900	2.58065300
C	4.19639900	2.81078200	4.50445500
H	5.85987300	4.04922700	3.88709700
H	2.39991300	1.65211700	4.84233900
H	4.60200800	2.62362500	5.50132000
C	4.54613800	0.79304500	0.74108200
C	5.13125100	1.67189400	-0.18488500
C	5.29311500	0.34780700	1.84170200
C	6.43332600	2.12708700	0.01501400
H	4.56245200	1.99147200	-1.05911500
C	6.60061100	0.79713200	2.02341500
H	4.83676100	-0.32440800	2.56936200
C	7.17476800	1.69410100	1.11854200
H	6.87784100	2.81536600	-0.70782400
H	7.16970200	0.45388400	2.89031600
H	8.19675500	2.04850800	1.26832800
H	-2.62907500	2.84282000	-1.33011800
C	-2.85661600	-0.16903400	-2.08964900
C	-2.76320000	0.29682800	-3.41709300
C	-3.50987500	-1.39732400	-1.86859100
C	-3.32217200	-0.42283600	-4.47219900
H	-2.22446100	1.22696300	-3.61523600
C	-4.05658400	-2.12491900	-2.92606700
H	-3.59216400	-1.77637800	-0.84601600
C	-3.97098000	-1.63983700	-4.23481100
H	-3.23998000	-0.03855300	-5.49246600
H	-4.55806300	-3.07587100	-2.72725900
H	-4.39944500	-2.20819700	-5.06379300

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.510655 (Hartree/Particle)
Thermal correction to Energy= 0.542103
Thermal correction to Enthalpy= 0.543047
Thermal correction to Gibbs Free Energy= 0.443789
Sum of electronic and zero-point Energies= -5384.208459
Sum of electronic and thermal Energies= -5384.177011
Sum of electronic and thermal Enthalpies= -5384.176066
Sum of electronic and thermal Free Energies= -5384.275324
HF= -5384.7191136
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.744497
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.700088
Solvent correction = -0.0444092
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.643043
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.278147

^{3}C-Ni^0

Ni	0.61236500	1.50197600	0.13966800
C	-1.27997200	2.06964000	0.62145100
C	-0.44395400	2.04528300	1.74837500
H	-0.46075900	1.16263900	2.40012300
Br	-2.57914500	0.66715200	0.34182700
C	2.98514300	2.78511000	-0.49869900
C	2.94750600	4.98197600	-1.15605900
C	1.53286000	4.51784300	-0.72495800
N	1.68049200	3.07288500	-0.56722500
H	3.01164700	5.07215600	-2.25638200
C	2.89761200	-0.72750400	0.33695200
C	4.41654800	-0.45198000	0.47802400
C	3.33570200	1.42292700	-0.29645300
N	2.33476200	0.58738300	0.03727200

H	5.04467400	-1.23752700	0.03523000
H	3.24512500	5.93938100	-0.70793000
H	4.69896200	-0.33990700	1.54317900
C	0.43431300	4.88725500	-1.70964400
H	0.64111400	4.45389900	-2.70112400
H	-0.53461500	4.49573500	-1.36592500
H	0.34335300	5.98083800	-1.81190000
C	2.25592500	-1.34823100	1.56938600
H	2.41740300	-0.70690600	2.45084400
H	1.16978900	-1.45302300	1.41944000
H	2.66933700	-2.34774400	1.77980500
H	1.28735500	4.95818300	0.25996900
H	2.73032600	-1.40320700	-0.52631600
N	3.81218400	3.89560300	-0.67138600
N	4.58259100	0.81185600	-0.24426400
C	4.98436600	4.14018500	0.05903500
C	5.90901800	5.08999900	-0.41031900
C	5.26103900	3.45958700	1.25895500
C	7.08313600	5.34210100	0.29728700
H	5.71203500	5.60857700	-1.35036700
C	6.44703000	3.70618100	1.94891000
H	4.53802000	2.74337800	1.64723000
C	7.36702800	4.64635300	1.47655000
H	7.79286800	6.07834900	-0.08806900
H	6.64825600	3.16290500	2.87589100
H	8.29468800	4.83533300	2.02081300
C	5.73651700	1.16446500	-0.94622800
C	5.66502400	1.91176800	-2.13701900
C	6.99849300	0.76516700	-0.46837300
C	6.83154000	2.27513300	-2.80608200
H	4.69190000	2.20405000	-2.52974400
C	8.15717900	1.12277200	-1.15623200
H	7.06974300	0.19876000	0.46156500
C	8.08553100	1.88772600	-2.32388400
H	6.75728100	2.86104800	-3.72576100
H	9.12869400	0.81147400	-0.76432800
H	8.99591000	2.17593700	-2.85353300
C	0.19901200	3.26256300	2.30054100
C	1.50478300	3.18637400	2.82257000
C	-0.43883500	4.51352900	2.27365300
C	2.15799600	4.32662000	3.28233300
H	2.02034700	2.22314800	2.81431100
C	0.21207200	5.65649000	2.74772500
H	-1.45791000	4.58805500	1.88846100
C	1.51305600	5.56988100	3.24762300
H	3.18230600	4.25283600	3.65433900
H	-0.30213600	6.62043700	2.72277700
H	2.02673400	6.46464000	3.60642700
H	-1.58757200	2.99870200	0.13768700

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.511640 (Hartree/Particle)
Thermal correction to Energy= 0.543227
Thermal correction to Enthalpy= 0.544171
Thermal correction to Gibbs Free Energy= 0.444084
Sum of electronic and zero-point Energies= -5384.222879
Sum of electronic and thermal Energies= -5384.191292
Sum of electronic and thermal Enthalpies= -5384.190348
Sum of electronic and thermal Free Energies= -5384.290435
HF= -5384.734519
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.772489
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.734464
Solvent correction = -0.0380243
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.654546
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.291024

^{3}C-TS-F^{trans}

Imaginary Frequency (cm^{-1}) = -108.96

Ni	0.86988300	1.47448500	0.14951000
C	-0.73665000	2.24973500	0.85819200
C	-0.43227900	2.50550000	2.18196100
H	-0.10154500	1.67154300	2.80807700
Br	-1.35018100	0.29172100	0.38312100
C	3.26105400	2.68332700	-0.46247900
C	3.19791900	4.91923200	-0.98290400
C	1.79042200	4.42412800	-0.56472500
N	1.94703900	2.97129000	-0.53226500
H	3.24561900	5.08153100	-2.07654000
C	3.10923200	-0.86251600	0.15704600
C	4.64562700	-0.66816400	0.19157400
C	3.59616600	1.31113500	-0.31944200
N	2.60182700	0.50373400	0.08199900
H	5.19392500	-1.43405600	-0.37402300
H	3.49856500	5.84808300	-0.47936100
H	5.01850400	-0.66958600	1.23416300
C	0.68152800	4.86969200	-1.50593400
H	0.88400500	4.52057900	-2.53071900
H	-0.28363400	4.44595700	-1.19229500
H	0.58463600	5.96732000	-1.51640600
C	2.54145000	-1.61540100	1.35066200
H	2.81149200	-1.10337300	2.28815300
H	1.44311500	-1.64843900	1.28652500
H	2.91765000	-2.65038300	1.39047400
H	1.56033500	4.79022700	0.45629500
H	2.83454900	-1.40860300	-0.77004000
N	4.06785200	3.80889400	-0.57831500
N	4.81671100	0.65166900	-0.42566300
C	5.33618900	3.99530400	-0.01773200
C	6.18542700	4.99055400	-0.53562400
C	5.78539100	3.21311800	1.06216400
C	7.45676700	5.18255500	0.00228000
H	5.85362100	5.59335700	-1.38283600
C	7.06532100	3.40330800	1.57964700
H	5.12509600	2.46202400	1.49426200
C	7.91189600	4.38470000	1.05632600
H	8.10502100	5.95470100	-0.41951800
H	7.40029200	2.78161000	2.41383700
H	8.91371400	4.52806900	1.46645000
C	5.90314300	0.99345500	-1.23297400
C	5.75444000	1.84877600	-2.34126400
C	7.17881800	0.47182900	-0.94544200
C	6.86164200	2.19395300	-3.11343700
H	4.76834900	2.23697900	-2.59305100

C	8.27512000	0.81333800	-1.73562500
H	7.31314600	-0.18043800	-0.08099600
C	8.12951000	1.68361600	-2.81982000
H	6.72715700	2.86480100	-3.96581000
H	9.25843500	0.40446800	-1.48990600
H	8.99269100	1.95863500	-3.42942500
C	-0.44732600	3.81441400	2.80888800
C	0.00492900	3.94545400	4.14170300
C	-0.87678000	4.98686100	2.14270600
C	0.02782600	5.18417900	4.77801700
H	0.34458700	3.05347700	4.67452100
C	-0.85543800	6.22207000	2.78294900
H	-1.22892700	4.92804900	1.11156100
C	-0.40114800	6.33215400	4.10349800
H	0.38321300	5.25620600	5.80889600
H	-1.19448300	7.11220500	2.24708900
H	-0.38220400	7.30447500	4.60070500
H	-1.31845800	2.93669200	0.23734300

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.509900 (Hartree/Particle)
Thermal correction to Energy= 0.541344
Thermal correction to Enthalpy= 0.542288
Thermal correction to Gibbs Free Energy= 0.441613
Sum of electronic and zero-point Energies= -5384.201218
Sum of electronic and thermal Energies= -5384.169773
Sum of electronic and thermal Enthalpies= -5384.168829
Sum of electronic and thermal Free Energies= -5384.269504
HF= -5384.7111171
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.750062
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.710705
Solvent correction = -0.0444092
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.634226
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.26819

C-Ni^{0}-*cis*

Ni	1.17557100	3.00569500	1.85941300
C	-0.68451900	2.94465500	2.06960900
C	-0.07045400	2.08680100	3.05614300
H	-0.14325100	2.44783300	4.09213700
Br	-1.89694700	2.26063800	0.63338300
C	3.28362500	3.66660200	0.15784100
C	2.91125600	5.17685900	-1.52262600
C	1.65391300	5.01407400	-0.61503500
N	2.02319400	3.93991700	0.32207600
H	2.73107600	4.76500000	-2.53155700
C	3.71436100	1.16908900	2.75021800
C	5.05996100	0.94634800	1.99566600
C	3.80626600	2.58836400	1.01026900
N	3.10483700	2.32523500	2.06932800
H	5.21494400	-0.09704000	1.68759200
H	3.24460000	6.21911000	-1.62796100
H	5.92421300	1.26406200	2.60540600
C	0.37811900	4.67523800	-1.36975300
H	0.51871600	3.76275400	-1.97040500
H	-0.44137400	4.47837100	-0.66511300
H	0.09140700	5.50022300	-2.04123300
C	3.86291300	1.42162400	4.24154700
H	4.53139500	2.27744500	4.42919500
H	2.87810900	1.64413800	4.67408400
H	4.27101600	0.53302500	4.74784600
H	1.48700700	5.92746800	-0.01560300
H	3.03654100	0.31265400	2.60090400
N	3.93053600	4.38487000	-0.81242800
N	4.91798000	1.81120700	0.80659700
C	5.31974700	4.57721100	-0.92716400
C	5.91172400	4.66483200	-2.19551000
C	6.12156900	4.68190100	0.22084100
C	7.29122400	4.83169800	-2.31080600
H	5.29056800	4.57013200	-3.08733300
C	7.50220700	4.83065800	0.09513500
H	5.65735300	4.65155700	1.20790600
C	8.09415300	4.90513500	-1.16884600
H	7.74417900	4.88715100	-3.30324100
H	8.11852400	4.90494500	0.99427200
H	9.17528400	5.02626300	-1.26378200
C	5.48240700	1.52096800	-0.45407800
C	4.66372600	1.39130600	-1.58700300
C	6.86978400	1.36642800	-0.57954700
C	5.23592300	1.15149400	-2.83629800
H	3.57990100	1.46851700	-1.48087000
C	7.43196000	1.10747600	-1.82895000
H	7.50333200	1.48187800	0.30117600
C	6.62053300	1.01011700	-2.96345400
H	4.59197600	1.05686400	-3.71388900
H	8.51512900	0.99949200	-1.91957800
H	7.06567100	0.81808600	-3.94205800
C	0.26329300	0.65669800	2.96077000
C	0.57781600	-0.05693800	4.13762400
C	0.41978700	-0.02922600	1.73242500
C	1.05197000	-1.36854400	4.09709500
H	0.45803800	0.44338700	5.10258100
C	0.88663400	-1.34196000	1.69392100
H	0.17668800	0.48212000	0.80162900
C	1.21818500	-2.02253100	2.87227000
H	1.29170600	-1.88511100	5.03067500
H	0.99835500	-1.84117200	0.72727300
H	1.58841700	-3.04989700	2.83594600
H	-1.20539800	3.82615800	2.45983900

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.513062 (Hartree/Particle)
Thermal correction to Energy= 0.544438
Thermal correction to Enthalpy= 0.545382
Thermal correction to Gibbs Free Energy= 0.447146
Sum of electronic and zero-point Energies= -5384.232491
Sum of electronic and thermal Energies= -5384.201115
Sum of electronic and thermal Enthalpies= -5384.200170
Sum of electronic and thermal Free Energies= -5384.298407
HF= -5384.7455528

M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.768336
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.722567
Solvent correction = -0.0457688
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.671044
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.309076

C-TS-F*cis*

Imaginary Frequency (cm^{-1}) = -263.28

Ni	0.76189800	1.46049300	0.38128200
C	-0.80662200	2.16982500	0.95785500
C	-0.09102600	2.66900200	2.04337800
H	-0.11309500	3.76616400	2.11540100
Br	-1.27284100	0.10236000	0.83244800
C	2.90871400	2.73510300	-0.66316500
C	2.69666700	4.93140600	-1.25075300
C	1.31135900	4.28195300	-0.98199800
N	1.60753900	2.84178300	-0.82546500
H	2.84568800	5.11107600	-2.33134400
C	3.18893200	-0.66110900	0.52217700
C	4.69790600	-0.32200600	0.39491200
C	3.40247000	1.41725000	-0.32712500
N	2.52712200	0.62186500	0.23653000
H	5.28466600	-1.10686100	-0.10209600
H	2.84670700	5.87904100	-0.71564800
H	5.14289100	-0.12317500	1.38837600
C	0.28033100	4.52462800	-2.07152800
H	0.64529600	4.14217800	-3.03771500
H	-0.65497600	3.99849200	-1.83091500
H	0.05976300	5.59899500	-2.17769100
C	2.77284500	-1.21432100	1.87367600
H	3.03663300	-0.51216400	2.67822700
H	1.68280700	-1.35291400	1.90165900
H	3.25781900	-2.18406000	2.06951700
H	0.91054800	4.63958600	-0.01664200
H	2.89974500	-1.37516400	-0.27266500
N	3.63221000	3.90833100	-0.75893600
N	4.67456200	0.90181600	-0.41696300
C	4.78437100	4.19134100	0.00163600
C	5.74621000	5.08339500	-0.49663600
C	4.99353300	3.57683300	1.24865200
C	6.90529800	5.34249100	0.23365700
H	5.59180900	5.54582800	-1.47312600
C	6.16477200	3.82880600	1.96244200
H	4.23257700	2.91359700	1.66304600
C	7.12762800	4.70899800	1.46053700
H	7.65135300	6.03127800	-0.16964900
H	6.31619700	3.34162800	2.92898500
H	8.04322000	4.90419900	2.02288800
C	5.75615600	1.41573000	-1.14282700
C	5.54751500	2.06745000	-2.37100600
C	7.06348200	1.28676300	-0.64638000
C	6.62620700	2.61478500	-3.06255700
H	4.53836200	2.13643200	-2.77847500
C	8.13685000	1.82613700	-1.35471300
H	7.23263800	0.79065600	0.31032200
C	7.92600100	2.50185700	-2.55977200
H	6.44958600	3.12374000	-4.01334800
H	9.14732100	1.72939300	-0.95064800
H	8.76853800	2.93029700	-3.10658700
C	0.73072800	2.02026000	3.07224700
C	1.91750500	2.67247500	3.48748100
C	0.37931200	0.82712200	3.74346000
C	2.73927000	2.13228200	4.47332700
H	2.19920700	3.61146000	3.00315600
C	1.20241900	0.29451300	4.73376600
H	-0.54455100	0.31647000	3.47594300
C	2.39451700	0.92931100	5.10148400
H	3.65563600	2.65774900	4.75694200
H	0.90483700	-0.63289400	5.23065200
H	3.03482800	0.50341900	5.87728900
H	-1.57451400	2.74397800	0.42953200

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.510387 (Hartree/Particle)
Thermal correction to Energy= 0.541701
Thermal correction to Enthalpy= 0.542645
Thermal correction to Gibbs Free Energy= 0.445091
Sum of electronic and zero-point Energies= -5384.203255
Sum of electronic and thermal Energies= -5384.171941
Sum of electronic and thermal Enthalpies= -5384.170997
Sum of electronic and thermal Free Energies= -5384.268551
HF= -5384.7136418
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.732669
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.691846
Solvent correction = -0.0408235
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.636739
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.275864

E*trans*

Ni	-0.83698900	1.18902800	0.21933700
C	-2.37638300	2.13655800	-0.24164400
C	-3.41413200	1.74481500	-1.00218900
H	-3.46605700	0.69521500	-1.31417300
Br	-2.00727400	-0.55131300	1.19484200
C	1.59539200	2.28669500	-0.53542200
C	1.52088800	4.41318100	-1.36507400
C	0.10604100	3.77264000	-1.33678700
N	0.31457000	2.51126100	-0.60390600
H	1.77373900	4.82688500	-2.35199200
C	1.47397900	-0.88484700	1.19408600
C	2.92569200	-1.00185000	0.64112900
C	1.95503600	0.97262000	0.02172300
N	0.96987000	0.35421200	0.58897400
H	3.02367700	-1.77488000	-0.13880400
H	1.64275500	5.20865300	-0.61051000
H	3.65920200	-1.21239200	1.43360300
C	-0.45585600	3.48424100	-2.72719600
H	0.24664300	2.86095300	-3.30396500

H	-1.41156000	2.95028300	-2.63983100
H	-0.61946900	4.42603200	-3.27438100
C	1.40077200	-0.78465100	2.71555600
H	2.01396200	0.05567200	3.08063200
H	0.35564400	-0.62535400	3.01461700
H	1.76853600	-1.71454100	3.17785900
H	-0.60625100	4.39770200	-0.77960200
H	0.83024400	-1.71234300	0.86217600
N	2.40565200	3.27770600	-1.01863700
N	3.16691200	0.33167600	0.03525800
C	3.73240100	3.50986200	-0.56451600
C	4.70816000	3.92582200	-1.47767400
C	4.06288200	3.34610400	0.78768900
C	6.01152600	4.16158700	-1.04206500
H	4.44301600	4.03173400	-2.53057800
C	5.37292900	3.56842500	1.21410200
H	3.29307800	3.04473100	1.50078500
C	6.34960700	3.97685400	0.30210300
H	6.77231200	4.47420400	-1.76050100
H	5.62803800	3.43219700	2.26754500
H	7.37365900	4.15294800	0.63846000
C	4.16035500	0.50034900	-0.96629900
C	3.79876500	0.65999600	-2.31138700
C	5.51254100	0.48538400	-0.60449500
C	4.78676000	0.83655100	-3.28109700
H	2.74421800	0.64290400	-2.59388400
C	6.49551200	0.64574900	-1.58038600
H	5.78124300	0.37662100	0.44723400
C	6.13642200	0.82952000	-2.91926300
H	4.49941800	0.96730800	-4.32696500
H	7.54861000	0.64444700	-1.29090800
H	6.90839300	0.96406200	-3.68007400
H	-2.35916900	3.18405100	0.10869700
C	-4.53863700	2.57409200	-1.46971800
C	-5.60785100	1.96217900	-2.15328100
C	-4.60291300	3.97050800	-1.28246500
C	-6.69462400	2.70343900	-2.61973100
H	-5.57898300	0.88063700	-2.31140800
C	-5.68717500	4.71286000	-1.74571000
H	-3.78600700	4.47936000	-0.76593500
C	-6.74258300	4.08532900	-2.41846400
H	-7.51066700	2.19802200	-3.14320700
H	-5.71055800	5.79413400	-1.58385100
H	-7.59131600	4.66941200	-2.78259300

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.513502 (Hartree/Particle)
Thermal correction to Energy= 0.545152
Thermal correction to Enthalpy= 0.546097
Thermal correction to Gibbs Free Energy= 0.446489
Sum of electronic and zero-point Energies= -5384.260387
Sum of electronic and thermal Energies= -5384.228737
Sum of electronic and thermal Enthalpies= -5384.227793
Sum of electronic and thermal Free Energies= -5384.327400
HF= -5384.7738896
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.836213
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.783286
Solvent correction = -0.0529276
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.69933
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.329464

E-TS
Imaginary Frequency (cm^{-1}) = -62.98

Ni	-0.42322800	0.56718700	-1.41246400
C	-2.08869400	0.53913000	-0.95198600
C	-2.34420200	0.50015100	-2.30839100
H	-2.35729400	1.43384500	-2.88878800
Br	1.15468400	-0.80453900	-2.61334400
C	1.70509900	2.06471800	-0.36890800
C	2.25675200	3.97193300	-1.50410600
C	0.90257100	3.39275300	-2.00195600
N	0.78579100	2.11992100	-1.27633600
H	3.05096600	3.83016100	-2.25927900
C	1.14271000	-1.20197400	1.09421400
C	2.62908100	-1.01027600	1.51307000
C	1.80739200	0.80347300	0.39467700
N	0.73503600	0.10603000	0.55399600
H	3.28542200	-1.81906100	1.16387800
H	2.21042900	5.03734300	-1.23868800
H	2.73649600	-0.91503200	2.60905500
C	0.82732000	3.16758200	-3.50465200
H	1.61000000	2.46300200	-3.82323000
H	-0.14123900	2.72150100	-3.77168000
H	0.94333900	4.11745800	-4.05020500
C	0.22805800	-1.67245500	2.21329000
H	0.24471000	-0.96319400	3.05650500
H	-0.80733200	-1.74884400	1.84987200
H	0.53820100	-2.66261100	2.58343800
H	0.06508300	4.03990200	-1.68162500
H	1.08112800	-1.90182900	0.24069500
N	2.53109900	3.15419100	-0.31336400
N	2.98255200	0.25516700	0.84310800
C	3.47028100	3.47181600	0.68104600
C	4.67882900	4.09195400	0.33230800
C	3.20341500	3.17890200	2.02848200
C	5.61838000	4.38896400	1.31908400
H	4.89570300	4.30893900	-0.71404700
C	4.15701200	3.46460300	3.00393300
H	2.24657100	2.73404500	2.30576100
C	5.36880600	4.06943300	2.65620000
H	6.56211400	4.86008500	1.03529700
H	3.94309200	3.22683400	4.04867900
H	6.11064800	4.29729700	3.42445100
C	4.26340700	0.53208800	0.30534600
C	4.42341900	0.70222800	-1.07811300
C	5.36716200	0.64434200	1.16025300
C	5.67914100	1.03501000	-1.58923500
H	3.56946700	0.53374400	-1.74077000
C	6.62215300	0.95354300	0.63672900
H	5.22736200	0.52151100	2.23530100
C	6.77979300	1.16426600	-0.73669100
H	5.80123000	1.16802400	-2.66698700
H	7.47796300	1.05114000	1.30847200
H	7.76182700	1.41782400	-1.14257600

H	-2.58011400	0.12950600	-0.06383300
C	-2.90366300	-0.67422700	-3.01061300
C	-2.61056500	-1.98304900	-2.58659300
C	-3.74621300	-0.50239400	-4.12272800
C	-3.17400600	-3.08242400	-3.23276800
H	-1.90074000	-2.12478100	-1.76964700
C	-4.30623900	-1.60310900	-4.77242500
H	-3.96788600	0.50938700	-4.47372000
C	-4.02733000	-2.89847900	-4.32589300
H	-2.92958300	-4.09261700	-2.89459300
H	-4.96166200	-1.45012300	-5.63373300
H	-4.46029800	-3.76151700	-4.83754800

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.510437
(Hartree/Particle)
Thermal correction to Energy= 0.542055
Thermal correction to Enthalpy= 0.542999
Thermal correction to Gibbs Free Energy= 0.444184
Sum of electronic and zero-point Energies= -5384.214706
Sum of electronic and thermal Energies= -5384.183088
Sum of electronic and thermal Enthalpies= -5384.182144
Sum of electronic and thermal Free Energies= -5384.280959
HF= -5384.7251428
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.767644
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.723072
Solvent correction = -0.0408235
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.646548
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.280707

E*cis*

Ni	-1.00295000	0.98013100	0.26717400
C	-2.59147700	1.97363000	0.13749800
C	-2.72448000	3.20307300	0.67978600
H	-3.64561300	3.78478300	0.52852500
Br	-2.08504600	-0.69467500	1.46618200
C	1.34083700	2.14947900	-0.66422500
C	1.08156800	4.22993000	-1.56189100
C	-0.25596800	3.45076700	-1.56517000
N	0.04808000	2.25243500	-0.76671100
H	1.32921400	4.66014800	-2.54301300
C	1.49307500	-0.89312200	1.28045400
C	2.95412300	-0.90995700	0.75148100
C	1.81007000	0.90710900	-0.02458200
N	0.87287700	0.20459600	0.52825800
H	3.12490800	-1.69779000	-0.00198400
H	1.08527000	5.03102500	-0.80403000
H	3.69335000	-1.03035200	1.55657900
C	-0.73401900	3.02997600	-2.95208800
H	0.04452000	2.45760100	-3.48217300
H	-1.62843300	2.39769800	-2.85809300
H	-0.99021700	3.91517700	-3.55541300
C	1.39412300	-0.60765100	2.77864500
H	1.90208100	0.33909100	3.02575200
H	0.33604900	-0.53448500	3.06511200
H	1.86664000	-1.41997900	3.35357500
H	-1.04818500	4.01682800	-1.06402400
H	0.95420900	-1.82464800	1.05544300
N	2.06870100	3.19357900	-1.16997000
N	3.08471600	0.41728200	0.10160600
C	3.32555900	3.59434200	-0.63329500
C	4.33344800	4.03720900	-1.49613200
C	3.54128900	3.57766100	0.75117800
C	5.56205400	4.44374400	-0.97635200
H	4.15437400	4.03118200	-2.57218300
C	4.77852400	3.97044600	1.26339900
H	2.73235000	3.27426800	1.41748400
C	5.79079500	4.40370500	0.40256900
H	6.35145100	4.77708500	-1.65345900
H	4.94623200	3.95156400	2.34279100
H	6.75719200	4.71417300	0.80607100
C	4.12654200	0.65317600	-0.83503700
C	3.85663900	0.69364400	-2.20990300
C	5.43839900	0.81798900	-0.37579400
C	4.89249200	0.92859500	-3.11508100
H	2.83560500	0.54175800	-2.56532500
C	6.47148800	1.03626500	-1.28636400
H	5.63231200	0.80328000	0.69765100
C	6.20154300	1.09898800	-2.65688400
H	4.67612200	0.96702900	-4.18523500
H	7.49147600	1.17622300	-0.92193900
H	7.01147800	1.27924300	-3.36712100
H	-3.45525800	1.54916100	-0.39325800
C	-1.64818100	3.88583900	1.42418500
C	-1.42862600	5.26941700	1.27674400
C	-0.75390700	3.16510200	2.24365800
C	-0.32116900	5.89384300	1.85633300
H	-2.12555000	5.85473000	0.66948200
C	0.34846400	3.78854800	2.82878100
H	-0.95451400	2.10896300	2.43362400
C	0.58385800	5.15290700	2.62471800
H	-0.16324900	6.96572500	1.70957900
H	1.02056100	3.20580300	3.46562200
H	1.45050800	5.64021800	3.07803000

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.514027
(Hartree/Particle)
Thermal correction to Energy= 0.545171
Thermal correction to Enthalpy= 0.546115
Thermal correction to Gibbs Free Energy= 0.449919
Sum of electronic and zero-point Energies= -5384.272495
Sum of electronic and thermal Energies= -5384.241351
Sum of electronic and thermal Enthalpies= -5384.240407
Sum of electronic and thermal Free Energies= -5384.336603
HF= -5384.7865225
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.842928
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.796719
Solvent correction = -0.0462081

(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.709588
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.338354

^{3}F*trans*

Ni	0.44540900	1.44836500	-0.58525500
C	0.00031400	2.56584600	0.97554600
C	0.85725200	3.36031700	1.64513300
H	1.88624500	3.46251900	1.26924800
Br	-0.84633800	-0.39188900	-1.29689300
C	2.95012000	2.67337300	-0.98405000
C	3.03763500	4.88674500	-1.54726200
C	1.59337200	4.31940300	-1.67945800
N	1.74845400	2.87655700	-1.42714100
H	3.46808300	5.13315300	-2.53403300
C	2.69352100	-0.73461000	0.24213600
C	4.24184000	-0.57810500	0.31733100
C	3.25618800	1.30593000	-0.52241700
N	2.23575500	0.59994600	-0.16461300
H	4.79064600	-1.39327000	-0.17408800
H	3.09840000	5.77650000	-0.90554000
H	4.58606700	-0.50153400	1.36426800
C	0.93322300	4.59154200	-3.02190300
H	1.53547600	4.17527500	-3.84499700
H	-0.06300900	4.12682200	-3.05638600
H	0.81536700	5.67436700	-3.18508300
C	2.02290200	-1.17705400	1.53256700
H	2.23954400	-0.46615400	2.34520400
H	0.93463400	-1.21022300	1.37940900
H	2.37056300	-2.17887800	1.82975700
H	0.95247300	4.70631900	-0.86837000
H	2.40317000	-1.42801300	-0.56713400
N	3.76976200	3.76487800	-0.92874400
N	4.47173400	0.69529900	-0.39418400
C	4.89244700	3.92013600	-0.08362600
C	6.02341900	4.60271300	-0.55027600
C	4.87974500	3.40127100	1.22036900
C	7.13806200	4.74829200	0.27483800
H	6.03348000	4.99194600	-1.56940000
C	6.00572400	3.53712100	2.03295700
H	3.98444500	2.90688000	1.59970000
C	7.13787800	4.20916200	1.56482300
H	8.01968900	5.27312000	-0.09955500
H	5.98786900	3.12985600	3.04646200
H	8.01555900	4.31869100	2.20536200
C	5.67840200	1.07864800	-1.00972500
C	5.67330900	1.59628200	-2.31451200
C	6.89120100	0.94686800	-0.31912400
C	6.86665500	2.01642200	-2.90106000
H	4.73447900	1.65774600	-2.86773800
C	8.08159200	1.35266200	-0.92128900
H	6.89264800	0.55523200	0.69898000
C	8.07477200	1.89807600	-2.20837600
H	6.85333300	2.42283200	-3.91508700
H	9.02086400	1.25676000	-0.37215900
H	9.00857400	2.22206500	-2.67259700
C	0.63581400	4.15936500	2.86485100
C	1.68678700	4.94931500	3.37080400
C	-0.58804000	4.17580700	3.56307100
C	1.52709100	5.72442300	4.52093300
H	2.64686200	4.95071200	2.84552200
C	-0.75028500	4.94897700	4.71068800
H	-1.41922000	3.57011700	3.19620500
C	0.30542300	5.72926200	5.19866400
H	2.36090400	6.32787700	4.88980900
H	-1.71031600	4.94371000	5.23377000
H	0.17469700	6.33374100	6.09950100
H	-1.02286700	2.48069400	1.37818700

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.511935 (Hartree/Particle)
Thermal correction to Energy= 0.544429
Thermal correction to Enthalpy= 0.545373
Thermal correction to Gibbs Free Energy= 0.442103
Sum of electronic and zero-point Energies= -5384.261982
Sum of electronic and thermal Energies= -5384.229487
Sum of electronic and thermal Enthalpies= -5384.228543
Sum of electronic and thermal Free Energies= -5384.331814
HF= -5384.7739164
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.860809
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.811014
Solvent correction = -0.0497947
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.695606
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.3183203

^{3}F-TS

Imaginary Frequency (cm^{-1}) = -649.88

Ni	-0.75955300	1.71943000	-0.27458400
C	-2.43502600	2.13047400	-1.04128600
C	-2.37134300	0.75393900	-1.13377000
H	-2.00075300	0.29224400	-2.07003300
Br	-1.06861900	2.75632900	1.95636800
C	1.87095900	2.60629300	0.10447700
C	2.22490500	4.85880900	0.25315400
C	0.96031000	4.52444900	-0.59008900
N	0.96242000	3.05455500	-0.69872100
H	3.02690400	5.30493700	-0.36183900
C	0.99176900	-0.87900200	0.71192900
C	2.47171400	-0.91087700	1.20367200
C	1.91560500	1.14291100	0.35569900
N	0.79842700	0.50360900	0.24868600
H	3.07368100	-1.70890200	0.74484200
H	2.01411800	5.52790900	1.09858200
H	2.52417100	-1.02015800	2.30048000
C	0.91851500	5.19532100	-1.95370800
H	1.80313900	4.92291100	-2.55186600
H	0.02055900	4.87817200	-2.50409100
H	0.89161700	6.29168900	-1.84958300
C	-0.02022100	-1.22685500	1.79690400
H	0.04383800	-0.50086600	2.62118800
H	-1.04178700	-1.19065600	1.39865300
H	0.16894000	-2.24015300	2.18583200

H	0.05168300	4.77955200	-0.01679600
H	0.84944200	-1.55404900	-0.15048000
N	2.63314000	3.53231100	0.75413400
N	2.97969400	0.40800700	0.79323000
C	3.28644400	3.33424400	1.99794400
C	4.58313000	3.82647000	2.18790900
C	2.63020500	2.64821500	3.02976700
C	5.23571200	3.60744700	3.40074700
H	5.08456500	4.34941600	1.37224100
C	3.30101300	2.41461300	4.23160800
H	1.58873100	2.34262200	2.89038200
C	4.60258000	2.88951300	4.42013600
H	6.25165200	3.98248200	3.54279400
H	2.79014900	1.87912600	5.03547300
H	5.12004500	2.71037200	5.36545600
C	4.34099300	0.75561500	0.74591100
C	4.84581000	1.51025200	-0.32528300
C	5.20509300	0.33657200	1.76749200
C	6.19040800	1.87779200	-0.34421900
H	4.18388600	1.80026200	-1.14285000
C	6.55218600	0.69443300	1.72936900
H	4.81326500	-0.23883900	2.60667300
C	7.05005700	1.47350900	0.68156000
H	6.57287300	2.47100800	-1.17820500
H	7.21463900	0.37416800	2.53658900
H	8.10427100	1.75747300	0.65966500
H	-2.92177500	3.04719900	-1.35776000
C	-2.98412700	-0.22651300	-0.20937200
C	-3.56040800	0.16379800	1.01531500
C	-2.96222900	-1.59570800	-0.53268300
C	-4.08550500	-0.79022300	1.88431500
H	-3.55083600	1.21925200	1.29230800
C	-3.49221000	-2.54934600	0.33829400
H	-2.51706800	-1.91110800	-1.48096600
C	-4.05408000	-2.15117800	1.55468400
H	-4.51659700	-0.46949100	2.83610700
H	-3.46484500	-3.60806200	0.06704600
H	-4.46473000	-2.89480800	2.24202100

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.508645 (Hartree/Particle)
Thermal correction to Energy= 0.540978
Thermal correction to Enthalpy= 0.541923
Thermal correction to Gibbs Free Energy= 0.440543
Sum of electronic and zero-point Energies= -5384.216413
Sum of electronic and thermal Energies= -5384.184080
Sum of electronic and thermal Enthalpies= -5384.183135
Sum of electronic and thermal Free Energies= -5384.284515
HF= -5384.725058
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.783063
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.740852
Solvent correction = -0.0422116
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.644673
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.278215

^{3}F*cis*

Ni	-1.04650200	2.20376700	0.11952700
C	-0.86524800	1.19188000	-1.56619900
C	-1.42272600	-0.01029500	-1.81762000
H	-1.19068300	-0.57452500	-2.73500000
Br	-2.63078400	3.83222100	0.85529000
C	1.58330000	2.86193700	0.89000900
C	2.31176600	5.01241600	0.64919300
C	0.83313000	4.86035200	0.19172000
N	0.61044600	3.40667200	0.23857900
H	2.98569200	5.16783500	-0.21314400
C	0.38837100	-0.55051600	1.28055800
C	1.90233200	-0.79229600	1.55877100
C	1.47063200	1.40894800	1.12256500
N	0.27446500	0.91538000	1.15641000
H	2.34574600	-1.56828300	0.91928300
H	2.46827900	5.82692600	1.36949300
H	2.07985700	-1.06332200	2.61466600
C	0.51198400	5.43603500	-1.17632700
H	1.14091200	4.97370200	-1.95371900
H	-0.54367100	5.23810700	-1.41110800
H	0.67555500	6.52502100	-1.18916400
C	-0.53375000	-1.10806200	2.35198100
H	-0.29638500	-0.67111800	3.33528800
H	-1.58014500	-0.88431100	2.10819400
H	-0.42698500	-2.20200000	2.41632300
H	0.14152600	5.29901000	0.93264400
H	0.09922700	-0.96695500	0.30182500
N	2.58144700	3.70763400	1.28311300
N	2.49894300	0.52021000	1.25400700
C	3.57305100	3.45861100	2.25105300
C	4.87842100	3.93063000	2.05600800
C	3.25959800	2.73773200	3.41407600
C	5.86406800	3.66076500	3.00483500
H	5.12301400	4.48184600	1.14701000
C	4.25659900	2.45666100	4.34766000
H	2.23255000	2.41126600	3.58693400
C	5.56190600	2.91494800	4.14777000
H	6.88122800	4.02319300	2.84044300
H	4.00567600	1.89107200	5.24806900
H	6.33887200	2.69927900	4.88418800
C	3.83140800	0.72479500	0.83814500
C	4.10095900	1.42912600	-0.34555600
C	4.89025800	0.22569100	1.60824400
C	5.42131300	1.66775000	-0.72687200
H	3.27322200	1.77377200	-0.96846800
C	6.20687600	0.45184800	1.20863900
H	4.67636100	-0.31060200	2.53380100
C	6.47845900	1.18197800	0.04772200
H	5.62421400	2.22077800	-1.64697900
H	7.02746100	0.06952200	1.81966400
H	7.51124900	1.36501100	-0.25632200
H	-0.19483700	1.58191000	-2.35028300
C	-2.34251700	-0.69393400	-0.88708900
C	-3.17891700	0.03533200	-0.01774800
C	-2.39038000	-2.09969300	-0.81553500
C	-3.99101000	-0.61127500	0.91470000
H	-3.22610500	1.12474700	-0.10187400
C	-3.20409700	-2.74897300	0.11507000

H	-1.76466900	-2.68659400	-1.49452500
C	-4.00440300	-2.00799500	0.99159400
H	-4.62624400	-0.01517600	1.57474100
H	-3.21546900	-3.84152400	0.15708300
H	-4.64329900	-2.51596000	1.71809400

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.512116
(Hartree/Particle)
Thermal correction to Energy= 0.544284
Thermal correction to Enthalpy= 0.545228
Thermal correction to Gibbs Free Energy= 0.444184
Sum of electronic and zero-point Energies= -5384.267068
Sum of electronic and thermal Energies= -5384.234900
Sum of electronic and thermal Enthalpies= -5384.233956
Sum of electronic and thermal Free Energies= -5384.335000
HF= -5384.7791837
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.864299
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5382.817199
Solvent correction = -0.0471001
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5386.699301
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5385.321349

Figure A4.4
B-TS-G$^{s\text{-}z}$-Td

Ni	-0.78173700	1.38940200	0.56334800
C	-1.86459200	0.52178500	1.98244000
C	-1.91520400	-0.81118800	2.20100200
H	-2.38625800	-1.21679700	3.11134700
Br	-0.19185900	3.64110700	1.51070600
C	1.61310000	1.88179700	-0.89883500
C	1.59368000	3.61337000	-2.39169800
C	0.15673200	3.07328700	-2.11090100
N	0.36075500	1.93870200	-1.19913800
H	1.89035300	3.46487100	-3.44401900
C	1.67010000	-0.27007100	2.03304400
C	3.17931200	-0.36190200	1.64686600
C	2.00315800	0.90976500	0.14650500
N	1.08570700	0.58812600	0.99342000
H	3.52873600	-1.39487800	1.50166200
H	1.70901600	4.67724000	-2.14014300
H	3.81977400	0.12188600	2.40369200
C	-0.61151800	2.65932900	-3.35805100
H	-0.04649800	1.90344300	-3.92753000
H	-1.57316000	2.22084500	-3.06129100
H	-0.78927600	3.52841500	-4.01164300
C	1.42963800	0.32183200	3.41612400
H	1.85140500	1.33673500	3.47838500
H	0.35157600	0.38975600	3.61042500
H	1.89526800	-0.31180100	4.18816400
H	-0.42457700	3.82129300	-1.54479300
H	1.18872100	-1.25773400	1.96793100
N	2.43488200	2.79648800	-1.49277800
N	3.23777100	0.37209500	0.37136200
C	3.63704000	3.28108000	-0.91318300
C	4.76503400	3.48308700	-1.71657800
C	3.68827200	3.55469700	0.46134300
C	5.95302300	3.93356100	-1.14150000
H	4.71260700	3.25288700	-2.78162500
C	4.88823500	3.98357000	1.03141100
H	2.77876000	3.45745300	1.06141200
C	6.02175900	4.17193500	0.23470800
H	6.83557400	4.07902700	-1.76834600
H	4.92925400	4.19311300	2.10296700
H	6.95690100	4.51354700	0.68448700
C	4.31568100	0.30890100	-0.52983400
C	4.08763500	0.10957500	-1.90058200
C	5.62910600	0.43679200	-0.05622000
C	5.16256000	0.08575300	-2.78837500
H	3.06833800	-0.03349100	-2.26280500
C	6.69856200	0.39228200	-0.94959500
H	5.80540500	0.60487300	1.00681100
C	6.47177900	0.22732600	-2.31891700
H	4.97548800	-0.06271200	-3.85457200
H	7.71759700	0.50533800	-0.57286300
H	7.31180000	0.20118300	-3.01630700
H	-2.34468900	1.13224600	2.75990700
C	-1.27266100	-1.83326400	1.35557400
C	-0.87905600	-3.06427500	1.91788200
C	-0.96525800	-1.60790200	-0.00337200
C	-0.15553900	-4.00273500	1.17961800
H	-1.12445500	-3.26804100	2.96415800
C	-0.23792700	-2.54286000	-0.73981500
H	-1.32462600	-0.70367200	-0.49883400
C	0.18317200	-3.74097500	-0.15224200
H	0.15055000	-4.94249900	1.64715900
H	-0.00813500	-2.33694300	-1.78882500
H	0.75295500	-4.47183600	-0.73136500
C	-4.04143100	3.12227100	1.95421800
H	-3.25184000	3.39726900	2.67521800
C	-3.40030800	3.02609400	0.61915100
H	-2.71487200	3.81573400	0.30193400
H	-4.44339900	2.14294400	2.25284800
O	-2.46914800	1.09866600	-1.12749600
O	-4.51860000	2.56190400	-1.74180200
O	-4.79153000	0.76812700	0.04261800
P	-3.69790800	1.78118600	-0.57455000
C	-5.18737900	4.17750300	2.05595000
C	-6.33592800	3.79257600	1.11062600
H	-7.17413000	4.50177400	1.20843700
H	-6.00745000	3.79569600	0.06021400
H	-6.71334700	2.78247300	1.33632700
C	-4.65583300	5.57191800	1.69267500
H	-3.78614400	5.84094200	2.31350000
H	-4.34377700	5.62059700	0.63798500
H	-5.43530300	6.33603200	1.84536800
C	-5.68817300	4.17887500	3.50721300
H	-6.51040900	4.90123400	3.63751200
H	-6.06323100	3.18408400	3.79793100
H	-4.88157700	4.45334300	4.20601100
C	-4.62221400	-0.65141400	0.09874700
H	-4.56701400	-0.96143600	1.15010400
H	-5.49140600	-1.11804400	-0.38860700
H	-3.69806700	-0.95904400	-0.40749900
C	-4.97605800	1.83497200	-2.87868300

H	-5.36899400	2.56617600	-3.59769700
H	-4.15173500	1.26984000	-3.34300100
H	-5.78125300	1.13694500	-2.59515900

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.769589 (Hartree/Particle)
Thermal correction to Energy= 0.819181
Thermal correction to Enthalpy= 0.820125
Thermal correction to Gibbs Free Energy= 0.679570
Sum of electronic and zero-point Energies= -6266.331688
Sum of electronic and thermal Energies= -6266.282096
Sum of electronic and thermal Enthalpies= -6266.281152
Sum of electronic and thermal Free Energies= -6266.421707
HF= -6267.1012769
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.336363
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.292200
Solvent correction = -0.0441628
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.781629
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.95335

G$^{s\text{-}z}$-Td

Ni	-0.72037800	1.50599900	0.90030900
C	-1.45699600	0.59013400	2.39530700
C	-1.82081900	-0.67983700	2.63569900
H	-2.20997400	-0.88083800	3.64526400
Br	0.11866500	3.58860900	2.17050700
C	1.47681600	2.31302300	-0.65641800
C	1.31383000	4.30783100	-1.75875800
C	-0.09140600	3.69856100	-1.46796200
N	0.19591600	2.41550500	-0.80380300
H	1.50470700	4.40513700	-2.84035500
C	1.81677800	-0.25782600	1.88430900
C	3.18005500	-0.47379200	1.17132000
C	1.95973600	1.16710300	0.14925000
N	1.10476300	0.66008500	0.97980000
H	3.23499100	-1.43268000	0.62852400
H	1.46126900	5.28786900	-1.28340600
H	4.02866200	-0.41625300	1.86786600
C	-0.95379400	3.52508300	-2.71223200
H	-0.44042600	2.88870100	-3.45140500
H	-1.92353800	3.06219700	-2.47763100
H	-1.14479500	4.50528500	-3.17739000
C	1.95603500	0.38139000	3.26414300
H	2.50538600	1.33235800	3.19890200
H	0.96492900	0.59699700	3.68185900
H	2.49192900	-0.30317100	3.94087600
H	-0.61954800	4.31839700	-0.72385200
H	1.25253200	-1.19697900	1.96964400
N	2.23763600	3.32503200	-1.15434400
N	3.21275100	0.63673600	0.19657100
C	3.51609500	3.70095600	-0.65640400
C	4.54013100	4.02448800	-1.55319400
C	3.73503000	3.76309600	0.72653900
C	5.79612300	4.38551700	-1.06630500
H	4.35382400	3.96120800	-2.62628500
C	5.00163600	4.10567900	1.20351300
H	2.90055600	3.57423900	1.40885200
C	6.03308000	4.41505400	0.31161800
H	6.59848700	4.62753100	-1.76663400
H	5.17505200	4.15264500	2.28121000
H	7.02037100	4.68953200	0.69031800
C	4.19618900	0.72730000	-0.81645800
C	3.83246500	0.69769400	-2.17010900
C	5.54543600	0.83485600	-0.45743900
C	4.81371900	0.81268800	-3.15526100
H	2.78277200	0.58393200	-2.44688700
C	6.52157800	0.92969800	-1.44801300
H	5.81856300	0.88046000	0.59751800
C	6.16006200	0.92747900	-2.79856400
H	4.52428900	0.79773100	-4.20854000
H	7.57107600	1.02628700	-1.16188800
H	6.92670000	1.01172400	-3.57176800
H	-1.55157500	1.31098600	3.21442400
C	-1.84361200	-1.86806300	1.76748700
C	-2.72835400	-2.91810300	2.08328000
C	-1.01038100	-2.03556200	0.64532100
C	-2.80462000	-4.06909500	1.29832800
H	-3.37662500	-2.81498000	2.95759300
C	-1.07595500	-3.18992600	-0.13480700
H	-0.31596800	-1.24384100	0.37882900
C	-1.97867100	-4.21156800	0.17955400
H	-3.51027300	-4.86079200	1.56283800
H	-0.41144500	-3.29680600	-0.99664600
H	-2.02953100	-5.11358800	-0.43494000
C	-3.43315600	2.65303000	1.75259100
H	-2.77100900	3.06476700	2.53037000
C	-2.53533500	2.24154400	0.59746800
H	-2.21603900	3.12882800	0.03702700
H	-3.92141900	1.76577800	2.18103800
O	-3.74564600	1.57936400	-1.91552400
O	-4.09213100	0.08290500	0.22114200
O	-1.79569100	0.21179200	-0.91579300
P	-3.16026400	1.10165900	-0.62072100
C	-4.51047500	3.73154700	1.45756000
C	-5.58755700	3.20558200	0.49559300
H	-6.38782600	3.95323700	0.36668600
H	-5.17776900	2.98262200	-0.50035800
H	-6.04493900	2.28149100	0.88367900
C	-3.86088800	4.99524800	0.86854600
H	-3.01231600	5.33072500	1.48629400
H	-3.48768600	4.82035400	-0.15285400
H	-4.59365900	5.81642600	0.80900500
C	-5.16597100	4.08664600	2.80256200
H	-5.95977800	4.83974300	2.66940300
H	-5.62042500	3.19575000	3.26635100
H	-4.42572800	4.49411300	3.51008300
C	-1.37674100	-0.14777500	-2.22320300
H	-0.35846800	0.23959400	-2.37959700
H	-1.37453400	-1.24527600	-2.31114800
H	-2.05313700	0.28664600	-2.97337600
C	-4.61011200	-1.08299600	-0.41331600
H	-5.37146700	-1.50546100	0.25499800
H	-5.06793200	-0.82838200	-1.38252000
H	-3.81168600	-1.82779000	-0.55856900

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.774338 (Hartree/Particle)
Thermal correction to Energy= 0.822645
Thermal correction to Enthalpy= 0.823589
Thermal correction to Gibbs Free Energy= 0.690376
Sum of electronic and zero-point Energies= -6266.361184
Sum of electronic and thermal Energies= -6266.312877
Sum of electronic and thermal Enthalpies= -6266.311933
Sum of electronic and thermal Free Energies= -6266.445146
HF= -6267.1355215
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.355035
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.307826
Solvent correction = -0.0472088
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.810853
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.984863

G-TS-H^{S-Z}-Td

Ni	-0.75088500	1.55992100	1.19147600
C	-1.91505300	1.07908900	2.64188400
C	-2.29992400	-0.13917200	3.11645600
H	-2.53530900	-0.15929500	4.18975500
Br	0.10674800	3.71005400	2.17821000
C	1.33961700	2.19340700	-0.64479400
C	1.17356000	4.09102300	-1.90745400
C	-0.22501000	3.52799400	-1.51916500
N	0.06433300	2.25238200	-0.83882600
H	1.35974400	4.01477000	-2.99358100
C	1.80404400	-0.32893300	1.95303800
C	3.27124100	-0.20072300	1.45384500
C	1.85659500	1.09716100	0.20998700
N	1.06646300	0.64470800	1.12894400
H	3.75301200	-1.16674200	1.24768300
H	1.32050600	5.13399600	-1.59537600
H	3.89267500	0.35651900	2.17726500
C	-1.18603900	3.35066300	-2.68549300
H	-0.74521100	2.69384400	-3.45350200
H	-2.13239200	2.90047800	-2.34954700
H	-1.40953000	4.32367100	-3.15124100
C	1.61568900	-0.03789100	3.43452000
H	1.91712300	0.99640600	3.65916000
H	0.55666700	-0.14610000	3.70707300
H	2.21329300	-0.73439800	4.04375500
H	-0.68324200	4.17921700	-0.75312900
H	1.40803900	-1.33541400	1.72849300
N	2.09174000	3.21016900	-1.15962900
N	3.11745500	0.57286900	0.21177900
C	3.36217600	3.62307700	-0.68623700
C	4.36053700	3.98039100	-1.60090900
C	3.61577600	3.67291000	0.69209700
C	5.62053500	4.35929300	-1.13885200
H	4.15302700	3.92831300	-2.67073400
C	4.88720800	4.03183000	1.14308000
H	2.80072400	3.47037000	1.39274800
C	5.89212700	4.37295700	0.23279500
H	6.40024300	4.62685800	-1.85544700
H	5.08366500	4.07036800	2.21729600
H	6.88303800	4.66068600	0.59159800
C	4.08701000	0.66303600	-0.80158400
C	3.70386000	0.65472600	-2.15243200
C	5.44539300	0.74942600	-0.46568300
C	4.66976400	0.77749500	-3.14987300
H	2.65048100	0.54643700	-2.41574700
C	6.40475700	0.85412700	-1.47213800
H	5.74467200	0.76954900	0.58259800
C	6.02371800	0.87838000	-2.81630000
H	4.36180200	0.77751100	-4.19811700
H	7.45954700	0.93442900	-1.20025000
H	6.77820400	0.96797000	-3.60060200
H	-1.86908800	1.87005900	3.39303900
C	-2.43412000	-1.44764200	2.46649000
C	-3.44644000	-2.33296100	2.88966700
C	-1.54702800	-1.90240000	1.47221000
C	-3.59442200	-3.59532700	2.31574000
H	-4.13687400	-2.00751800	3.67217500
C	-1.69009200	-3.16587200	0.89836900
H	-0.73972300	-1.24770600	1.15523000
C	-2.71988400	-4.01919700	1.30927100
H	-4.39688400	-4.25500800	2.65612800
H	-0.98156600	-3.49464300	0.13284900
H	-2.82976800	-5.00990200	0.86172900
C	-3.79262600	2.82962700	2.09886900
H	-3.17066900	3.34599200	2.84613200
C	-2.81046900	2.08437400	1.19898200
H	-2.24143400	2.85707400	0.65073200
H	-4.41696000	2.10589300	2.64485200
O	-3.93476000	1.56134300	-1.38749900
O	-4.43551600	0.02828400	0.67474000
O	-2.03769400	0.15268200	-0.35022300
P	-3.41538300	1.01120300	-0.09466800
C	-4.70055600	3.91030900	1.44699300
C	-5.88319300	3.28212000	0.69025700
H	-6.57671000	4.06883100	0.35007300
H	-5.55423100	2.72795000	-0.19885800
H	-6.44686600	2.59494200	1.34194700
C	-3.88690700	4.80426100	0.49622200
H	-2.97507600	5.18225600	0.98741500
H	-3.59146800	4.25571400	-0.41102200
H	-4.48741700	5.67025100	0.17414000
C	-5.25220000	4.76653700	2.60065200
H	-5.94863600	5.53210800	2.22256200
H	-5.79927500	4.14421700	3.32803100
H	-4.44008900	5.28101600	3.13935200
C	-1.67504500	-0.36675600	-1.62566400
H	-0.65700300	-0.02033300	-1.84810900
H	-1.70711300	-1.46639700	-1.58487200
H	-2.36239700	0.00593200	-2.39845600
C	-5.03688200	-1.06872400	-0.00969500
H	-5.88397100	-1.40738700	0.60022000
H	-5.39593200	-0.75798800	-1.00345100
H	-4.31604000	-1.89577700	-0.10648500

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.772677 (Hartree/Particle)

Thermal correction to Energy= 0.821003
Thermal correction to Enthalpy= 0.821947
Thermal correction to Gibbs Free Energy= 0.687729
Sum of electronic and zero-point Energies= -6266.342941
Sum of electronic and thermal Energies= -6266.294615
Sum of electronic and thermal Enthalpies= -6266.293671
Sum of electronic and thermal Free Energies= -6266.427889
HF= -6267.1156181
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.337807
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.291649
Solvent correction = -0.0461581
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.790861
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.970169

H

Ni	-0.86955800	0.86556900	0.23468800
Br	-3.06442600	0.80384900	0.86222800
C	1.41429000	2.13566300	-0.69410200
C	1.13240000	3.99637200	-2.00229500
C	-0.23054800	3.47899600	-1.47636900
N	0.10982900	2.19253600	-0.86167700
H	1.24964100	3.78108100	-3.08055300
C	1.52578800	-0.96125200	1.16268400
C	3.04238400	-0.63721300	1.16800000
C	1.88169200	0.93168400	-0.03882300
N	0.92338900	0.21368600	0.52100800
H	3.67212800	-1.49312000	0.88964000
H	1.28561500	5.07215200	-1.84231700
H	3.36655700	-0.27291500	2.16026800
C	-1.32121100	3.32562600	-2.52393800
H	-0.98147600	2.67117400	-3.34238900
H	-2.20675900	2.86529000	-2.06055800
H	-1.60976900	4.30121400	-2.94577400
C	0.91496700	-1.21033300	2.53302200
H	1.10813400	-0.35593300	3.20082000
H	-0.17551200	-1.32433400	2.43902700
H	1.32731800	-2.12135000	2.99457500
H	-0.60141700	4.14517500	-0.67328200
H	1.32964800	-1.83816400	0.51661200
N	2.10073600	3.21664000	-1.20902700
N	3.15471000	0.43060000	0.15957500
C	3.34187300	3.71958000	-0.78938300
C	4.12148500	4.47376000	-1.68215600
C	3.81462100	3.49600700	0.51445900
C	5.36072300	4.97158600	-1.28252400
H	3.76327100	4.64510900	-2.69871600
C	5.06437100	3.98115400	0.89661100
H	3.19955000	2.94501000	1.22614100
C	5.84594900	4.71943600	0.00402100
H	5.95956500	5.54982700	-1.99015400
H	5.42383100	3.79152600	1.91083700
H	6.82233800	5.10051300	0.31002500
C	4.26583900	0.58025400	-0.68261300
C	4.11339500	0.89865800	-2.04290500
C	5.55889000	0.39784300	-0.16269400
C	5.23662400	1.06993300	-2.85036400
H	3.11435700	1.00793700	-2.46515800
C	6.67395100	0.55283300	-0.98467000
H	5.68692000	0.16037600	0.89476000
C	6.52251500	0.90016600	-2.33029500
H	5.10228900	1.32590200	-3.90409500
H	7.67274400	0.41486400	-0.56374500
H	7.39848700	1.03218800	-2.96855400

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.387828 (Hartree/Particle)
Thermal correction to Energy= 0.412497
Thermal correction to Enthalpy= 0.413441
Thermal correction to Gibbs Free Energy= 0.328202
Sum of electronic and zero-point Energies= -5075.528354
Sum of electronic and thermal Energies= -5075.503685
Sum of electronic and thermal Enthalpies= -5075.502741
Sum of electronic and thermal Free Energies= -5075.587980
HF= -5075.916182
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5073.908529
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5073.863646
Solvent correction = -0.044883
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5077.516169
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -5076.433871

B-TS-G'$^{S-Z}$-SP

Ni	-0.76449500	1.81001200	0.09554600
C	-2.09920600	3.18350200	-0.44649600
C	-3.44608300	3.22915900	-0.57355300
H	-3.92541800	4.18424100	-0.84263000
Br	-0.49547000	-0.34030600	-1.05830100
C	2.03435200	2.37105700	-0.33617000
C	2.56952100	3.68948400	-2.12820200
C	1.02880100	3.63588400	-1.90298400
N	0.86941400	2.69001400	-0.78856800
H	2.85546300	3.15945800	-3.05370000
C	1.34100800	0.07415800	2.40522200
C	2.74785800	-0.45534400	1.98518600
C	2.09072900	1.33458400	0.72168500
N	1.11028500	1.25618900	1.55488700
H	2.73963100	-1.51222400	1.68318600
H	2.97547500	4.71021800	-2.17003700
H	3.49271600	-0.32362800	2.78909900
C	0.23797600	3.18025500	-3.12181800
H	0.55102100	2.16873300	-3.42138300
H	-0.83429900	3.14146700	-2.88498200
H	0.39492100	3.87320700	-3.96379500
C	1.22323000	0.41441700	3.88526900
H	1.98991100	1.15384300	4.16965900

H	0.23445500	0.83640500	4.11891700
H	1.37378400	-0.48801700	4.49946800
H	0.65074500	4.61845000	-1.56826800
H	0.56905000	-0.66316400	2.13205400
N	3.09057700	2.97953500	-0.94949000
N	3.07493800	0.39332300	0.82555900
C	4.42866400	3.01144600	-0.51854100
C	5.46851300	2.96615800	-1.45736600
C	4.72877700	3.09637300	0.85045600
C	6.79454500	2.97669000	-1.02586500
H	5.23705500	2.88784400	-2.52006900
C	6.05755000	3.08678600	1.27187100
H	3.91965600	3.18037000	1.57788200
C	7.09628000	3.02589200	0.33771300
H	7.59862500	2.92877600	-1.76352200
H	6.28239400	3.14708400	2.33928700
H	8.13611700	3.02649300	0.67122400
C	3.94624700	0.00042700	-0.21900700
C	3.45579400	-0.13320400	-1.52648600
C	5.29650900	-0.24722600	0.05684200
C	4.33491000	-0.46289200	-2.55944600
H	2.38505800	-0.01148700	-1.71282400
C	6.16145000	-0.60020700	-0.97853200
H	5.66771900	-0.12811300	1.07575000
C	5.68744000	-0.69486100	-2.29065400
H	3.95224700	-0.56472900	-3.57780200
H	7.21641400	-0.78215500	-0.76189100
H	6.36969100	-0.96094100	-3.10122300
H	-1.62136900	4.15703500	-0.65833800
C	-4.41537400	2.14613800	-0.35425000
C	-5.75950900	2.46772000	-0.07930700
C	-4.06454600	0.78414500	-0.41736000
C	-6.71027200	1.47419400	0.15607600
H	-6.05271800	3.52048300	-0.03783900
C	-5.01446700	-0.21020800	-0.18548200
H	-3.04267600	0.50533900	-0.67317600
C	-6.34150500	0.12562700	0.10920500
H	-7.74477000	1.75194300	0.37507700
H	-4.71594700	-1.25997200	-0.25194000
H	-7.08445800	-0.65650700	0.28480800
C	-0.19856100	4.19759400	2.39612400
H	0.03085500	4.72180900	1.45028200
C	-1.64001400	3.81747700	2.35887400
H	-2.39204200	4.54965200	2.06260600
H	0.43225200	3.29809700	2.41641600
O	-1.90301600	1.81513100	4.32894800
O	-1.95123500	1.14885700	1.84359300
O	-3.89130300	2.60638800	2.80750800
P	-2.31412100	2.31306500	2.97783800
C	0.24523400	5.12995900	3.56620900
C	0.15294500	4.37659500	4.90075000
H	0.45018300	5.03152100	5.73616700
H	-0.86227700	4.00167400	5.09161500
H	0.81853300	3.49895000	4.90225000
C	-0.62951200	6.39024800	3.61110300
H	-0.62281000	6.91741200	2.64230600
H	-1.67407100	6.14357800	3.85623100
H	-0.26378200	7.09123700	4.37869100
C	1.70654400	5.52398200	3.30117400
H	2.10071700	6.15151600	4.11664800
H	2.34706700	4.62926700	3.22647400
H	1.80645700	6.08989300	2.36021500
C	-4.87986900	1.70887000	3.31123100
H	-4.51663800	1.19888200	4.21716100
H	-5.76834100	2.30520500	3.55851200
H	-5.15121000	0.97588000	2.53760800
C	-2.17462500	-0.23418100	2.17289500
H	-1.66395700	-0.81896200	1.39792100
H	-1.77463600	-0.44973100	3.17297100
H	-3.25035000	-0.45542500	2.13897900

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.770242 (Hartree/Particle)
Thermal correction to Energy= 0.819192
Thermal correction to Enthalpy= 0.820136
Thermal correction to Gibbs Free Energy= 0.683996
Sum of electronic and zero-point Energies= -6266.328716
Sum of electronic and thermal Energies= -6266.279766
Sum of electronic and thermal Enthalpies= -6266.278822
Sum of electronic and thermal Free Energies= -6266.414962
HF= -6267.0989579
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.261606
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.214503
Solvent correction = -0.0471028
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.776903
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.947631

G'$^{S\text{-}Z}$-SP

Ni	-0.74779400	1.88380100	0.35047500
C	-2.13148500	2.88931500	-0.52048500
C	-3.46759500	2.84569800	-0.62744400
H	-3.92772800	3.68359400	-1.17408400
Br	-0.72327200	0.00147500	-1.23264800
C	2.00448200	2.41651900	-0.30254300
C	2.56636300	4.22626400	-1.58612800
C	1.03696800	3.93212400	-1.63965500
N	0.84747000	2.85634800	-0.66094500
H	3.01656900	4.26243000	-2.58942400
C	1.12238500	-0.27538200	1.97929500
C	2.39869000	-0.88995400	1.34254300
C	2.00192600	1.21192100	0.55411400
N	0.93180200	0.98455700	1.24031800
H	2.16307600	-1.68880700	0.62115800
H	2.80566000	5.16667500	-1.06217100
H	3.10213100	-1.27752300	2.09396000
C	0.55883000	3.46322100	-3.01319800
H	1.14708900	2.59299600	-3.34250900
H	-0.49351700	3.15166700	-2.96852300
H	0.66820100	4.27018800	-3.75514600
C	1.26746400	-0.00578600	3.47572300
H	2.16219100	0.60957500	3.66631400
H	0.39178600	0.52574100	3.87566500
H	1.38466600	-0.95682000	4.01978500
H	0.45411700	4.81210000	-1.32306500

H	0.25132700	-0.91500300	1.78685400
N	3.08589600	3.08591900	-0.80574400
N	2.97871600	0.25747600	0.60986200
C	4.38970500	3.07504800	-0.25914900
C	5.49580300	3.13938800	-1.11596600
C	4.58231700	3.01006000	1.12865700
C	6.78576500	3.11954500	-0.58777700
H	5.33720500	3.16768300	-2.19492100
C	5.87688000	2.96875500	1.64789000
H	3.71881100	2.99728000	1.79626000
C	6.98171800	3.02378500	0.79344100
H	7.64450500	3.15868600	-1.26155400
H	6.02111200	2.91008200	2.72915700
H	7.99365100	2.99834000	1.20350900
C	3.92061200	0.04066900	-0.43646500
C	3.49764000	0.04522700	-1.77289000
C	5.26294300	-0.18889900	-0.11911900
C	4.43545600	-0.13869000	-2.79054000
H	2.43532500	0.17432500	-1.99888800
C	6.19046400	-0.39144700	-1.14098400
H	5.57385100	-0.17275000	0.92644900
C	5.78112200	-0.35541300	-2.47753300
H	4.10875700	-0.13010200	-3.83303200
H	7.24090600	-0.55840700	-0.89308300
H	6.51098900	-0.50405100	-3.27669700
H	-1.64385100	3.75213600	-0.99156900
C	-4.45732600	1.88020800	-0.11758800
C	-5.72134400	2.34979900	0.28772700
C	-4.21768300	0.49629200	-0.07095900
C	-6.70148400	1.47554100	0.75867000
H	-5.92742800	3.42268500	0.24186500
C	-5.20146100	-0.37957400	0.39167700
H	-3.25842100	0.11521300	-0.42220500
C	-6.44419900	0.10201700	0.81746200
H	-7.67144000	1.86615700	1.07772200
H	-4.99877200	-1.45402500	0.40792300
H	-7.21152800	-0.58845400	1.17670600
C	0.29763300	3.75353500	2.44842000
H	1.04778400	3.86702600	1.65060300
C	-1.00253400	3.23053000	1.84718500
H	-1.65915400	4.03889200	1.51323900
H	0.70815900	3.00818400	3.14555300
O	-1.44612200	1.76927100	4.27677500
O	-2.06519900	0.84921100	1.93546400
O	-3.43227700	2.82322200	2.92440000
P	-1.94806400	2.17303100	2.92464300
C	0.20911100	5.12110700	3.17480100
C	-0.86028400	5.09831600	4.27847400
H	-0.84390200	6.03891400	4.85308900
H	-1.87140900	4.98398000	3.85843200
H	-0.69884700	4.25833600	4.97008900
C	-0.11024600	6.23197900	2.16161700
H	0.65924100	6.28053400	1.37199800
H	-1.08384200	6.06935000	1.67364800
H	-0.14845200	7.21679000	2.65475300
C	1.58482800	5.39528400	3.80357600
H	1.60933800	6.38014200	4.29775700
H	1.83006800	4.63199400	4.55971400
H	2.38115000	5.38285500	3.03975200
C	-4.49846900	2.17701500	3.61884700
H	-4.14255300	1.75613000	4.57258000
H	-5.26715400	2.93571500	3.81702600
H	-4.93729800	1.38692700	2.99108200
C	-2.34518200	-0.46492800	2.40538100
H	-2.03975100	-1.15313200	1.60607600
H	-1.78732200	-0.66741000	3.33159600
H	-3.42291600	-0.58642600	2.58681300

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.773858 (Hartree/Particle)
Thermal correction to Energy= 0.822228
Thermal correction to Enthalpy= 0.823172
Thermal correction to Gibbs Free Energy= 0.689368
Sum of electronic and zero-point Energies= -6266.358834
Sum of electronic and thermal Energies= -6266.310464
Sum of electronic and thermal Enthalpies= -6266.309520
Sum of electronic and thermal Free Energies= -6266.443324
HF= -6267.132692
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.353268
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.307696
Solvent correction = -0.0455716
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.808557
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.983529

G-TS-H'$^{S\text{-}Z}$-SP

Ni	-0.69623900	2.23397000	0.28532600
C	-1.82308900	3.76044100	-0.12985500
C	-3.10322700	3.79307300	-0.58087400
H	-3.36507300	4.64074000	-1.22997100
Br	-0.59082700	0.24301600	-1.20444800
C	2.13314800	2.54348300	-0.14125400
C	2.83043300	3.98591600	-1.78025300
C	1.28683800	4.05391400	-1.57680700
N	1.01456300	3.05331300	-0.53389600
H	3.08224900	3.56492300	-2.76884700
C	1.21349500	0.02779400	2.32709000
C	2.40461600	-0.70672900	1.64137300
C	2.06912500	1.38403400	0.77767900
N	1.08239500	1.30406500	1.60260100
H	2.07914800	-1.57295600	1.04443200
H	3.33389500	4.95855500	-1.67804300
H	3.16671500	-1.03822700	2.36436400
C	0.49487800	3.74339800	-2.84197900
H	0.73233400	2.72943800	-3.19639800
H	-0.58466500	3.77373900	-2.64223900
H	0.73450600	4.47237000	-3.63269400
C	1.41515600	0.28035500	3.81832800
H	2.34274900	0.85206100	3.98799900
H	0.56455900	0.85201900	4.21560400
H	1.49544300	-0.67507300	4.36206800
H	0.99058700	5.04643300	-1.19140500
H	0.28433600	-0.53865200	2.17603700
N	3.25724300	3.07678100	-0.70847400
N	2.94135000	0.32740000	0.73691600

C	4.58816400	2.92168600	-0.28535600
C	5.62388200	2.90713800	-1.23044200
C	4.89108600	2.79388200	1.07999300
C	6.94353200	2.73605500	-0.81378000
H	5.39051400	2.99303500	-2.29208200
C	6.21175600	2.60461800	1.48369600
H	4.09156000	2.84923100	1.82024600
C	7.24419200	2.57322000	0.54110700
H	7.74194400	2.71302400	-1.55885800
H	6.43697700	2.49826200	2.54748400
H	8.27824400	2.43174400	0.86243500
C	3.75513900	-0.00948200	-0.37819700
C	3.23728100	0.06007600	-1.67930500
C	5.07951200	-0.41029900	-0.16651100
C	4.06806600	-0.22487900	-2.76486100
H	2.18090400	0.30588200	-1.82303500
C	5.89521300	-0.71523000	-1.25579100
H	5.47108000	-0.44595200	0.85113900
C	5.39629100	-0.60997400	-2.55784500
H	3.66479000	-0.16746600	-3.77883900
H	6.93178400	-1.01564200	-1.08755400
H	6.04018500	-0.83784900	-3.41055300
H	-1.19777700	4.61200100	-0.42129500
C	-4.21791800	2.87847700	-0.27688700
C	-5.46269300	3.40744700	0.11497200
C	-4.09405500	1.48286400	-0.39436400
C	-6.53719400	2.57158700	0.41981000
H	-5.57703200	4.49172000	0.19785100
C	-5.17378000	0.64756500	-0.10089500
H	-3.15109300	1.05660200	-0.73924700
C	-6.39634400	1.18344700	0.31708000
H	-7.49055100	3.00428700	0.73438100
H	-5.06104600	-0.43378200	-0.21721500
H	-7.23949800	0.52595000	0.54416000
C	-0.06949400	4.30628500	2.23824200
H	0.48721500	4.64567700	1.35117700
C	-1.39158900	3.69258300	1.77478700
H	-2.17641000	4.44967200	1.82645700
H	0.55301400	3.52730500	2.69949300
O	-1.41979900	1.92992600	4.07473100
O	-2.08723000	1.16713200	1.67986600
O	-3.59920800	2.85370100	2.95631800
P	-2.06097300	2.36748700	2.79933700
C	-0.19189800	5.52014200	3.19521800
C	-1.04429000	5.18580100	4.42979200
H	-1.03620400	6.02819000	5.14048700
H	-2.09526300	4.99689400	4.15989400
H	-0.67448900	4.28632200	4.94232000
C	-0.80741500	6.71596700	2.45081600
H	-0.19234400	7.00273400	1.58157500
H	-1.82216200	6.49254100	2.08395900
H	-0.88550400	7.59307200	3.11311700
C	1.23120800	5.88550500	3.64656700
H	1.22673400	6.77735200	4.29383000
H	1.68727000	5.05812700	4.21364600
H	1.88049000	6.10035100	2.78130600
C	-4.57045900	2.04944500	3.62173900
H	-4.11638900	1.50086000	4.46218600
H	-5.34752400	2.72354300	4.00629800
H	-5.03025700	1.34974600	2.90719800
C	-2.34906400	-0.20524300	1.97280200
H	-1.87316800	-0.78314100	1.16965500
H	-1.92883800	-0.46804000	2.95463200
H	-3.43405200	-0.38547100	1.96348600

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.772431 (Hartree/Particle)
Thermal correction to Energy= 0.820875
Thermal correction to Enthalpy= 0.821819
Thermal correction to Gibbs Free Energy= 0.687069
Sum of electronic and zero-point Energies= -6266.342268
Sum of electronic and thermal Energies= -6266.293824
Sum of electronic and thermal Enthalpies= -6266.292880
Sum of electronic and thermal Free Energies= -6266.427629
HF= -6267.1146987
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.338677
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.293482
Solvent correction = -0.0451952
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.790061
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.968074

B-TS-G$^{S\text{-}E}$-Td

Ni	-0.48987500	1.80373900	0.91282600
C	-1.54178000	1.13446500	2.45127300
C	-1.92689400	-0.15443500	2.55897100
H	-1.75961200	-0.82042900	1.70236200
Br	0.44548900	3.86709400	1.97238200
C	1.75138100	2.19773100	-0.83428900
C	1.84208700	4.04500800	-2.17559600
C	0.40376100	3.79034500	-1.63957800
N	0.50489500	2.50453400	-0.93724300
H	1.90782300	3.87277000	-3.26461100
C	1.77872800	-0.34952700	1.76901200
C	3.16924300	-0.66048800	1.13323400
C	2.09138000	1.02935800	0.01375100
N	1.20853900	0.67552700	0.88858000
H	3.23799400	-1.67604200	0.71147100
H	2.21362000	5.05481000	-1.95507700
H	3.98749100	-0.53124300	1.85886600
C	-0.68229600	3.77043400	-2.70435300
H	-0.47167600	2.99807400	-3.46167200
H	-1.65776400	3.54526600	-2.24982500
H	-0.75039500	4.74721500	-3.20920100
C	1.86594300	0.18244800	3.19677400
H	2.47102300	1.10141100	3.22607700
H	0.86189900	0.42824000	3.56674000
H	2.31926500	-0.57286300	3.85860600
H	0.15093400	4.53184800	-0.86014600
H	1.12269600	-1.23469800	1.75132700
N	2.64514200	3.04017200	-1.44538700
N	3.26500100	0.33269300	0.04657700
C	3.94256500	3.31363700	-0.93951200
C	5.01158200	3.49124800	-1.82576500
C	4.14842500	3.40782800	0.44491500

C	6.29112000	3.73518300	-1.32783200
H	4.83752300	3.40385000	-2.89921800
C	5.43719300	3.62828600	0.93391000
H	3.29059000	3.34382100	1.12122700
C	6.51041000	3.78986100	0.05226800
H	7.12536100	3.86274900	-2.02130700
H	5.59713700	3.69902300	2.01245100
H	7.51583300	3.96978800	0.43984100
C	4.24392600	0.27133000	-0.96795600
C	3.87213200	0.25776700	-2.32038700
C	5.59957800	0.21291200	-0.61809100
C	4.85403600	0.22574400	-3.31060100
H	2.81487300	0.27092000	-2.59028700
C	6.57364800	0.16129100	-1.61406100
H	5.88580600	0.24471100	0.43389000
C	6.20696400	0.17644700	-2.96289400
H	4.55770300	0.22379600	-4.36220900
H	7.62861100	0.12899800	-1.33315900
H	6.97297600	0.14557700	-3.74073500
H	-1.70012200	1.80595900	3.30571400
C	-2.57380700	-0.81320100	3.70526600
C	-2.78031300	-2.20731300	3.68016700
C	-3.03137800	-0.10602300	4.83663600
C	-3.41024000	-2.86949800	4.73540500
H	-2.43355500	-2.77508500	2.81154100
C	-3.65912900	-0.76529600	5.89107300
H	-2.89584700	0.97624600	4.87843000
C	-3.85349200	-2.15166500	5.84929200
H	-3.55602100	-3.95203300	4.68820800
H	-4.00616500	-0.19258200	6.75523200
H	-4.34884200	-2.66504500	6.67687000
C	-4.27718200	2.60279600	2.18336800
H	-3.71889700	2.99146200	3.05284800
C	-3.38251700	2.66336500	0.99385800
H	-2.84248300	3.58947500	0.77233800
H	-4.52758600	1.55581800	2.40894300
O	-1.95161500	0.79481900	-0.53889100
O	-3.85331300	2.20577500	-1.57792900
O	-4.44966500	0.35040800	0.07209300
P	-3.29441900	1.43484800	-0.25341800
C	-5.60158400	3.41930200	2.06860200
C	-6.44821400	2.89965400	0.89664500
H	-7.40757600	3.44002700	0.84396500
H	-5.92799400	3.03572400	-0.06370200
H	-6.66210000	1.82543700	1.00621200
C	-5.28814500	4.90826600	1.86049300
H	-4.65315200	5.30019500	2.67183200
H	-4.76363200	5.07914100	0.90755700
H	-6.21652700	5.50194800	1.84056400
C	-6.37161000	3.23414300	3.38428900
H	-7.32435200	3.78789600	3.36387900
H	-6.60084300	2.17099700	3.56223100
H	-5.78621300	3.60028300	4.24347100
C	-4.21309100	-1.05158800	0.19501600
H	-4.30165000	-1.34554900	1.25065400
H	-4.97556500	-1.57649500	-0.39940500
H	-3.21053800	-1.31127400	-0.17319600
C	-3.86183800	1.51751800	-2.82603300
H	-4.10627200	2.25365200	-3.60361300
H	-2.87592700	1.07178900	-3.03152400
H	-4.62860200	0.72473500	-2.82481400

(U)B3LYP-D3(BJ)/def2-SVP

Zero-point correction= 0.770114 (Hartree/Particle)
Thermal correction to Energy= 0.819383
Thermal correction to Enthalpy= 0.820327
Thermal correction to Gibbs Free Energy= 0.679827
Sum of electronic and zero-point Energies= -6266.326188
Sum of electronic and thermal Energies= -6266.276919
Sum of electronic and thermal Enthalpies= -6266.275975
Sum of electronic and thermal Free Energies= -6266.416474
HF= -6267.0963017
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.333626
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.283708
Solvent correction = -0.0499174
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.777738
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.948642

$G^{S\text{-}E}$-Td

Ni	-0.89170000	1.62385600	0.99970000
C	-1.64142500	0.74446800	2.49551800
C	-1.86165000	-0.57668100	2.52815600
H	-1.70123300	-1.14955900	1.60813600
Br	0.02376200	3.66180500	2.27116700
C	1.31099100	2.27111300	-0.59505500
C	1.25384500	4.32431100	-1.59499800
C	-0.18035500	3.76179000	-1.35959200
N	0.03820500	2.47544400	-0.68217000
H	1.44628500	4.54616200	-2.65661200
C	1.51210500	-0.33704800	1.91770900
C	2.84570600	-0.64818700	1.17751800
C	1.73318900	1.09235500	0.19513000
N	0.87350400	0.67017600	1.06220600
H	2.82782700	-1.61294400	0.64361900
H	1.45453100	5.22719800	-0.99947600
H	3.70889100	-0.64185100	1.85910700
C	-0.98865400	3.58055900	-2.64007700
H	-0.45064000	2.92765200	-3.34635300
H	-1.96278100	3.12010800	-2.42459200
H	-1.15858600	4.55464100	-3.12594700
C	1.71911800	0.23273900	3.31906900
H	2.35309900	1.13141700	3.28015600
H	0.75490500	0.52388300	3.75418900
H	2.19509300	-0.51996200	3.96751200
H	-0.72632800	4.40665100	-0.65212000
H	0.86382700	-1.22354800	1.97422100
N	2.12721100	3.22865900	-1.11983500
N	2.93534000	0.45008500	0.19289100
C	3.44151400	3.49588600	-0.63848600
C	4.47860900	3.72361300	-1.54872600
C	3.68181700	3.54434000	0.74156100
C	5.76753500	3.97520300	-1.07890500
H	4.27294300	3.66950400	-2.61870600
C	4.97911500	3.77735900	1.20212600

H	2.84365500	3.42695100	1.43570500
C	6.02245400	3.99086300	0.29596000
H	6.57990400	4.14072800	-1.78986500
H	5.16986200	3.81182400	2.27735900
H	7.03478400	4.17830900	0.66154400
C	3.88987400	0.46443900	-0.84914300
C	3.48364700	0.48756300	-2.19107800
C	5.25435200	0.44552600	-0.53267900
C	4.44108600	0.53009900	-3.20508400
H	2.42000200	0.46930700	-2.43521600
C	6.20431000	0.46799700	-1.55256600
H	5.56326800	0.44984600	0.51345700
C	5.80287500	0.51930300	-2.89085900
H	4.11896400	0.55615600	-4.24868100
H	7.26661100	0.46545500	-1.29883400
H	6.54983200	0.54633700	-3.68717400
H	-1.79278200	1.39720800	3.36123100
C	-2.32123300	-1.37274300	3.67945700
C	-2.49534300	-2.76153300	3.52508800
C	-2.60692000	-0.81091200	4.94013800
C	-2.93435900	-3.56017000	4.58296300
H	-2.28097000	-3.21459300	2.55288800
C	-3.04398400	-1.60676700	5.99671400
H	-2.48512700	0.26381200	5.08895600
C	-3.21083500	-2.98679500	5.82634600
H	-3.06135300	-4.63583800	4.43509500
H	-3.25906900	-1.14730700	6.96499300
H	-3.55486500	-3.60742100	6.65714800
C	-3.58096500	2.85138300	1.78747300
H	-2.91151700	3.26196800	2.56020400
C	-2.69543500	2.36080600	0.65483600
H	-2.41176900	3.18625500	-0.00763800
H	-4.11277900	2.00285700	2.24465100
O	-2.07541500	0.00215200	-0.58226200
O	-3.74382600	1.63850500	-1.75202500
O	-4.53715800	0.30099900	0.24824000
P	-3.19566000	0.98912200	-0.35458600
C	-4.60679000	3.96081800	1.43889500
C	-5.64532900	3.46756600	0.41989200
H	-6.40749600	4.24349800	0.23765000
H	-5.18000100	3.21980800	-0.54480700
H	-6.15585500	2.56147400	0.78139100
C	-3.88212900	5.19961300	0.88483800
H	-3.06641500	5.51539400	1.55459700
H	-3.44385700	5.00391400	-0.10676100
H	-4.58410500	6.04141200	0.76834500
C	-5.32110500	4.34329000	2.74552700
H	-6.07151500	5.13174900	2.57137800
H	-5.84031200	3.47308800	3.17964600
H	-4.60432300	4.71632600	3.49491000
C	-4.59732800	-1.04985800	0.70103000
H	-4.55981200	-1.07949700	1.79934200
H	-5.54971700	-1.47691100	0.35354700
H	-3.75905600	-1.63510500	0.29708900
C	-4.16302300	0.76417400	-2.79497100
H	-4.28445300	1.37005500	-3.70323600
H	-3.40995800	-0.02036300	-2.97246200
H	-5.12713500	0.29392400	-2.54013100

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.773202 (Hartree/Particle)
Thermal correction to Energy= 0.822267
Thermal correction to Enthalpy= 0.823211
Thermal correction to Gibbs Free Energy= 0.685631
Sum of electronic and zero-point Energies= -6266.362151
Sum of electronic and thermal Energies= -6266.313087
Sum of electronic and thermal Enthalpies= -6266.312143
Sum of electronic and thermal Free Energies= -6266.449723
HF= -6267.1353534
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.354763
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.307479
Solvent correction = -0.0472843
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.813401
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.987731

G-TS-H$^{S\text{-}E}$-Td

Ni	-0.79858200	1.54355900	1.21097400
C	-1.87279600	0.74306700	2.53827700
C	-2.08449000	-0.59749100	2.51734100
H	-2.09497900	-1.10575300	1.54998900
Br	0.02371700	3.54159800	2.45537300
C	1.25978900	2.19660300	-0.59346700
C	1.13884900	4.18030500	-1.72144800
C	-0.26530900	3.68781500	-1.26209700
N	-0.01909800	2.35776400	-0.67649200
H	1.23733800	4.16844700	-2.82123200
C	1.66167700	-0.49219300	1.82920500
C	3.10581400	-0.47080200	1.24603400
C	1.75444100	1.02555500	0.16731400
N	0.98355400	0.59315300	1.10832300
H	3.47623300	-1.46143000	0.94672500
H	1.38317900	5.18723400	-1.35615800
H	3.81854300	-0.03116100	1.96635000
C	-1.30766300	3.63640300	-2.36878700
H	-0.96713500	2.98809800	-3.19220400
H	-2.25314700	3.23074200	-1.98250600
H	-1.49582600	4.64464700	-2.77090400
C	1.59440400	-0.27664200	3.33484800
H	1.99117600	0.71640300	3.59440900
H	0.55293300	-0.32668000	3.67872500
H	2.17406700	-1.05138300	3.86139500
H	-0.63084900	4.31906800	-0.43230400
H	1.15091700	-1.43743100	1.57238100
N	2.04518300	3.18964900	-1.10808400
N	2.96530600	0.40166000	0.06820000
C	3.34365000	3.50760200	-0.63199600
C	4.35525300	3.84447400	-1.53891100
C	3.60855200	3.47729200	0.74510100
C	5.63921900	4.12361700	-1.07158500
H	4.13689100	3.85187800	-2.60771900
C	4.90263500	3.73570200	1.20069000
H	2.78938000	3.28708900	1.44507800
C	5.91999900	4.05626100	0.29667300
H	6.42979800	4.37453300	-1.78222400

H	5.10905700	3.71008400	2.27335200
H	6.92952800	4.26414000	0.65870900
C	3.90344600	0.50247600	-0.97290300
C	3.47472600	0.61620200	-2.30521000
C	5.27547200	0.48050600	-0.68433300
C	4.41247000	0.75219100	-3.32758600
H	2.40816300	0.58960800	-2.53395800
C	6.20513500	0.59942600	-1.71686200
H	5.61079200	0.40391600	0.35045000
C	5.78083900	0.74562300	-3.04024200
H	4.06972700	0.84635100	-4.36074200
H	7.27162900	0.59371200	-1.48090700
H	6.51241300	0.84517100	-3.84486700
H	-1.88416000	1.30030400	3.47773300
C	-2.24809000	-1.46224600	3.68628100
C	-2.37902500	-2.85417900	3.49159100
C	-2.27522000	-0.98384700	5.01495300
C	-2.53207400	-3.72756500	4.56841800
H	-2.35895100	-3.24575700	2.47068100
C	-2.42634700	-1.85703800	6.08937300
H	-2.17891700	0.08691800	5.20523400
C	-2.55585500	-3.23521700	5.87635700
H	-2.63306400	-4.80064900	4.38548600
H	-2.44486500	-1.45915700	7.10739700
H	-2.67477500	-3.91614100	6.72234200
C	-3.73381900	2.61857100	2.33681200
H	-3.03145000	3.00751900	3.09032100
C	-2.85477100	1.96906700	1.27135900
H	-2.36188400	2.78076600	0.70774300
H	-4.34961800	1.85225100	2.83296500
O	-2.53305100	-0.14231300	-0.49730700
O	-4.07385700	1.87035700	-1.12288700
O	-4.89115400	0.21062900	0.59081400
P	-3.51351200	0.86098500	0.03055500
C	-4.63720000	3.81380700	1.92387100
C	-5.90800500	3.34967900	1.19491900
H	-6.56536000	4.21086400	0.98948100
H	-5.67396400	2.86876400	0.23779300
H	-6.47342800	2.62939800	1.80721800
C	-3.85702600	4.80490200	1.04410700
H	-2.89093300	5.06897800	1.50449100
H	-3.66041800	4.38523300	0.04567400
H	-4.43624800	5.73172600	0.90213400
C	-5.04942600	4.51770400	3.22918300
H	-5.73839600	5.35305000	3.02461300
H	-5.56211200	3.81826800	3.91007900
H	-4.17106600	4.92175500	3.75768200
C	-5.00459500	-1.16419400	0.95549700
H	-4.80411500	-1.29273600	2.02951500
H	-6.03429200	-1.47855100	0.73315300
H	-4.29725700	-1.77938200	0.37996600
C	-4.61820300	1.30751800	-2.31560200
H	-4.68507300	2.11556500	-3.05639300
H	-3.96578700	0.50698600	-2.69781600
H	-5.62463000	0.90164000	-2.12355400

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.771963 (Hartree/Particle)
Thermal correction to Energy= 0.820838
Thermal correction to Enthalpy= 0.821782
Thermal correction to Gibbs Free Energy= 0.683755
Sum of electronic and zero-point Energies= -6266.344552
Sum of electronic and thermal Energies= -6266.295676
Sum of electronic and thermal Enthalpies= -6266.294732
Sum of electronic and thermal Free Energies= -6266.432759
HF= -6267.1165143
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.338614
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.29066
Solvent correction = -0.047954
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.796003
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.975739

B-TS-G'$^{S-E}$-SP

Ni	-0.78307700	1.25917300	0.32546100
C	-2.52362100	1.88706100	-0.36827600
C	-2.87042300	3.11239700	-0.81826400
H	-2.10120900	3.89794800	-0.86651600
Br	-0.05362500	-0.83940000	-0.71149600
C	1.76547400	2.44343200	-0.20537700
C	2.05932100	3.69419800	-2.08859600
C	0.55414700	3.38091200	-1.84918100
N	0.56769300	2.47464400	-0.68729800
H	2.45460400	3.10417600	-2.93517900
C	1.50907400	0.14646000	2.60914300
C	3.01968300	-0.02742300	2.28445700
C	2.02565000	1.49050600	0.89872200
N	1.07184400	1.25278800	1.73350000
H	3.31301800	-1.07118000	2.10712700
H	2.26967800	4.75712700	-2.27064100
H	3.65557900	0.39389400	3.08383100
C	-0.13653200	2.74518000	-3.04629300
H	0.34771800	1.78884200	-3.29568900
H	-1.18892000	2.53870600	-2.81359300
H	-0.08493600	3.41556600	-3.91906600
C	1.20365400	0.41894100	4.07523800
H	1.81462000	1.25695200	4.45004000
H	0.14685600	0.69319900	4.20318900
H	1.42123100	-0.46842900	4.69001800
H	0.01464100	4.29745400	-1.54917000
H	0.95103800	-0.73998200	2.25991100
N	2.67620700	3.24474800	-0.83265500
N	3.16907800	0.76285000	1.04784100
C	3.98209000	3.54860900	-0.41291600
C	5.01578700	3.66938200	-1.35182500
C	4.25354900	3.74394700	0.95135100
C	6.31269400	3.95201600	-0.92361500
H	4.81034100	3.50896300	-2.41049000
C	5.55666000	4.00793000	1.36938900
H	3.43914100	3.69922600	1.67671000
C	6.59266600	4.11207700	0.43585300
H	7.11448000	4.03164000	-1.66102700
H	5.76001800	4.15271900	2.43301500
H	7.61108100	4.32669200	0.76630300

C	4.13002400	0.51480700	0.04126900
C	3.70874700	0.25127200	-1.27096000
C	5.49483500	0.53654500	0.35377900
C	4.66140600	0.06737500	-2.27401200
H	2.63992200	0.15007700	-1.47866900
C	6.43779100	0.32779700	-0.65240400
H	5.81040900	0.75014900	1.37598800
C	6.02591200	0.10786000	-1.97038000
H	4.33219900	-0.13747800	-3.29555000
H	7.50198200	0.35644300	-0.40804600
H	6.76780000	-0.04533000	-2.75737500
H	-3.34172600	1.15291300	-0.28749700
C	-4.20301700	3.59415400	-1.21414800
C	-4.37383900	4.94665900	-1.57116900
C	-5.34188300	2.76223500	-1.23477300
C	-5.62349700	5.45048900	-1.93477800
H	-3.50286200	5.60888600	-1.56007200
C	-6.58918100	3.26284700	-1.59982800
H	-5.23875100	1.71131200	-0.95636500
C	-6.73964000	4.61003200	-1.95278300
H	-5.72695700	6.50456400	-2.20612500
H	-7.45658600	2.59738500	-1.60949400
H	-7.71996100	4.99949300	-2.23792600
C	-0.91899300	3.78320900	2.25048500
H	-0.76256800	4.20277300	1.24045800
C	-2.17263600	2.97448800	2.20476900
H	-3.07045600	3.41405300	1.77012300
H	-0.05374800	3.14411700	2.46705700
O	-2.05755900	1.29083600	4.46181100
O	-1.77502000	0.33074400	2.05655500
O	-4.05631100	1.17986100	2.77665600
P	-2.47844800	1.45511100	3.03497800
C	-0.90401700	4.97497600	3.25598700
C	-0.96299600	4.44448400	4.69528800
H	-0.94690900	5.27700300	5.41773200
H	-1.86659400	3.84429800	4.87268000
H	-0.10343300	3.78875300	4.90860100
C	-2.08641700	5.91695300	2.98954200
H	-2.08647100	6.27302200	1.94558900
H	-3.04879600	5.41493000	3.17417400
H	-2.03972400	6.79925000	3.64816700
C	0.41614100	5.73071400	3.03963200
H	0.50994900	6.57349700	3.74343800
H	1.28178800	5.06519000	3.19477500
H	0.48193900	6.13619300	2.01634500
C	-4.93175500	0.75845600	3.82149600
H	-4.44886200	0.86753200	4.80378500
H	-5.84142300	1.37517400	3.78033300
H	-5.20493600	-0.29759400	3.66650600
C	-1.99487400	-1.06508900	2.30806000
H	-1.29365500	-1.60841000	1.66287200
H	-1.81463500	-1.28436600	3.37128400
H	-3.02698400	-1.33116800	2.03376700

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.769122 (Hartree/Particle)
Thermal correction to Energy= 0.818951
Thermal correction to Enthalpy= 0.819895
Thermal correction to Gibbs Free Energy= 0.676814
Sum of electronic and zero-point Energies= -6266.324327
Sum of electronic and thermal Energies= -6266.274499
Sum of electronic and thermal Enthalpies= -6266.273555
Sum of electronic and thermal Free Energies= -6266.416636
HF= -6267.0934496
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.269727
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.221596
Solvent correction = -0.048131
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.773548
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.944033

G'$^{S\text{-}E}$-SP

Ni	-0.73990000	1.26288900	0.37012100
C	-2.31203100	1.65634600	-0.64012300
C	-3.59741300	1.75322200	-0.27622000
H	-3.87789400	1.71735200	0.78129900
Br	-0.31383500	-0.67649800	-1.11081100
C	1.82706700	2.34951100	-0.23794400
C	2.11032900	4.12695500	-1.63751200
C	0.60423800	3.80795000	-1.41923700
N	0.62206400	2.55060100	-0.65369900
H	2.43216500	3.84449700	-2.65662300
C	1.45184400	-0.49174500	2.00337000
C	2.77378600	-0.89422100	1.29179400
C	2.04352100	1.14909000	0.59679600
N	1.04873000	0.75113100	1.31799200
H	2.62161500	-1.69264500	0.54855300
H	2.36841300	5.18116900	-1.46605200
H	3.55942600	-1.19647700	1.99967400
C	-0.19624500	3.70507700	-2.70785700
H	0.16597400	2.86360600	-3.31803900
H	-1.25964400	3.54078900	-2.49014900
H	-0.10280300	4.63476500	-3.29132200
C	1.62394500	-0.24577600	3.50035100
H	2.41709300	0.49982600	3.67750300
H	0.69062100	0.12426700	3.94742100
H	1.91606200	-1.18180300	4.00326500
H	0.14393500	4.57446300	-0.76743800
H	0.66651700	-1.23891400	1.82450800
N	2.75778000	3.26647300	-0.63716500
N	3.14762300	0.34985300	0.58016900
C	4.07171200	3.42120400	-0.16182900
C	5.10362500	3.75629800	-1.04947000
C	4.35269400	3.25207000	1.20331300
C	6.40843900	3.89354700	-0.57696000
H	4.88695700	3.87644800	-2.11165600
C	5.66386300	3.37265500	1.66163300
H	3.54103800	3.03651100	1.90009900
C	6.69729800	3.69262400	0.77570300
H	7.20892200	4.14411600	-1.27665100
H	5.87552900	3.23339800	2.72432900
H	7.72169400	3.79444100	1.14009900
C	4.07881100	0.33674400	-0.49690800
C	3.61700200	0.34772600	-1.82067300

C	5.45047200	0.31572300	-0.22549700
C	4.53868200	0.38333800	-2.86896500
H	2.54112600	0.30295700	-2.01215700
C	6.36438300	0.33147600	-1.27906700
H	5.78941200	0.32210000	0.81125800
C	5.91111400	0.37756500	-2.60107200
H	4.18091800	0.39583900	-3.90122700
H	7.43551800	0.32825900	-1.06600200
H	6.62899500	0.40080800	-3.42422900
H	-2.03152600	1.70895400	-1.69710400
C	-4.74510100	1.92939900	-1.18639500
C	-6.00265400	2.25737900	-0.64496700
C	-4.64981600	1.78326100	-2.58473800
C	-7.11684300	2.45056800	-1.46359100
H	-6.09694500	2.36619500	0.43920800
C	-5.76090900	1.97710200	-3.40319300
H	-3.69504800	1.49581500	-3.02985200
C	-7.00173400	2.31458700	-2.84935700
H	-8.08085500	2.70779800	-1.01668400
H	-5.66244400	1.85410400	-4.48507800
H	-7.87192700	2.46195600	-3.49360200
C	-0.21238400	3.44561000	2.37692500
H	0.47425900	3.74000600	1.56775100
C	-1.31402600	2.56023400	1.80664600
H	-2.15946400	3.13765500	1.42261500
H	0.39279000	2.86160300	3.08659600
O	-1.26620800	1.12255000	4.27247500
O	-1.79662600	0.02101100	1.94839900
O	-3.54552700	1.53124000	3.07577900
P	-1.92760800	1.32905900	2.94756100
C	-0.67482600	4.75522200	3.06903100
C	-1.70048100	4.46748900	4.17717700
H	-1.94682900	5.39085500	4.72640900
H	-2.63921500	4.07087600	3.76022900
H	-1.31491600	3.72437000	4.89062300
C	-1.28746000	5.70938000	2.03144200
H	-0.55347700	5.96683300	1.24892500
H	-2.16492700	5.26486400	1.53647300
H	-1.61471000	6.64934800	2.50461400
C	0.56859000	5.41416700	3.68706900
H	0.31859900	6.38148000	4.15254500
H	1.01007300	4.76906500	4.46376800
H	1.34180300	5.59862200	2.92215800
C	-4.24229700	1.19222600	4.27429600
H	-3.53955800	1.09227100	5.11441400
H	-4.96496900	1.99336500	4.48579800
H	-4.78522900	0.24345600	4.13422000
C	-2.65593300	-1.11161900	1.91556300
H	-2.30637600	-1.73543900	1.08255800
H	-2.59305300	-1.66994500	2.86356900
H	-3.69466600	-0.79958000	1.72826000

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.772738 (Hartree/Particle)
Thermal correction to Energy= 0.821968
Thermal correction to Enthalpy= 0.822912
Thermal correction to Gibbs Free Energy= 0.684312
Sum of electronic and zero-point Energies= -6266.358239
Sum of electronic and thermal Energies= -6266.309009
Sum of electronic and thermal Enthalpies= -6266.308065
Sum of electronic and thermal Free Energies= -6266.446665
HF= -6267.1309765
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.34726
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.300569
Solvent correction = -0.0466902
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.806943
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.980676

G-TS-H'$^{S\text{-}E}$-SP

Ni	-0.68580800	1.00556800	0.37577300
C	-2.44626800	1.54251400	-0.14481400
C	-2.77147500	2.63675300	-0.87360000
H	-2.18501700	3.54922000	-0.72972100
Br	-0.00853400	-0.85336600	-1.11079700
C	1.76487600	2.33173900	-0.24075500
C	1.84647400	3.99936900	-1.81177500
C	0.41886800	3.38776000	-1.69123900
N	0.51997500	2.44063900	-0.56808500
H	2.23633500	3.92174900	-2.83832400
C	1.78502600	-0.28535800	2.28464500
C	3.03645900	-0.69566000	1.46751900
C	2.11512300	1.23436100	0.68773300
N	1.21177700	0.84493400	1.52701400
H	2.83792100	-1.54918000	0.79906200
H	1.89674800	5.05574000	-1.50063000
H	3.90741400	-0.91940900	2.10093200
C	-0.02579600	2.64758800	-2.95001800
H	0.70487300	1.86695500	-3.20953100
H	-0.99262100	2.15641900	-2.78323800
H	-0.11929800	3.35153300	-3.79237200
C	2.11151500	0.15214300	3.71087100
H	2.85602000	0.96557500	3.70056900
H	1.19573300	0.49947900	4.20607400
H	2.53299700	-0.69200400	4.28076300
H	-0.31785900	4.16730100	-1.44505100
H	1.04964500	-1.09933300	2.30224400
N	2.63068100	3.17287000	-0.88053800
N	3.27183900	0.50565700	0.63929000
C	3.94457300	3.49289100	-0.48438600
C	4.90896500	3.78402700	-1.45910900
C	4.29440800	3.53262600	0.87411200
C	6.21495200	4.08685800	-1.07738800
H	4.64073300	3.73470500	-2.51500100
C	5.60840800	3.81699200	1.24531600
H	3.53621900	3.34353100	1.63570800
C	6.57401800	4.09502900	0.27361200
H	6.96290300	4.29962900	-1.84443200
H	5.87445400	3.83696500	2.30476700
H	7.60038600	4.32371100	0.56846700
C	4.14107500	0.44434300	-0.48830800
C	3.61702100	0.27572700	-1.77696100
C	5.52262000	0.54338500	-0.29277900
C	4.48398600	0.25396800	-2.87136200

H	2.53916600	0.13452300	-1.90127900
C	6.38293100	0.50102300	-1.38980800
H	5.90885900	0.68703000	0.71737100
C	5.86475500	0.36882800	-2.68180400
H	4.07657600	0.12655200	-3.87720300
H	7.46052800	0.59172400	-1.23662700
H	6.53890900	0.34661900	-3.54134100
H	-3.10253100	0.66417800	-0.13687200
C	-3.84031200	2.74998900	-1.86296700
C	-4.09708000	4.00228900	-2.46061600
C	-4.63151900	1.65482200	-2.27404900
C	-5.10589700	4.16054800	-3.41050900
H	-3.49226200	4.86351100	-2.16210000
C	-5.63967700	1.81462300	-3.22122300
H	-4.44051600	0.66523900	-1.85434000
C	-5.88686000	3.06743900	-3.79639900
H	-5.28426600	5.14427700	-3.85277500
H	-6.23656000	0.94976100	-3.52247100
H	-6.67636400	3.18696800	-4.54199300
C	-1.21023000	3.24216500	2.11793500
H	-0.90827700	3.74169300	1.18452700
C	-2.01515600	1.99429900	1.76021100
H	-3.08441200	2.22387800	1.74705200
H	-0.27452600	2.93335000	2.60767500
O	-1.00332800	0.61540900	4.09076100
O	-1.63743900	-0.55668300	1.81818300
O	-3.48160700	0.35159000	3.34892400
P	-1.93033100	0.61586200	2.92008800
C	-1.93896800	4.29369400	2.99242700
C	-2.48317100	3.66361400	4.28454400
H	-2.90086200	4.43942500	4.94640800
H	-3.29117300	2.94629700	4.07226700
H	-1.69449000	3.12387800	4.82936100
C	-3.09145000	4.92758800	2.19758500
H	-2.71803100	5.43482700	1.29312500
H	-3.82931400	4.17670000	1.87301700
H	-3.62578100	5.67363200	2.80752900
C	-0.91394500	5.38065600	3.35202800
H	-1.38109600	6.19003500	3.93598600
H	-0.09012300	4.96179000	3.95217400
H	-0.47661000	5.82945100	2.44466600
C	-3.82853100	-0.11592500	4.65124800
H	-2.99263200	0.02849500	5.35147900
H	-4.70449700	0.45269300	4.99545400
H	-4.08937500	-1.18581000	4.60706600
C	-1.51349900	-1.94242000	2.12435400
H	-0.99063500	-2.39532500	1.27150800
H	-0.93620900	-2.08259200	3.05159500
H	-2.51275500	-2.39214600	2.23709500

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.771983 (Hartree/Particle)
Thermal correction to Energy= 0.820746
Thermal correction to Enthalpy= 0.821690
Thermal correction to Gibbs Free Energy= 0.684374
Sum of electronic and zero-point Energies= -6266.344388
Sum of electronic and thermal Energies= -6266.295626
Sum of electronic and thermal Enthalpies= -6266.294682
Sum of electronic and thermal Free Energies= -6266.431997
HF= -6267.1163714
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.342372
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6265.295573
Solvent correction = -0.0467989
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6269.793818
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6267.973518

Figure A4.5
F-TS-G^S-L9

Ni	-0.68555800	1.80958200	0.92172400
C	-1.61713100	1.08697200	2.46096700
C	-1.73957400	-0.23877800	2.62634000
H	-1.53661700	-0.88976300	1.76710600
Br	0.20913700	3.83608600	2.15721100
C	1.54126000	2.36059900	-0.67990200
C	1.54395200	4.37560400	-1.77433500
C	0.09544100	3.88919700	-1.46112700
N	0.28346900	2.63191600	-0.73689800
H	1.72015000	4.53670500	-2.84822100
C	1.59551400	-0.35566900	1.74248400
C	2.96278700	-0.65350500	1.05652700
C	1.91140200	1.14872400	0.09162700
N	1.03431000	0.73998200	0.94590700
H	2.97489700	-1.61940500	0.52752100
H	1.79624300	5.29888200	-1.23330300
H	3.80095400	-0.63800300	1.76756300
H	-0.39702800	4.59096900	-0.76878600
H	0.92113900	-1.22243800	1.66699200
N	2.38557400	3.26784200	-1.26471500
N	3.08173500	0.44297200	0.07209800
C	3.71153200	3.49134700	-0.81268500
C	4.73886200	3.69635100	-1.74061100
C	3.99104900	3.48512600	0.56147900
C	6.05488900	3.81368200	-1.30332100
H	4.51037000	3.70518300	-2.80670900
C	5.31064900	3.58709800	0.99596500
H	3.16736200	3.41164100	1.27582000
C	6.34390900	3.72825300	0.06333100
H	6.86143400	3.92066300	-2.02886800
H	5.53679700	3.55996400	2.06305600
C	4.06481700	0.47500800	-0.93455900
C	3.69964500	0.55675300	-2.28741100
C	5.42035900	0.43794600	-0.57972900
C	4.68256400	0.66980000	-3.26639600
H	2.64497500	0.54536500	-2.56609200
C	6.40039300	0.54244800	-1.56148900
H	5.70505700	0.38751300	0.47142200
C	6.03359000	0.67880600	-2.90447700
H	4.40053200	0.75126200	-4.31722800
H	7.45225500	0.56433900	-1.27579900
H	-1.81511800	1.79442200	3.27447400
C	-2.04795000	-0.96532600	3.86987400
C	-2.11706000	-2.37177100	3.84695100
C	-2.23544700	-0.31865600	5.10843500

C	-2.36487200	-3.10582500	5.00869400
H	-1.96746900	-2.89178200	2.89613400
C	-2.48251100	-1.04987900	6.26826500
H	-2.17669100	0.77038600	5.15762000
C	-2.54833400	-2.44830500	6.22742300
H	-2.41209500	-4.19696400	4.96236300
H	-2.62145900	-0.52553700	7.21726600
H	-2.73874400	-3.01834900	7.13976100
C	-3.99366200	3.10283100	1.72594400
H	-3.35527900	3.66257000	2.43279100
C	-3.16933000	2.78503500	0.52319800
H	-2.72730600	3.61594000	-0.03444700
H	-4.29029900	2.17098700	2.22920200
O	-1.90647000	0.53173000	-0.54484900
O	-3.83082600	1.69473400	-1.82352300
O	-4.37412100	0.37457100	0.30622600
P	-3.21542300	1.28155300	-0.36485900
C	-5.27019000	3.95305700	1.45045800
C	-6.20751900	3.20868600	0.48718000
H	-7.13526400	3.78228400	0.32752100
H	-5.73127700	3.05187000	-0.49271300
H	-6.47801100	2.21771900	0.88339500
C	-4.88283700	5.31262400	0.84895200
H	-4.17450100	5.84985400	1.50056600
H	-4.41308900	5.19700500	-0.14046500
H	-5.77356400	5.94842000	0.71852100
C	-5.97879900	4.17342600	2.79498000
H	-6.89340800	4.77472700	2.66539000
H	-6.26789900	3.21266300	3.25113900
H	-5.32448000	4.70146700	3.50755300
C	-4.23429700	-1.01524400	0.59403700
H	-4.24064200	-1.16143500	1.68319200
H	-5.08725600	-1.54569500	0.14429200
H	-3.29333700	-1.40775300	0.18368800
C	-3.99292200	0.68755300	-2.81559300
H	-4.31238900	1.18590000	-3.74067800
H	-3.04609200	0.15264400	-2.99058600
H	-4.76942400	-0.03569800	-2.51374500
C	1.67291400	0.04926600	3.22395500
C	1.96719100	-1.15288800	4.12891700
C	2.62885000	1.21468400	3.50152000
H	0.66116100	0.40260500	3.46992500
C	1.91484500	-0.74763100	5.60580000
H	2.96776500	-1.56617700	3.89537400
H	1.23547200	-1.95482300	3.93279800
C	2.57269100	1.61740500	4.97819000
H	3.66692400	0.93303700	3.24099200
H	2.34080500	2.07500000	2.88002500
C	2.85333100	0.42743400	5.90172300
H	2.16150400	-1.61046900	6.24631500
H	0.87706800	-0.46128800	5.85223300
H	3.28508900	2.43549600	5.17490900
H	1.56828200	2.02497700	5.18735500
H	2.76312100	0.73073100	6.95804000
H	3.90022000	0.09841300	5.76059100
C	-0.81376400	3.66922700	-2.68056200
C	-1.13931200	4.98906800	-3.39145200
C	-0.26162000	2.62259400	-3.65865200
H	-1.76062300	3.26503100	-2.28437200
C	-2.08407100	4.76833500	-4.57684900
H	-0.20576300	5.45566900	-3.75779200
H	-1.58180400	5.69918700	-2.67242800
C	-1.19278800	2.42108100	-4.85855100
H	0.73224300	2.94077500	-4.02501500
H	-0.11965900	1.67087600	-3.12245300
C	-1.51002000	3.74452100	-5.56140600
H	-2.28595300	5.72448100	-5.08681600
H	-3.05461700	4.40160200	-4.19687100
H	-0.74783100	1.70346200	-5.56773600
H	-2.13378200	1.96785200	-4.50480700
H	-2.21160600	3.57775900	-6.39542500
H	-0.58409900	4.15116800	-6.00903900
C	7.08618300	0.94654300	-3.94442700
C	7.77634100	3.67948500	0.51855800
F	8.23026100	2.40058400	0.53306500
F	8.59302500	4.36851700	-0.29276700
F	7.93315600	4.15620900	1.76286800
F	8.26333800	0.38453300	-3.63264800
F	6.72473700	0.49993400	-5.15844200
F	7.30931800	2.27733800	-4.07180700

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 1.026109 (Hartree/Particle)
Thermal correction to Energy= 1.091081
Thermal correction to Enthalpy= 1.092025
Thermal correction to Gibbs Free Energy= 0.915541
Sum of electronic and zero-point Energies= -7330.190590
Sum of electronic and thermal Energies= -7330.125618
Sum of electronic and thermal Enthalpies= -7330.124674
Sum of electronic and thermal Free Energies= -7330.301157
HF= -7331.2166987
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -7329.776222
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -7329.726339
Solvent correction = -0.0498832
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -7335.107563
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -7332.67124

F-TS-G^{R}-L9

Ni	-0.36142700	2.01713700	0.94176600
C	-1.25990800	1.24743300	2.43132200
C	-1.56731000	-0.02385000	2.74239300
H	-1.46791100	-0.78856600	1.96252400
Br	-0.08732200	-0.09157000	-0.49753500
C	2.14152600	2.89278600	-0.06975000
C	2.17440600	4.42361200	-1.78190600
C	0.72544200	4.17282300	-1.26504400
N	0.88401900	3.10852900	-0.26511800
H	2.31923700	4.04242700	-2.80545000
C	1.99874200	0.33676300	2.49193400
C	3.43404000	0.04239900	1.97128700
C	2.47351400	1.81882900	0.89276400
N	1.63770400	1.61597400	1.85533400
H	3.56830500	-0.99978300	1.65449900
H	2.46535400	5.48311000	-1.76175500

H	4.21498400	0.29483600	2.70875200
H	0.34607900	5.06278100	-0.73340000
H	1.30143500	-0.40064300	2.05673000
N	2.99053500	3.65624900	-0.82377900
N	3.51950400	0.94115100	0.79949600
C	4.38685100	3.72537000	-0.71470100
C	5.18452300	3.76027700	-1.86770900
C	4.99547000	3.73871100	0.55194500
C	6.57144200	3.74018300	-1.75614100
H	4.72195900	3.74242700	-2.85439500
C	6.38183700	3.71209800	0.65799800
H	4.37576600	3.76394200	1.44926200
C	7.17408100	3.69573000	-0.49531400
H	7.18457100	3.71445600	-2.65705600
H	6.85368900	3.70732200	1.64182300
C	4.24977100	0.68320700	-0.37780000
C	3.57905200	0.61659900	-1.61013300
C	5.64241800	0.53713800	-0.32747900
C	4.31257400	0.50359100	-2.78790700
H	2.48598700	0.62791300	-1.62343200
C	6.37041100	0.41170800	-1.50704000
H	6.15856200	0.58259300	0.63212500
C	5.70915000	0.42540800	-2.74018500
H	3.79684300	0.46657400	-3.74898000
H	7.45832600	0.35343900	-1.46977000
H	-1.33721400	2.00150400	3.23640700
C	-1.92691100	-0.54501300	4.07367400
C	-2.00541300	-1.93791900	4.26799400
C	-2.14470500	0.28167500	5.19557700
C	-2.27479900	-2.48377500	5.52429900
H	-1.83819000	-2.59705100	3.41172000
C	-2.41919200	-0.26053400	6.44982900
H	-2.08706000	1.36619300	5.08076000
C	-2.48259300	-1.64809300	6.62491900
H	-2.32138000	-3.56919300	5.64519800
H	-2.58121500	0.40429900	7.30250600
H	-2.69197300	-2.07166800	7.60996300
C	-3.92661800	0.28825400	-0.01254700
H	-4.31265500	0.46849700	1.00143400
C	-3.14032700	1.45360100	-0.48850500
H	-2.44265200	1.31863800	-1.31817300
H	-3.23558700	-0.56965700	0.04716500
O	-1.87250200	3.62427200	0.69754900
O	-4.36128400	3.11349400	1.31163800
O	-3.80526600	3.97707300	-0.98730900
P	-3.19219300	3.06204200	0.20074800
C	-5.12079300	-0.09861200	-0.93961100
C	-4.60631000	-0.42324500	-2.35025500
H	-5.42976800	-0.77629800	-2.99183100
H	-4.16589700	0.46328400	-2.83273800
H	-3.83377800	-1.20835000	-2.32160100
C	-6.12560700	1.06205600	-1.00355400
H	-6.49190600	1.32621300	0.00122800
H	-5.66656000	1.96479000	-1.43583300
H	-6.99481600	0.79127300	-1.62470600
C	-5.79514800	-1.33923600	-0.33784500
H	-6.65613400	-1.65325400	-0.95001100
H	-5.09210100	-2.18576700	-0.28168000
H	-6.16119300	-1.13656400	0.68173400
C	-3.89583400	5.39227200	-0.81413300
H	-4.13225500	5.82229700	-1.79604300
H	-4.69612500	5.64065000	-0.09923500
H	-2.93974900	5.79994100	-0.45088400
C	-4.10421300	3.04803400	2.71851700
H	-3.95669700	2.00576900	3.03598900
H	-3.20792000	3.63045300	2.97477600
H	-4.98403300	3.47165500	3.22097300
C	-0.31657500	3.79163400	-2.32210500
C	-0.70700200	4.97875000	-3.21076700
C	0.05535200	2.56594600	-3.16484200
H	-1.20778300	3.52605500	-1.73702800
C	-1.85664000	4.59839400	-4.15106700
H	0.16660700	5.30355300	-3.80785600
H	-0.99637400	5.83959400	-2.58308700
C	-1.09241000	2.18692400	-4.10601500
H	0.95472900	2.78229900	-3.77115100
H	0.29222200	1.71892900	-2.50335200
C	-1.51116200	3.36434700	-4.99192600
H	-2.11677100	5.44947100	-4.80205800
H	-2.74906600	4.37661900	-3.53953600
H	-0.80582300	1.31930700	-4.72181400
H	-1.95684500	1.86160700	-3.50015600
H	-2.36796400	3.08439600	-5.62686700
H	-0.68137800	3.61423100	-5.67904500
C	1.77848200	0.35104600	4.00207300
C	1.93689000	-1.04663300	4.61404600
C	2.61323500	1.38801200	4.76075700
H	0.72177900	0.63589200	4.12227100
C	1.57584500	-1.04190700	6.10265400
H	2.98130400	-1.39213900	4.48760100
H	1.29602200	-1.76128700	4.07184500
C	2.24108600	1.39969000	6.24784400
H	3.69046800	1.15612300	4.66255700
H	2.45949000	2.38332000	4.31205800
C	2.38544500	0.00720900	6.87301500
H	1.73310500	-2.04296800	6.53684800
H	0.49893500	-0.82368600	6.20351800
H	2.85941500	2.13250600	6.79281100
H	1.19272100	1.73345800	6.34978600
H	2.07473900	0.02927500	7.93086500
H	3.45360400	-0.28040000	6.86754500
C	8.66262600	3.52458600	-0.37885900
C	6.50298100	0.46255200	-4.01539700
F	7.70096700	-0.12846600	-3.89052100
F	5.85809300	-0.12591000	-5.03558900
F	6.73983800	1.74385500	-4.39847000
F	9.31896500	4.05518600	-1.42180500
F	8.99726600	2.21207500	-0.33327300
F	9.15070800	4.08293100	0.74169200

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 1.026295
(Hartree/Particle)
Thermal correction to Energy= 1.091501
Thermal correction to Enthalpy= 1.092445
Thermal correction to Gibbs Free Energy= 0.915694
Sum of electronic and zero-point Energies= -7330.177131
Sum of electronic and thermal Energies= -7330.111925
Sum of electronic and thermal Enthalpies= -7330.110981
Sum of electronic and thermal Free Energies= -7330.287732
HF= -7331.2034262

M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -7329.704544
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -7329.654717
Solvent correction = -0.0498271
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -7335.103307
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -7332.671649

F-TS-G^S-L8

Ni	-0.67211900	1.79917600	0.72806400
C	-2.35765100	2.74083600	0.43991800
C	-3.26722100	2.59243200	-0.53425100
H	-3.17892500	1.73565100	-1.21226000
Br	-0.67454800	0.30701400	-1.29737700
C	1.86718300	2.67788100	-0.09132900
C	1.97099700	4.56985700	-1.39752200
C	0.49897700	4.18476400	-1.06034800
N	0.63405000	3.04383800	-0.15710800
H	2.14956300	4.64541600	-2.47889700
C	1.62751700	-0.26850100	2.04165000
C	3.17586300	-0.24268000	1.83632100
C	2.14217000	1.43245800	0.66400200
N	1.16300400	0.92354600	1.32217400
H	3.59232400	-1.20600500	1.51927100
H	2.27973300	5.51734100	-0.92682500
H	3.70014600	0.08554700	2.74635400
N	2.74817000	3.45616700	-0.80474600
N	3.35029300	0.76676100	0.76452800
C	4.13165500	3.54915800	-0.55687500
C	4.62951800	3.53349700	0.75840700
C	5.04856700	3.62581400	-1.60997800
H	3.93288400	3.52926000	1.60362000
C	6.41044000	3.60336900	-1.31818500
H	4.69749400	3.64382800	-2.64291000
C	6.79104400	3.50351800	0.02187000
H	7.15694200	3.59902200	-2.11058800
C	4.16209600	0.55190300	-0.36755300
C	5.55684400	0.43797000	-0.22598100
C	3.61108000	0.48340700	-1.65462500
H	6.01296200	0.48546100	0.76797400
C	4.47605400	0.37603700	-2.74246500
H	2.52663500	0.51675000	-1.79977900
C	5.84862300	0.32042600	-2.49036100
H	4.09341100	0.33174300	-3.76204100
H	-2.45976600	3.59062500	1.12935100
C	-4.38498900	3.50908700	-0.82737500
C	-5.25176100	3.21761300	-1.89791400
C	-4.62553600	4.69078000	-0.09531700
C	-6.31228300	4.06442800	-2.22565600
H	-5.08074500	2.30755300	-2.47915500
C	-5.68153700	5.53905000	-0.42258600
H	-3.97309100	4.94360900	0.74309200
C	-6.53321000	5.23209000	-1.49093300
H	-6.96956500	3.81154800	-3.06173600
H	-5.84496900	6.44938100	0.16061900
H	-7.36095000	5.89818200	-1.74590300
C	-3.73563800	0.16940300	2.12397500
H	-3.67322600	-0.28543100	1.11987100
C	-2.34514200	0.49511900	2.55611900
H	-1.60303500	-0.30911600	2.57364900
H	-4.31302200	1.09724400	2.01069900
O	-0.60401200	2.61145900	2.87996700
O	-1.57311000	1.56653800	5.01455000
O	-3.15797400	2.82358600	3.54506300
P	-1.83409200	1.91810000	3.43583800
C	-4.51268300	-0.80454700	3.05904100
C	-4.68287300	-0.17612300	4.45059400
H	-5.27152900	-0.83717500	5.10747600
H	-3.71076100	0.00511900	4.93393800
H	-5.20218200	0.79270100	4.38462800
C	-3.76394900	-2.14085700	3.18000600
H	-3.59160700	-2.59191700	2.18879100
H	-2.78555300	-2.01496500	3.67023900
H	-4.34298900	-2.86006300	3.78145400
C	-5.89232400	-1.04790000	2.42996600
H	-6.49600100	-1.72727600	3.05357300
H	-6.44854500	-0.10295200	2.32172500
H	-5.79894600	-1.49904900	1.42888600
C	-3.08290200	4.15026700	4.06197400
H	-4.05066300	4.62701000	3.85984900
H	-2.89844500	4.13016200	5.14767500
H	-2.27952400	4.71768500	3.56632500
C	-0.29385900	1.12584100	5.44770000
H	-0.11731600	0.07526800	5.15482600
H	0.50266100	1.75746600	5.02503400
H	-0.27731200	1.18960700	6.54439600
C	8.24524500	3.34155900	0.42010100
C	6.85748400	0.32023900	-3.62135300
F	6.25808900	0.14663700	-4.81292300
F	7.50697200	1.50257100	-3.67364400
F	7.77542700	-0.63641500	-3.47865300
F	8.44201100	2.15398400	1.01469300
F	8.62941700	4.29328300	1.28024200
F	9.05569500	3.40314300	-0.64860000
N	5.92552900	3.49099500	1.03551100
N	6.37367600	0.32814000	-1.26489600
H	-0.00484900	3.79714800	-1.96232000
H	1.39656200	-0.10205500	3.10469800
C	-0.37966800	5.29775700	-0.46717400
H	-1.37807200	4.84397200	-0.37690100
C	0.88229300	-1.54280000	1.58330200
H	-0.14607700	-1.21180400	1.36427300
C	0.07709500	5.70330700	0.93572500
H	0.06952300	4.83778700	1.61568500
H	1.09409200	6.13319900	0.93073100
H	-0.59247900	6.46626400	1.35957400
C	1.43868100	-2.12730000	0.28371200
H	1.53660400	-1.35042800	-0.48531300
H	2.41155900	-2.62382200	0.43729400
H	0.74616700	-2.87356200	-0.12898300
C	-0.49987800	6.47238400	-1.45000600
H	-0.67782200	6.06591800	-2.46150300
H	0.46031700	7.01899600	-1.50289900
C	-1.62729700	7.44648400	-1.10746100
H	-1.71233000	8.23888300	-1.86722700
H	-2.59540300	6.92187700	-1.05740600
H	-1.46241400	7.93930100	-0.13645800
C	0.82982200	-2.56561800	2.72928400
H	0.43079700	-2.06235200	3.62882400
H	1.85912000	-2.87711000	2.99053300

C	-0.02241600	-3.79780000	2.43274000
H	-0.09193600	-4.45262700	3.31515400
H	-1.04694300	-3.50671300	2.14944900
H	0.39355100	-4.39637200	1.60840400

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.925823 (Hartree/Particle)
Thermal correction to Energy= 0.990253
Thermal correction to Enthalpy= 0.991197
Thermal correction to Gibbs Free Energy= 0.815624
Sum of electronic and zero-point Energies= -7207.532604
Sum of electronic and thermal Energies= -7207.468175
Sum of electronic and thermal Enthalpies= -7207.467231
Sum of electronic and thermal Free Energies= -7207.642804
HF= -7208.4584275
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (scf=qc)
HF = -7207.038375
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP (scf=qc)
HF = -7206.984202
Solvent correction = -0.0541731
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP (scf=qc)
HF = -7212.25336
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP (scf=qc)
HF = -7209.95028

F-TS-G^R-L8

Ni	-0.77343500	1.53834000	0.47957200
C	-2.00169600	0.37519000	1.45107900
C	-1.91964800	0.26039800	2.78665700
H	-1.32028300	0.99542900	3.33775000
Br	-0.61827900	0.07237700	-1.56729700
C	1.73119200	2.54613800	-0.37935100
C	1.81515800	3.95230200	-2.19711200
C	0.35744500	3.77185700	-1.67105400
N	0.48731400	2.78677600	-0.59655900
H	1.94971300	3.50048400	-3.19185800
C	1.55473200	-0.01121100	2.22051600
C	3.10368000	0.13496300	2.11593800
C	2.03640900	1.49016800	0.61284800
N	1.05423200	1.03516300	1.31106200
H	3.62571600	-0.82409200	2.01486000
H	2.13452400	5.00308700	-2.24260400
H	3.52419400	0.67803200	2.97612600
N	2.61414700	3.22756800	-1.18780400
N	3.27192900	0.94279100	0.88420600
C	3.95038700	3.51751500	-0.88425400
C	4.34366300	3.77034300	0.44438100
C	4.93663300	3.53406200	-1.87729300
H	3.58566900	3.83120600	1.23249100
C	6.26592800	3.70995000	-1.50030700
H	4.67190300	3.35425000	-2.92034500
C	6.54941000	3.86436500	-0.14169900
H	7.06863600	3.66822400	-2.23450900
C	4.18787200	0.62773700	-0.13896200
C	5.57141400	0.67882800	0.10815200
C	3.74894400	0.29744800	-1.42845800
H	5.94139500	0.93385200	1.10631900
C	4.70339300	0.10044900	-2.42477900
H	2.68124700	0.20401400	-1.64829000
C	6.05132900	0.22220200	-2.07980200
H	4.40810900	-0.14681000	-3.44435900
H	-2.57259300	-0.34400600	0.85300800
C	-2.46603700	-0.81962900	3.62475200
C	-2.07495700	-0.90871700	4.97482300
C	-3.34066100	-1.80709400	3.12767900
C	-2.52370600	-1.94668900	5.79376700
H	-1.39728600	-0.15093500	5.37905300
C	-3.79057700	-2.84233600	3.94420800
H	-3.66629100	-1.75761000	2.08683600
C	-3.38275500	-2.92209000	5.28164400
H	-2.19945200	-1.99516200	6.83652700
H	-4.46694500	-3.59726400	3.53512400
H	-3.73529300	-3.73706100	5.91804100
C	-4.54645700	1.62348200	0.16764800
H	-4.69813400	1.27976300	1.20136600
C	-3.35613300	2.52101500	0.10650200
H	-2.99052800	2.83657800	-0.87577700
H	-4.32637400	0.72769500	-0.44005600
O	-1.27524900	3.32395900	1.77910400
O	-3.72505100	3.22003900	2.69546000
O	-3.05887800	5.02284600	0.99998400
P	-2.74943300	3.47688800	1.43502000
C	-5.88071400	2.23863400	-0.35410100
C	-5.73880100	2.64298200	-1.82905800
H	-6.69775200	3.01551900	-2.22422600
H	-4.99491600	3.44489100	-1.95700200
H	-5.42644000	1.78718800	-2.44967700
C	-6.26494900	3.46702400	0.48488300
H	-6.34184400	3.21012700	1.55270700
H	-5.51453400	4.26646800	0.39097400
H	-7.23623700	3.87161500	0.15637000
C	-6.96794700	1.16214500	-0.22083100
H	-7.94104700	1.53860800	-0.57579400
H	-6.71619000	0.26627500	-0.81147300
H	-7.08898000	0.85065800	0.82942600
C	-2.70169000	6.08582000	1.87817100
H	-2.74440400	7.01819100	1.29902600
H	-3.41451200	6.14892600	2.71720600
H	-1.68274600	5.94623700	2.27153600
C	-3.26883900	3.01246300	4.03148200
H	-3.55287600	2.00078300	4.35280100
H	-2.17673300	3.11957400	4.09338600
H	-3.75356400	3.75703700	4.68092000
C	7.97534600	3.93440200	0.36663700
C	7.14230600	0.13632300	-3.12834100
F	6.65668200	-0.29449000	-4.30669400
F	7.68464400	1.35329100	-3.34568400
F	8.12859000	-0.68397400	-2.76471500
F	8.24342900	2.89299500	1.17015700
F	8.19451400	5.05361800	1.06962400
F	8.85802400	3.90764900	-0.64550500
N	5.61042400	3.91698400	0.80351800
N	6.47481100	0.48287400	-0.84300600
H	-0.26995000	3.31137500	-2.44956300
H	1.21872400	0.25357500	3.23322300
C	-0.33565900	5.04881100	-1.16083900
H	-1.30582400	4.71902600	-0.76054600
C	0.98621900	-1.40654100	1.88334300

H	-0.08421500	-1.24107200	1.70144700
C	0.43566300	5.69199400	-0.00669300
H	0.51726400	4.98965200	0.83466700
H	1.44711900	6.00919900	-0.31303200
H	-0.08435400	6.58634300	0.36356800
C	1.58229300	-2.00422200	0.60875000
H	1.43426500	-1.33086900	-0.24659000
H	2.65495400	-2.23943800	0.71568300
H	1.06848200	-2.94074700	0.34974900
C	-0.63295400	6.01333500	-2.31867700
H	-1.06844900	5.43532400	-3.15284500
H	0.30990800	6.44297500	-2.70483200
C	-1.59511300	7.14069600	-1.94222400
H	-1.85072400	7.75550500	-2.81897600
H	-2.53121400	6.73165100	-1.52839400
H	-1.16279100	7.81349500	-1.18521800
C	1.11084000	-2.32889700	3.10808600
H	0.77038300	-1.77397000	3.99923600
H	2.17590300	-2.57447000	3.28373200
C	0.29025800	-3.61309000	3.00298600
H	0.38067500	-4.21451700	3.92081400
H	-0.77704400	-3.37828300	2.86360000
H	0.61336800	-4.24355400	2.16018900

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.926546
(Hartree/Particle)
Thermal correction to Energy= 0.990503
Thermal correction to Enthalpy= 0.991448
Thermal correction to Gibbs Free Energy= 0.818452
Sum of electronic and zero-point Energies= -7207.551755
Sum of electronic and thermal Energies= -7207.487798
Sum of electronic and thermal Enthalpies= -7207.486853
Sum of electronic and thermal Free Energies= -7207.659849
HF= -7207.043719
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP (scf=qc)
HF = -7206.994343
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP (scf=qc)
HF = -7329.654717
Solvent correction = -0.0493753
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP (scf=qc)
HF = -7212.261244
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP (scf=qc)
HF = -7209.959959

Figure A4.6
E^{cis}-L9

Ni	-0.86677700	0.98664800	0.26250700
C	-2.47133900	1.94343900	0.08105100
C	-2.66834200	3.18601400	0.56973800
H	-3.61151200	3.71485800	0.36906700
Br	-1.95359900	-0.66622700	1.48194000
C	1.46989800	2.15716100	-0.66117100
C	1.21355600	4.22281700	-1.60669600
C	-0.13062400	3.45184400	-1.56465500
N	0.17852900	2.26604300	-0.75468000
H	1.46301000	4.60605700	-2.60590700
C	1.63379800	-0.89648900	1.25807100
C	3.10108300	-0.90340400	0.74107900
C	1.93953600	0.90172700	-0.05259500
N	1.00873200	0.19702400	0.50627500
H	3.28927500	-1.70913900	0.01247700
H	1.22075100	5.06010600	-0.89033600
H	3.83857200	-0.98966700	1.55112400
H	-0.90055300	4.03953400	-1.05573600
H	1.10837600	-1.83402900	1.02655200
N	2.19740200	3.20257700	-1.16947900
N	3.21407300	0.40713700	0.05779600
C	3.44985500	3.59388100	-0.63065100
C	4.45857300	4.05307000	-1.48513200
C	3.68180600	3.51688400	0.75043500
C	5.71351200	4.36988200	-0.97318600
H	4.27148000	4.10812300	-2.55793700
C	4.94037800	3.82465200	1.26030500
H	2.87533600	3.21180800	1.41813200
C	5.96209100	4.23295300	0.39684500
H	6.51307800	4.67895200	-1.64643000
H	5.12997900	3.74810800	2.33202200
C	4.25865200	0.67752400	-0.85669600
C	3.99592200	0.78691800	-2.23051900
C	5.56553100	0.84435800	-0.38183500
C	5.02188500	1.12109100	-3.11037100
H	2.98361700	0.62696800	-2.60427600
C	6.59155900	1.17197900	-1.26316700
H	5.76282800	0.76947700	0.68799600
C	6.31709500	1.32939800	-2.62586200
H	4.81650200	1.22269600	-4.17713100
H	-3.30567800	1.46651000	-0.45208300
C	-1.65433300	3.95783300	1.31232100
C	-1.53939300	5.35060300	1.13122200
C	-0.72200300	3.32950800	2.16425800
C	-0.49715300	6.07502000	1.71389000
H	-2.26761300	5.86316100	0.49577500
C	0.31282400	4.05473800	2.75703200
H	-0.84226400	2.26464700	2.37551000
C	0.44456700	5.42764900	2.52160400
H	-0.42104400	7.15186100	1.54116200
H	1.01048400	3.54865400	3.42896700
H	1.25718700	5.99302500	2.98410100
C	7.35794000	4.42242800	0.92515300
F	7.36512700	4.83162100	2.20349500
F	8.04784900	3.25591600	0.88712900
F	8.05801000	5.30996600	0.20386500
C	-0.69673400	3.01052400	-2.92544500
C	-1.18329600	4.21527900	-3.74219700
C	0.26306000	2.13474800	-3.74313400
H	-1.57928300	2.39588100	-2.67611900
C	-1.80294700	3.78263200	-5.07497900
H	-0.33358200	4.89344800	-3.94585900
H	-1.91067700	4.79407200	-3.14880000
C	-0.36099000	1.70719200	-5.07578000
H	1.19681600	2.69211900	-3.94344700
H	0.54091900	1.24453400	-3.15603200
C	-0.83568500	2.91623900	-5.88761000
H	-2.10967900	4.66793400	-5.65566900
H	-2.72323400	3.20599200	-4.87254700
H	0.35952200	1.10955500	-5.65827300
H	-1.22231400	1.04631500	-4.87164400
H	-1.31122200	2.58620100	-6.82565600

H	0.04051400	3.52516800	-6.17859500
C	1.48202900	-0.63175500	2.76908100
C	1.98988800	-1.80875000	3.61070200
C	2.11767700	0.68787600	3.22423700
H	0.39384600	-0.55383400	2.92679800
C	1.75201900	-1.56176300	5.10488600
H	3.07266400	-1.95998200	3.43850900
H	1.48631800	-2.73704500	3.29302000
C	1.87417500	0.93500800	4.71599900
H	3.20723600	0.67246900	3.03406100
H	1.70179200	1.51860600	2.63543900
C	2.37374000	-0.23883300	5.56452400
H	2.15224800	-2.40089700	5.69728900
H	0.66394600	-1.53497400	5.29123400
H	2.36091100	1.87308300	5.03194300
H	0.79095200	1.07230400	4.88169900
H	2.15521900	-0.06283400	6.63049800
H	3.47444700	-0.30492700	5.47755000
H	7.59776800	1.34948900	-0.88349300
C	7.39076200	1.82885700	-3.55392700
F	8.61790100	1.46981400	-3.15073400
F	7.37931300	3.18277000	-3.61771500
F	7.22150400	1.38391100	-4.80925100

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.770110
(Hartree/Particle)
Thermal correction to Energy= 0.817149
Thermal correction to Enthalpy= 0.818093
Thermal correction to Gibbs Free Energy= 0.683850
Sum of electronic and zero-point Energies= -6448.125651
Sum of electronic and thermal Energies= -6448.078613
Sum of electronic and thermal Enthalpies= -6448.077669
Sum of electronic and thermal Free Energies= -6448.211912
HF= -6448.8957617
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.282554
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.233698
Solvent correction = -0.0488562
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6452.037351
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6450.058898

E^{cis}-L9-conf2

Ni	-0.69966900	0.55069900	0.21370200
C	-2.40697700	1.14946700	-0.26897000
C	-3.16414100	0.88865400	-1.35225700
H	-4.12818500	1.40652900	-1.46023400
Br	-1.62727600	-1.14492000	1.50167100
C	1.52206800	1.99611200	-0.57715100
C	1.09493800	3.99542600	-1.60088600
C	-0.15153400	3.06869800	-1.62708100
N	0.23420800	1.94652300	-0.75478000
H	1.35925800	4.37829200	-2.59590900
C	1.92812000	-0.95081100	1.46759000
C	3.40335400	-0.83646200	0.97859300
C	2.09607300	0.82381400	0.10080500
N	1.22342600	0.07480400	0.69181800
H	3.68939800	-1.65623000	0.30000600
H	0.97216100	4.85241300	-0.91808400
H	4.12464000	-0.80604400	1.80714300
H	-1.03686100	3.56209800	-1.20277900
H	1.48957100	-1.93112500	1.23169200
N	2.15292500	3.10365100	-1.07507300
N	3.40601200	0.44135700	0.22714100
C	3.37168600	3.61383800	-0.56656700
C	4.31263800	4.15996300	-1.44816100
C	3.64864800	3.56366500	0.80779200
C	5.54364000	4.59888300	-0.96965500
H	4.09639400	4.18854500	-2.51658300
C	4.88276600	3.99764100	1.28437600
H	2.90350000	3.16867200	1.49964300
C	5.83739800	4.49997800	0.39456000
H	6.29316600	4.97745200	-1.66454000
H	5.10615400	3.94444200	2.35101400
C	4.42177700	0.76167300	-0.70381600
C	4.14062900	0.81537700	-2.07728200
C	5.71536700	1.04370300	-0.24653800
C	5.12792900	1.21319400	-2.97478200
H	3.14330200	0.56352800	-2.43941700
C	6.70345300	1.43402400	-1.14555700
H	5.92860800	1.00840200	0.82232700
C	6.40521000	1.53931900	-2.50841800
H	4.90469000	1.27211800	-4.04116000
H	-2.83366000	1.84594200	0.47138700
C	-2.84576300	-0.02085500	-2.46357500
C	-1.81578400	-0.98207400	-2.39238900
C	-3.57564100	0.06623500	-3.66607300
C	-1.52034800	-1.79870500	-3.48252100
H	-1.27546400	-1.10739600	-1.45225900
C	-3.27897300	-0.75027300	-4.75885100
H	-4.38731800	0.79580300	-3.73879100
C	-2.24437900	-1.68667900	-4.67558300
H	-0.72347000	-2.54253300	-3.39699900
H	-3.85960300	-0.65598800	-5.68026600
H	-2.01024700	-2.32941700	-5.52759100
C	7.21778000	4.83581800	0.89061300
F	7.20543800	5.27749700	2.15824400
F	8.01577900	3.74101600	0.86880500
F	7.81565100	5.76759200	0.13454700
C	-0.52388300	2.54006000	-3.02447600
C	-1.08301700	3.65488700	-3.91782700
C	0.61063500	1.77812900	-3.72329300
H	-1.33487800	1.82182100	-2.85169200
C	-1.53187700	3.10384900	-5.27554400
H	-0.31420700	4.43404200	-4.08140400
H	-1.92747200	4.14843200	-3.40744400
C	0.16335700	1.24206200	-5.08708100
H	1.48826100	2.43797500	-3.85878300
H	0.93006400	0.93716800	-3.08701000
C	-0.39431700	2.35608400	-5.97719600
H	-1.90789000	3.92241400	-5.91117300
H	-2.37361600	2.40828500	-5.11619500
H	1.00549400	0.73460600	-5.58676200
H	-0.61435300	0.47832800	-4.92902600
H	-0.74600700	1.93800600	-6.93463300
H	0.41343000	3.07062400	-6.22491200

C	1.72139800	-0.69755300	2.97337900
C	2.33976100	-1.81697000	3.82079700
C	2.20606800	0.68417400	3.43360500
H	0.62811500	-0.73423700	3.11108700
C	2.08032700	-1.59661400	5.31488100
H	3.43246000	-1.86140100	3.65079700
H	1.93124100	-2.79025600	3.50134600
C	1.94688800	0.89729000	4.92891400
H	3.28953200	0.79304700	3.23681200
H	1.69278400	1.46566300	2.84999200
C	2.57107400	-0.21924300	5.77150800
H	2.56199500	-2.39323100	5.90532300
H	0.99529300	-1.67623300	5.50416300
H	2.33159500	1.88111000	5.24540000
H	0.85630000	0.91574200	5.10154400
H	2.34513800	-0.06577800	6.83947800
H	3.67222700	-0.17493300	5.67543100
H	7.69570300	1.69969600	-0.78086700
C	7.42648800	2.10480900	-3.45760400
F	8.68221800	1.85526700	-3.05956500
F	7.30429800	3.45171700	-3.54827600
F	7.28323200	1.62140600	-4.70155900

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.769981
(Hartree/Particle)
Thermal correction to Energy= 0.817099
Thermal correction to Enthalpy= 0.818043
Thermal correction to Gibbs Free Energy= 0.683454
Sum of electronic and zero-point Energies= -6448.123103
Sum of electronic and thermal Energies= -6448.075985
Sum of electronic and thermal Enthalpies= -6448.075041
Sum of electronic and thermal Free Energies= -6448.209630
HF= -6448.8930838
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.280523
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.228751
Solvent correction = -0.0517716
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6452.034945
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6450.057003

E^{trans}-L9

Ni	-0.81450500	1.03518600	0.56128100
C	-2.45421300	1.74208000	0.02839300
C	-2.95285900	2.94304100	0.37428000
H	-2.44480200	3.52754400	1.15371200
Br	-1.85227600	-0.68722400	1.70146000
C	1.49777700	2.27262500	-0.33543800
C	1.24263200	4.35915500	-1.24570900
C	-0.12783300	3.64014300	-1.08774800
N	0.20490700	2.40475000	-0.36032900
H	1.42276200	4.70800200	-2.27223000
C	1.68968400	-0.81943800	1.52006300
C	3.12767800	-0.85399900	0.91777400
C	1.97106800	0.99909800	0.22947700
N	1.06504600	0.33640600	0.87116200
H	3.26349100	-1.67322700	0.19392400
H	1.34845600	5.21880900	-0.56474400
H	3.90820800	-0.93999500	1.68693400
H	-0.82287800	4.23042400	-0.47593300
H	1.11128800	-1.71812300	1.26117800
N	2.21701000	3.31162900	-0.86180000
N	3.22500800	0.44489700	0.20871600
C	3.54063100	3.62961300	-0.47374800
C	4.45112500	4.09076400	-1.43256900
C	3.94997100	3.47198200	0.85904500
C	5.77425100	4.33568700	-1.07677000
H	4.13097400	4.20383300	-2.46884700
C	5.27508500	3.71168000	1.21229900
H	3.23315100	3.14515700	1.61373900
C	6.19226200	4.12705100	0.24182500
H	6.49236000	4.64690700	-1.83536200
H	5.59903900	3.57398800	2.24504500
C	4.17182100	0.67152400	-0.81696700
C	3.75749800	0.83039600	-2.14832900
C	5.53314100	0.75518600	-0.49770900
C	4.68972200	1.13649800	-3.13600400
H	2.70205500	0.72897200	-2.40518400
C	6.46491200	1.05434900	-1.48726200
H	5.85147800	0.63870700	0.53875600
C	6.04187400	1.26589800	-2.80388700
H	4.36631400	1.27647400	-4.16861600
H	-2.99483000	1.13687000	-0.71542000
C	-4.09635300	3.64016200	-0.23880300
C	-4.82463900	3.11388200	-1.32652100
C	-4.45752500	4.92069600	0.22456600
C	-5.85908300	3.83544300	-1.91873500
H	-4.57179200	2.12420400	-1.71209400
C	-5.49339900	5.64559200	-0.36777300
H	-3.90822600	5.34982500	1.06759100
C	-6.20094300	5.10842600	-1.44600400
H	-6.40612200	3.40150100	-2.76005200
H	-5.74990700	6.63662400	0.01608400
H	-7.01122400	5.67278200	-1.91357800
C	7.64996100	4.24703300	0.59515400
F	7.83101400	4.62845700	1.86945400
F	8.27822600	3.05465200	0.45424200
F	8.29281400	5.12054800	-0.19277400
C	-0.84624500	3.30816900	-2.40613400
C	-1.39655700	4.57268000	-3.07767500
C	-0.00836500	2.46802900	-3.37767300
H	-1.71257700	2.69921100	-2.10781200
C	-2.18983300	4.22600600	-4.34127100
H	-0.56449800	5.25220200	-3.34459100
H	-2.03926600	5.11498600	-2.36489300
C	-0.80853800	2.12609600	-4.63962000
H	0.90566700	3.01884000	-3.66876800
H	0.31964600	1.54197300	-2.87697900
C	-1.35711600	3.38687600	-5.31588900
H	-2.54502000	5.14740000	-4.83070900
H	-3.09217300	3.66248000	-4.04535700
H	-0.18372800	1.55095300	-5.34286700
H	-1.65095300	1.46896200	-4.35925200
H	-1.95790200	3.11560300	-6.19943500
H	-0.51129300	3.99460300	-5.68852300
C	1.62412700	-0.64812700	3.04934800

C	2.15534100	-1.88938300	3.77765300
C	2.31083700	0.63016000	3.54991400
H	0.54696900	-0.56136700	3.26967100
C	2.03496500	-1.74169700	5.29810100
H	3.21847400	-2.05357500	3.51751300
H	1.60533100	-2.78173200	3.43514500
C	2.18934700	0.77078200	5.07104500
H	3.38254300	0.61829800	3.27430800
H	1.86116600	1.50633600	3.05496500
C	2.72688300	-0.46811200	5.79395400
H	2.45416900	-2.62913400	5.80003300
H	0.96517600	-1.70240900	5.56927300
H	2.71694600	1.67675600	5.41286900
H	1.12518800	0.90971200	5.33153100
H	2.59968000	-0.36157500	6.88373200
H	3.81503000	-0.55107000	5.61292600
H	7.51723200	1.16695900	-1.22642500
C	7.02514600	1.73576300	-3.84120600
F	8.26990900	1.30422400	-3.59288900
F	7.07860700	3.08970200	-3.87425600
F	6.68710600	1.33445800	-5.07680900

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.769418
(Hartree/Particle)
Thermal correction to Energy= 0.816986
Thermal correction to Enthalpy= 0.817930
Thermal correction to Gibbs Free Energy= 0.679838
Sum of electronic and zero-point Energies= -6448.114781
Sum of electronic and thermal Energies= -6448.067212
Sum of electronic and thermal Enthalpies= -6448.066268
Sum of electronic and thermal Free Energies= -6448.204361
HF= -6448.8841988
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.274747
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.220768
Solvent correction = -0.0539791
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6452.027992
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6450.050867

E^{trans}-L9-conf2

Ni	-0.90285800	1.10274100	0.62291200
C	-2.51824800	1.81698900	0.04352300
C	-3.34913000	1.27184000	-0.86360500
H	-3.20399200	0.22293200	-1.14777900
Br	-1.90934900	-0.65798200	1.72194300
C	1.41411500	2.35834200	-0.26117900
C	1.20367800	4.43094000	-1.21866100
C	-0.18790500	3.76415800	-0.99725300
N	0.12380200	2.51436700	-0.27680900
H	1.37133900	4.70623900	-2.26965800
C	1.58638800	-0.76250400	1.55027300
C	3.00671600	-0.81809200	0.90957700
C	1.87455300	1.07248100	0.28527600
N	0.97228200	0.42211000	0.94350400
H	3.10556700	-1.62878000	0.17043100
H	1.34919300	5.32944100	-0.59879700
H	3.80510700	-0.93254100	1.65645100
H	-0.82409000	4.39064000	-0.35335600
H	0.97773300	-1.63929400	1.28638600
N	2.15131600	3.38081800	-0.79068200
N	3.11400500	0.48909500	0.21726000
C	3.49077500	3.66525000	-0.44074400
C	4.38058300	4.12392800	-1.42067500
C	3.93897900	3.47658600	0.87561900
C	5.71922400	4.33385800	-1.10339800
H	4.03208100	4.26213800	-2.44464200
C	5.27969900	3.68109600	1.18946000
H	3.23943500	3.15409100	1.64805700
C	6.17478800	4.09316800	0.19717800
H	6.41917000	4.64269800	-1.87977900
H	5.63303400	3.51920100	2.20896400
C	4.02692700	0.70332700	-0.84178300
C	3.56638300	0.88469400	-2.15505100
C	5.40060400	0.75339100	-0.57306800
C	4.46757800	1.18245900	-3.17364700
H	2.50013300	0.80726400	-2.37345700
C	6.30116100	1.04392800	-1.59363200
H	5.75434600	0.61847100	0.44957000
C	5.83362700	1.28036500	-2.89083600
H	4.10895200	1.34059300	-4.19193200
H	-2.67051400	2.87341800	0.32440200
C	-4.37242800	1.98457300	-1.64660100
C	-4.80166800	3.29502100	-1.34953200
C	-4.89662600	1.37718900	-2.80512100
C	-5.69495600	3.96792300	-2.18085500
H	-4.42782100	3.79005200	-0.45083800
C	-5.78893200	2.05077700	-3.64139500
H	-4.58183100	0.35967400	-3.05274800
C	-6.19125000	3.35396900	-3.33738000
H	-6.01083100	4.98281900	-1.92481400
H	-6.17212600	1.55446900	-4.53688000
H	-6.88847000	3.88509400	-3.98956700
C	7.64525700	4.17630700	0.50437700
F	7.87605400	4.52070300	1.78126100
F	8.24508000	2.97668300	0.31158400
F	8.27869900	5.05816700	-0.28209400
C	-0.97200600	3.47176700	-2.28799900
C	-1.39126600	4.75365300	-3.01771500
C	-0.26650200	2.49125000	-3.23177700
H	-1.89174400	2.97569200	-1.95685300
C	-2.28177900	4.42431600	-4.22167600
H	-0.49929100	5.30984500	-3.36460000
H	-1.92860400	5.41920300	-2.32059100
C	-1.15774100	2.16738100	-4.43649400
H	0.69162700	2.91830500	-3.58602000
H	-0.02745000	1.56566700	-2.68320500
C	-1.59439500	3.43846300	-5.17186400
H	-2.55180900	5.34941800	-4.75699300
H	-3.22469700	3.98351500	-3.85670400
H	-0.63474300	1.48279300	-5.12471500
H	-2.05449800	1.63403700	-4.07647500
H	-2.26795100	3.18284400	-6.00607300
H	-0.70672300	3.92177900	-5.62215100
C	1.56396400	-0.62573700	3.08376200
C	2.07664500	-1.89922400	3.76839200

C	2.30067400	0.61937900	3.59661300
H	0.49537400	-0.51469500	3.33300600
C	2.00069400	-1.78549800	5.29459000
H	3.12718000	-2.08774100	3.47566800
H	1.49131000	-2.76619200	3.41953700
C	2.22321600	0.72621500	5.12343800
H	3.36412200	0.58248000	3.29282600
H	1.86581800	1.52051100	3.13424000
C	2.74258500	-0.54505700	5.80207900
H	2.40640900	-2.69677300	5.76382000
H	0.93998400	-1.72209200	5.59540100
H	2.78613600	1.60792000	5.47233800
H	1.17085000	0.88937600	5.41603700
H	2.64701400	-0.46167600	6.89711000
H	3.82272100	-0.65484400	5.59012600
C	6.78677200	1.74437400	-3.95840200
F	8.03140500	1.28651400	-3.76173100
F	6.86498700	3.09752600	-3.97697500
F	6.39576400	1.36537600	-5.18530100
H	7.36473900	1.13095800	-1.37141500

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.769573
(Hartree/Particle)
Thermal correction to Energy= 0.817113
Thermal correction to Enthalpy= 0.818057
Thermal correction to Gibbs Free Energy= 0.680883
Sum of electronic and zero-point Energies= -6448.114560
Sum of electronic and thermal Energies= -6448.067020
Sum of electronic and thermal Enthalpies= -6448.066076
Sum of electronic and thermal Free Energies= -6448.203250
HF= -6448.8841328
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.273114
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.220285
Solvent correction = -0.0528287
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6452.027398
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6450.051352

^{3}F^{trans}-L9

Ni	-0.73010600	0.80127700	0.38746200
C	-1.23043400	2.04888600	1.81308500
C	-2.47529200	2.08733800	2.33074300
H	-3.21848700	1.36614900	1.95993700
Br	-1.73033900	-1.10990600	-0.60304000
C	1.63928300	2.02540500	-0.51250500
C	1.53073600	4.07091600	-1.52931000
C	0.11490600	3.54289100	-1.15651600
N	0.36829100	2.17090200	-0.69647600
H	1.69398300	4.03937400	-2.62150700
C	1.72909400	-1.18645000	1.17888900
C	3.24092900	-1.07839800	0.81451000
C	2.06447300	0.73438300	0.06155800
N	1.17670500	0.10959800	0.76054300
H	3.63152400	-1.95821600	0.28641800
H	1.73187300	5.08923900	-1.17219700
H	3.85792000	-0.90306200	1.71341700
H	-0.28981900	4.09578000	-0.28801200
H	1.22342200	-1.95128000	0.56173600
N	2.41280900	3.10422400	-0.84765000
N	3.27178000	0.10326500	-0.06977600
C	3.73668600	3.34098400	-0.44198700
C	4.66746300	3.87637800	-1.34329100
C	4.13971300	3.01724000	0.86446400
C	5.99895700	4.02261400	-0.96514000
H	4.35878900	4.12703700	-2.35865100
C	5.47268900	3.15895400	1.23662000
H	3.40271100	2.65610100	1.58363100
C	6.40892300	3.64435400	0.31733300
H	6.72921200	4.39214900	-1.68494200
H	5.78849800	2.89747000	2.24781200
C	4.24361600	0.37163100	-1.04834200
C	3.85229900	0.69372500	-2.35880700
C	5.60552400	0.34703500	-0.71675000
C	4.80862300	1.06173100	-3.29994700
H	2.79708800	0.65037300	-2.63378000
C	6.55988500	0.70882900	-1.66306500
H	5.91258700	0.09717100	0.29930000
C	6.16259000	1.08911600	-2.94899600
H	4.50448800	1.32272600	-4.31484900
H	7.61382700	0.73686700	-1.38663100
H	-0.49883100	2.77667100	2.20722100
C	-3.00787800	2.99120200	3.36979200
C	-4.34601500	2.85106200	3.78460400
C	-2.23908500	4.00350800	3.97817200
C	-4.89557700	3.68110400	4.76335400
H	-4.96027100	2.07161700	3.32506300
C	-2.78412500	4.83344100	4.95552300
H	-1.19801000	4.13778500	3.67646700
C	-4.11706700	4.67851100	5.35563300
H	-5.93773000	3.54799700	5.06548200
H	-2.16533900	5.61074000	5.41220200
H	-4.54271100	5.33061700	6.12220800
C	1.45371600	-1.49565400	2.65220700
C	-0.04517500	-1.42859100	2.98084500
C	2.03472500	-2.86689800	3.03364000
H	1.97169400	-0.72074500	3.25123800
C	-0.32265800	-1.78716100	4.44250400
H	-0.59007600	-2.11776200	2.31233100
H	-0.43463400	-0.42372700	2.76126800
C	1.75245900	-3.22288700	4.49681100
H	1.58103000	-3.63240700	2.37722600
H	3.12184500	-2.89706400	2.84448300
C	0.25491200	-3.15646900	4.81092100
H	-1.40776600	-1.76007000	4.63091700
H	0.12452900	-1.01650100	5.09715000
H	2.15382900	-4.22429900	4.72393200
H	2.29252900	-2.51387200	5.15086000
H	0.07777700	-3.37944400	5.87604800
H	-0.27054900	-3.93921400	4.23403100
C	-0.91618100	3.60561500	-2.28349300
C	-2.23227500	2.92105700	-1.88266600
C	-1.16257400	5.06178700	-2.70982000
H	-0.49343800	3.05624100	-3.14700500
C	-3.29330100	3.03732700	-2.97983500
H	-2.60512700	3.38126600	-0.95009700

H	-2.05260800	1.85949500	-1.65558700
C	-2.22511700	5.16856500	-3.80814300
H	-1.49566800	5.63395900	-1.82385700
H	-0.22314100	5.53112700	-3.04984700
C	-3.53373100	4.49343300	-3.38723500
H	-4.23020200	2.56846900	-2.63950700
H	-2.96286700	2.46226400	-3.86400800
H	-2.39725500	6.22732400	-4.06245300
H	-1.84507900	4.68398400	-4.72607100
H	-4.27291500	4.55057600	-4.20310400
H	-3.96648800	5.04415300	-2.53210700
C	7.86864100	3.66693400	0.67882300
C	7.17650600	1.62001700	-3.92461100
F	6.84317700	1.34968900	-5.19695100
F	8.40218100	1.12351500	-3.70441100
F	7.27689400	2.96865500	-3.82986100
F	8.54883800	4.59209700	-0.01315900
F	8.45020800	2.47202500	0.41316200
F	8.06114000	3.90431000	1.98647400

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.767062
(Hartree/Particle)
Thermal correction to Energy= 0.815767
Thermal correction to Enthalpy= 0.816711
Thermal correction to Gibbs Free Energy= 0.671792
Sum of electronic and zero-point Energies= -6448.111905
Sum of electronic and thermal Energies= -6448.063200
Sum of electronic and thermal Enthalpies= -6448.062256
Sum of electronic and thermal Free Energies= -6448.207174
HF= -6448.8789664
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.304465
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.248691
Solvent correction = -0.0557741
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6452.018542
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6450.035781

^{3}F^{trans}-L9-conf2

Ni	-1.12765000	0.68509000	0.11800800
C	-1.16133300	1.94598900	1.61925200
C	-1.83324000	1.71171400	2.76325900
H	-2.53138100	0.86400300	2.78986700
Br	-2.52362000	-1.20865300	0.11926600
C	1.19622400	1.94171800	-0.83645400
C	1.01607300	4.12645900	-1.51996400
C	-0.35667300	3.38386400	-1.58388800
N	-0.06635200	2.02535900	-1.11146700
H	1.34373100	4.49496600	-2.50362500
C	1.34495100	-1.20831700	0.95241200
C	2.86497400	-1.09016600	0.61234500
C	1.66030800	0.65752900	-0.27350900
N	0.73949700	-0.06517800	0.26918400
H	3.23030800	-1.92207600	-0.00849000
H	1.00656600	4.97507800	-0.82050100
H	3.49196900	-1.03138000	1.51436300
H	-1.07414500	3.83521000	-0.87878700
H	0.90830500	-2.12864700	0.53363100
N	1.93421700	3.08211100	-1.01850600
N	2.93438100	0.16953200	-0.16043200
C	3.11345100	3.38718600	-0.29741300
C	4.18570200	4.00974600	-0.94814600
C	3.22112400	3.04683300	1.05979200
C	5.38059200	4.22908300	-0.26880600
H	4.10005000	4.26841300	-2.00399600
C	4.41989700	3.25894500	1.73536300
H	2.37152500	2.60253300	1.58003500
C	5.50654700	3.83183900	1.06669500
H	6.23082600	4.66602700	-0.79264300
H	4.51108400	2.97711100	2.78551700
C	4.04372200	0.56594500	-0.92712100
C	3.88738500	0.91483300	-2.27875200
C	5.31192500	0.64125800	-0.33350900
C	4.97083400	1.40515600	-3.00114700
H	2.91244700	0.80972800	-2.75688500
C	6.39450600	1.12546000	-1.06095200
H	5.43726700	0.37594700	0.71645700
C	6.22215100	1.53015900	-2.38874900
H	4.84587900	1.69143300	-4.04660400
H	7.36642000	1.23107900	-0.57884200
H	-0.46397300	2.80527500	1.61788300
C	-1.72114400	2.43575300	4.04400600
C	-2.53241100	2.04799100	5.12752700
C	-0.80018600	3.48052900	4.26025300
C	-2.43139300	2.67208200	6.37221400
H	-3.25079000	1.23657500	4.98173000
C	-0.69704800	4.10599400	5.50090900
H	-0.15063100	3.79848300	3.44165700
C	-1.51152200	3.70537100	6.56727000
H	-3.07396400	2.34865000	7.19529400
H	0.02746700	4.91266600	5.64227300
H	-1.42718400	4.19488900	7.54048200
C	0.98950600	-1.15739100	2.44896400
C	1.46536100	-2.41515200	3.18697100
C	1.47947200	0.11718000	3.15042600
H	-0.11391000	-1.14325000	2.47318100
C	1.04811400	-2.38864500	4.66154000
H	2.56836600	-2.48720100	3.12624400
H	1.06336200	-3.31467600	2.69089100
C	1.05607800	0.13817200	4.62192500
H	2.58289500	0.18108300	3.08975900
H	1.06451200	0.99696300	2.63776700
C	1.53293800	-1.11477900	5.36155400
H	1.42858900	-3.28473500	5.17892800
H	-0.05381900	-2.43561900	4.71925100
H	1.43202500	1.05053700	5.11206600
H	-0.04353600	0.20101400	4.67051300
H	1.18537200	-1.09811000	6.40746900
H	2.63868300	-1.12012000	5.39949600
C	-1.01559500	3.34269200	-2.97201700
C	-1.42288900	4.74356900	-3.44939400
C	-0.16053900	2.62245200	-4.02423100
H	-1.93904900	2.75067300	-2.83956700
C	-2.12094400	4.69525400	-4.81270200
H	-0.52290400	5.38139500	-3.53130100
H	-2.07607700	5.21974500	-2.69873200

C	-0.86205600	2.57876000	-5.38582000
H	0.80797000	3.14463400	-4.13754800
H	0.06638200	1.60228900	-3.67591400
C	-1.25913900	3.98073300	-5.85864900
H	-2.36864600	5.71570400	-5.14746500
H	-3.08086400	4.15894400	-4.70599700
H	-0.21342000	2.08898800	-6.13045200
H	-1.76853400	1.95302900	-5.30210200
H	-1.79310400	3.92445000	-6.82118500
H	-0.34470900	4.57485400	-6.04299700
C	6.84318900	3.91972800	1.75182500
C	7.35183000	2.19740900	-3.12332300
F	6.72242400	4.09682200	3.07657900
F	7.59724100	4.91740700	1.26847300
F	7.54773200	2.77482200	1.57575600
F	8.55246500	1.77917500	-2.69776700
F	7.31733400	3.54044700	-2.94038100
F	7.28727000	1.98938900	-4.44831600

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.767831
(Hartree/Particle)
Thermal correction to Energy= 0.816141
Thermal correction to Enthalpy= 0.817086
Thermal correction to Gibbs Free Energy= 0.674081
Sum of electronic and zero-point Energies= -6448.110454
Sum of electronic and thermal Energies= -6448.062144
Sum of electronic and thermal Enthalpies= -6448.061199
Sum of electronic and thermal Free Energies= -6448.204204
HF= -6448.8782851
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.297271
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6447.243878
Solvent correction = -0.0533931
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6452.01918
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6450.037051

Figure A4.7
E^{cis}-L8

Ni	-1.19622300	0.67448400	0.23843200
C	-2.79608000	1.06302600	-0.65593100
C	-2.95103600	1.05910300	-1.99644000
H	-3.90696100	1.37909400	-2.43595000
Br	-2.27624600	-0.91238200	1.53260300
C	1.07758900	2.04481100	-0.51862000
C	0.75429200	3.83412300	-1.90748500
C	-0.59420400	3.30976400	-1.34068100
N	-0.21246300	2.06059400	-0.66152300
H	0.85904500	3.59292900	-2.97757900
C	1.40794800	-0.90045000	1.56017800
C	2.91526600	-0.51045400	1.46408400
C	1.60438800	0.90889200	0.24386100
N	0.72081800	0.21990400	0.89041300
H	3.56452200	-1.34924100	1.18254800
H	0.89993000	4.91330400	-1.76644700
H	3.29150500	-0.07269000	2.40201800
H	-1.27956200	3.06200300	-2.15724400
H	1.07142600	-0.92352300	2.60583700
N	1.74832200	3.08009800	-1.11460600
N	2.91162300	0.51338000	0.39316500
C	3.01786500	3.54565300	-0.74512800
C	3.40972800	3.54549100	0.60755300
C	3.94579700	3.97620500	-1.70017300
H	2.68376100	3.28016400	1.38324100
C	5.23575800	4.29785400	-1.28438900
H	3.67553800	4.00250400	-2.75715200
C	5.53959800	4.17447600	0.07355800
H	6.00491500	4.58046200	-2.00118500
C	3.87967800	0.62956900	-0.61650700
C	5.23146100	0.84784200	-0.28836400
C	3.52659800	0.57674300	-1.97205400
H	5.54046700	0.90023300	0.76043400
C	4.51148700	0.79893900	-2.93145600
H	2.49694500	0.37527700	-2.27287500
C	5.81366200	1.04654300	-2.49225800
H	-3.67051400	1.32108900	-0.04373500
C	-1.89255600	0.72271900	-2.96441900
C	-1.78704800	1.42076900	-4.18407500
C	-0.91706400	-0.25487700	-2.68257400
C	-0.71711500	1.20328700	-5.05475300
H	-2.54858100	2.16482200	-4.43525800
C	0.14418300	-0.48552300	-3.55941800
H	-1.02793300	-0.85198400	-1.77497100
C	0.26233500	0.25393200	-4.74193000
H	-0.65130300	1.77020100	-5.98713000
H	0.87242800	-1.26857200	-3.33337300
H	1.09124300	0.06872300	-5.42980100
C	6.94936900	4.38183400	0.59164100
F	7.78673300	4.73221700	-0.39812300
F	6.99387600	5.34288000	1.52379500
F	7.42008200	3.25545500	1.14745000
C	-1.32779500	4.24561300	-0.36037100
C	-1.90356100	5.45329200	-1.11620500
C	-2.84645100	6.32383800	-0.28651800
H	-1.07774100	6.07719600	-1.50589600
H	-2.44584000	5.07818600	-2.00162200
H	-3.28968800	7.12221200	-0.90157300
H	-3.67209400	5.72432600	0.13039800
H	-2.32822100	6.80805600	0.55541700
C	1.04477100	-2.25345900	0.91260700
C	1.55611000	-3.40975100	1.78524200
C	1.07914300	-4.78868700	1.33046100
H	2.66209800	-3.39719100	1.82006700
H	1.21538100	-3.23685700	2.82074500
H	1.39919900	-5.56990500	2.03726400
H	-0.02054900	-4.82132400	1.26745500
H	1.47915300	-5.05816700	0.34063000
H	4.27358300	0.77888000	-3.99485700
C	6.92067000	1.40046500	-3.46503000
F	6.51653300	1.24761700	-4.73990400
F	8.00720000	0.64826100	-3.28532600
F	7.28792200	2.68896800	-3.31676300
N	4.64294700	3.83177200	0.99848800
N	6.16567500	1.05265000	-1.20664500
H	-2.17650600	3.64613900	0.00952300
H	-0.05600300	-2.28208500	0.92743000

C	1.50761300	-2.34504200	-0.54198400
H	1.16576200	-1.47441300	-1.11690800
H	2.60570900	-2.40837200	-0.63215200
H	1.08832300	-3.23471400	-1.03265800
C	-0.46361400	4.63438900	0.84138700
H	-0.09516500	3.74124300	1.36810500
H	0.40495000	5.24736600	0.54561800
H	-1.04141500	5.21907700	1.57084000

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.670237
(Hartree/Particle)
Thermal correction to Energy= 0.716518
Thermal correction to Enthalpy= 0.717462
Thermal correction to Gibbs Free Energy= 0.584929
Sum of electronic and zero-point Energies= -6325.493046
Sum of electronic and thermal Energies= -6325.446764
Sum of electronic and thermal Enthalpies= -6325.445820
Sum of electronic and thermal Free Energies= -6325.578354
HF= -6326.1632825
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6324.551569
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6324.502558
Solvent correction = -0.0490106
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6329.18937
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6327.354506

E*trans*-L8

Ni	-1.13089500	0.50655400	0.29794500
C	-2.80369700	0.94883300	-0.40369700
C	-3.10594700	0.89309300	-1.71520300
H	-2.34335600	0.54061400	-2.42357100
Br	-2.10292900	-0.84518700	1.90693300
C	1.12022000	1.81620300	-0.63123800
C	0.77722900	3.51875200	-2.12319200
C	-0.57197400	2.96762300	-1.57583900
N	-0.16816500	1.77653400	-0.80504100
H	0.93805700	3.24441700	-3.17764800
C	1.44803400	-1.08705900	1.49254600
C	2.96047800	-0.71703100	1.40333500
C	1.66725300	0.72820600	0.18622100
N	0.78026400	0.04087900	0.82945100
H	3.59438500	-1.55616200	1.08715000
H	0.87241200	4.60806000	-2.02536100
H	3.34778100	-0.32401400	2.35709300
H	-1.22240500	2.63903800	-2.39645900
H	1.10377900	-1.12404100	2.53529600
N	1.77364400	2.84280000	-1.26260100
N	2.97290200	0.34296700	0.36786800
C	2.97311000	3.42079000	-0.81910800
C	3.93687200	3.86310800	-1.74577800
C	3.26145900	3.54391700	0.54605200
H	3.74649000	3.77681000	-2.82020200
C	4.50489100	4.04183800	0.92927700
H	2.52106700	3.24971700	1.29170400
C	5.40084400	4.41241300	-0.07554000
H	4.77316500	4.14428900	1.98055200
C	4.00331400	0.55055800	-0.56226700
C	3.73283000	0.51545600	-1.94387100
C	5.30982400	0.84299600	-0.15489400
H	2.73907700	0.21885800	-2.29553900
C	6.25662800	1.17264200	-1.12194100
H	5.56289100	0.86467000	0.90652300
C	5.85131900	1.19641300	-2.45875600
H	-3.57649400	1.26422700	0.31030700
C	-4.36802200	1.29477600	-2.36012800
C	-4.47100100	1.24754100	-3.76417500
C	-5.48742600	1.75941200	-1.63918400
C	-5.63390900	1.65008900	-4.42343400
H	-3.61699700	0.88495900	-4.34388800
C	-6.64849200	2.16213300	-2.29533100
H	-5.44462200	1.79888200	-0.54900500
C	-6.73090200	2.11209000	-3.69238300
H	-5.68406200	1.60067000	-5.51439200
H	-7.50237700	2.51620600	-1.71163900
H	-7.64369700	2.42720900	-4.20352000
C	6.80877900	4.87051900	0.25089400
F	6.97818200	5.01447700	1.57831700
F	7.71150200	3.96354500	-0.16997200
F	7.10375300	6.03418700	-0.33000700
C	-1.37899000	3.94397600	-0.69766600
C	1.05328300	-2.41736800	0.81431200
C	1.42718900	-2.44958400	-0.66936800
H	1.05719300	-3.36778500	-1.14655800
H	0.97181200	-1.60573300	-1.20974300
H	2.51914400	-2.41732100	-0.82846200
C	-0.57896600	4.45198100	0.50347400
H	-0.21383700	3.61397600	1.11694100
H	0.28615600	5.06601500	0.19918000
H	-1.20560600	5.07533000	1.15673000
C	1.61445900	-3.60529300	1.61091100
C	1.06797400	-4.96362800	1.17212000
H	1.37223700	-3.45121200	2.67685000
H	2.71894600	-3.61678600	1.54569800
H	1.43980600	-5.76811100	1.82550600
H	-0.03294300	-4.97551800	1.21642000
H	1.36392000	-5.21502100	0.14186100
H	-0.04550000	-2.44712700	0.89276500
H	-2.21957200	3.34326400	-0.31726400
C	-1.97062300	5.06721700	-1.56374500
C	-3.03671600	5.90150900	-0.85489600
H	-2.41978600	4.60990600	-2.46214500
H	-1.16213600	5.73002600	-1.92528600
H	-3.46533500	6.65333100	-1.53531300
H	-3.86144400	5.26120500	-0.50244800
H	-2.63163300	6.43935000	0.01640000
C	6.78016800	1.67059400	-3.55967000
F	7.98748600	1.99864300	-3.07178000
F	6.27604000	2.75347200	-4.16968700
F	6.95883600	0.72600000	-4.49227100
H	7.26895300	1.46165800	-0.84466100
N	5.11656300	4.34116100	-1.37578600
N	4.62843100	0.85177000	-2.86109700

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.669614
(Hartree/Particle)

Thermal correction to Energy= 0.716414
Thermal correction to Enthalpy= 0.717358
Thermal correction to Gibbs Free Energy= 0.580946
Sum of electronic and zero-point Energies= -6325.482279
Sum of electronic and thermal Energies= -6325.435479
Sum of electronic and thermal Enthalpies= -6325.434535
Sum of electronic and thermal Free Energies= -6325.570947
HF= -6326.1518927
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6324.545548
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6324.490555
Solvent correction = -0.0549929
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6329.179713
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6327.347035

^{3}F^{cis}-L8

Ni	-0.94285800	0.76391000	0.32737800
C	-1.28217300	1.60583500	2.08363600
C	-1.25682500	0.94141600	3.25703200
H	-1.32483500	1.47414400	4.21868700
Br	-2.02312300	-0.39926500	-1.45162900
C	1.48257700	1.99042300	-0.46570500
C	1.44841800	3.97083100	-1.62171500
C	0.02081500	3.55390400	-1.15639900
N	0.21690200	2.20756100	-0.60124400
H	1.56878000	3.87533700	-2.71275000
C	1.49459000	-1.32915100	1.02035700
C	3.03065400	-1.08844100	0.97396900
C	1.87429400	0.68474000	0.09803900
N	0.93560900	-0.02550100	0.62619200
H	3.58721100	-1.91079300	0.50659500
H	1.72249300	4.99262900	-1.32778900
H	3.44756000	-0.90119900	1.97587500
N	2.30756100	2.99319600	-0.92304700
N	3.13571200	0.13360800	0.14253300
C	3.59272200	3.26948800	-0.43423500
C	3.91253000	3.01982900	0.91457100
C	4.60032800	3.76347200	-1.27031900
H	3.12945500	2.70143800	1.61099200
C	5.88862200	3.90172100	-0.75934300
H	4.38890100	3.98284600	-2.31813800
C	6.11123900	3.53682000	0.57034100
H	6.71299600	4.22716900	-1.39143200
C	4.13526300	0.34234600	-0.82128700
C	5.48849000	0.40320100	-0.43721500
C	3.82221900	0.52191300	-2.17453900
H	5.76691600	0.26705400	0.61255500
C	4.84934700	0.81604400	-3.06895600
H	2.78984400	0.43199200	-2.51569200
C	6.15099600	0.89687300	-2.56993700
H	-1.41460300	2.69459100	2.17603500
C	-1.11481000	-0.52289100	3.37174300
C	-0.38919300	-1.10253100	4.43060200
C	-1.69529200	-1.38661400	2.42167400
C	-0.21586900	-2.48553800	4.51456700
H	0.05440600	-0.45091100	5.18864500
C	-1.52819500	-2.76906500	2.50685400
H	-2.31167500	-0.96897800	1.62132200
C	-0.78215300	-3.32713900	3.54979000
H	0.36022600	-2.91169900	5.34018100
H	-1.99519100	-3.41383400	1.75830100
H	-0.65701100	-4.41025300	3.62081400
H	-0.65579300	3.46680000	-2.01884600
H	1.16578700	-1.55277400	2.04320000
C	-0.63099800	4.49001300	-0.11771900
C	-1.06990800	5.80181000	-0.78862300
H	-1.53994700	3.96129900	0.21639600
C	-1.89418100	6.72250500	0.11034900
H	-0.17912100	6.34754600	-1.15181800
H	-1.66049300	5.55268900	-1.68749700
H	-2.25038500	7.60180800	-0.44810000
H	-2.77802800	6.19802200	0.50871300
H	-1.31132200	7.09193700	0.96789600
C	0.97161200	-2.43850200	0.08229800
C	1.41179600	-3.81585500	0.60381400
H	-0.12553000	-2.37929300	0.15128800
C	0.66239700	-4.98611700	-0.03119300
H	2.49848500	-3.94540600	0.44441000
H	1.25372100	-3.84266500	1.69440100
H	0.98066200	-5.94468900	0.40755400
H	-0.42350100	-4.88711900	0.12776400
H	0.83308600	-5.04796600	-1.11698300
C	0.26318100	4.70838600	1.10567800
H	0.57329900	3.75116700	1.54802100
H	1.16534600	5.29240400	0.85730000
H	-0.27429000	5.25893800	1.89032600
C	1.34570500	-2.20122100	-1.38226700
H	0.93695400	-1.24556300	-1.74088500
H	2.43753000	-2.22066700	-1.54238600
H	0.90635100	-2.97907400	-2.02208800
C	7.50474300	3.53228300	1.16758700
F	7.57672200	4.30981500	2.25545300
F	8.41544400	3.97583800	0.28557900
F	7.85844600	2.29033200	1.53180500
C	7.30939600	1.31391100	-3.45444500
F	8.33801500	0.47040500	-3.36613700
F	7.75431300	2.53800200	-3.10529600
F	6.93693400	1.38163500	-4.74590700
H	4.64812800	0.97310300	-4.12847600
N	5.14358900	3.13013900	1.39190000
N	6.46349800	0.67692700	-1.29299500

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.669029 (Hartree/Particle)
Thermal correction to Energy= 0.715826
Thermal correction to Enthalpy= 0.716770
Thermal correction to Gibbs Free Energy= 0.581595
Sum of electronic and zero-point Energies= -6325.486138
Sum of electronic and thermal Energies= -6325.439342
Sum of electronic and thermal Enthalpies= -6325.438398
Sum of electronic and thermal Free Energies= -6325.573573

HF= -6326.1551676
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6324.578138
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6324.529802
Solvent correction = -0.0483352
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6329.177996
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6327.338851

^{3}F^{trans}-L8

Ni	-0.53721800	0.65963300	0.61716100
C	-0.75282500	1.35775700	2.43661900
C	-1.94098000	1.63548400	3.00964800
H	-2.86126300	1.39915300	2.45629900
Br	-2.01434600	-0.19006600	-1.03555500
C	1.75549600	1.99816400	-0.35493000
C	1.54565100	4.02921900	-1.41250800
C	0.15710700	3.45835100	-0.98517400
N	0.47521300	2.15288300	-0.38454900
H	1.64419500	4.09740400	-2.50692000
C	2.06623900	-1.29976700	1.16831100
C	3.56891700	-1.05542500	0.83060500
C	2.25389100	0.70215800	0.15525400
N	1.40574300	-0.04461500	0.77878200
H	4.00657500	-1.86137100	0.22484700
H	1.74886500	5.02035500	-0.98157300
H	4.18010700	-0.92466700	1.73664900
N	2.49681800	3.04024900	-0.86466300
N	3.53133800	0.20059700	0.04986600
C	3.81448500	3.35050600	-0.49311100
C	4.26994300	3.09264300	0.81405100
C	4.71993200	3.89364300	-1.41157900
H	3.56731500	2.73855600	1.57620000
C	6.04589000	4.06916800	-1.02333000
H	4.40174600	4.12295400	-2.42977900
C	6.40718600	3.69000300	0.27154400
H	6.79418200	4.43399600	-1.72482100
C	4.40549300	0.46804500	-1.01932400
C	5.78875700	0.58775000	-0.79024400
C	3.93042700	0.64277400	-2.32470300
H	6.19203100	0.45581400	0.21867900
C	4.83351100	0.99324300	-3.32647600
H	2.86979700	0.51011500	-2.54618600
C	6.17857100	1.13174700	-2.97711200
H	0.15059200	1.59351600	3.02529100
C	-2.19187200	2.27278300	4.31694100
C	-3.51591800	2.41440900	4.77411400
C	-1.16110300	2.78252700	5.13195500
C	-3.80209500	3.03085600	5.99361300
H	-4.33088500	2.03010400	4.15435000
C	-1.44338000	3.39853500	6.34921100
H	-0.12485800	2.69896500	4.79777100
C	-2.76646100	3.52664200	6.78950200
H	-4.83987200	3.12535700	6.32381000
H	-0.62530300	3.78721500	6.96161000
H	-2.98591700	4.01177100	7.74365600
H	-0.45601100	3.25320600	-1.87582200
H	1.94107800	-1.42272700	2.25432600
C	-0.65842800	4.37037600	-0.04467500
C	0.04722200	4.55359700	1.31002000
H	-0.68874000	5.35381900	-0.55308900
C	-0.69081000	5.45903200	2.29428400
H	0.17733000	3.56346400	1.77107500
H	1.06101300	4.95915600	1.13730600
H	-0.08197900	5.63451200	3.19435500
H	-0.92545900	6.44091600	1.84913100
H	-1.63242200	5.00101200	2.63043200
C	1.42938600	-2.51948300	0.46662100
C	1.39931100	-2.33828900	-1.06100800
H	2.10062000	-3.36777000	0.70230500
C	0.89947700	-3.56125500	-1.82765600
H	0.75095000	-1.47938500	-1.30007200
H	2.41473500	-2.08451000	-1.41674800
H	0.99424800	-3.40729500	-2.91365100
H	1.47094700	-4.46782200	-1.56570400
H	-0.16282800	-3.75580900	-1.61941600
C	-2.09683800	3.86057800	0.07573100
H	-2.55265300	3.72991400	-0.91754800
H	-2.12857400	2.89167000	0.58935100
H	-2.72073400	4.56324200	0.64548900
C	0.05072600	-2.82949800	1.05812400
H	0.09238700	-2.87580000	2.15758700
H	-0.68998700	-2.06888600	0.76898100
H	-0.32393300	-3.79823300	0.69831800
C	7.85185000	3.71810300	0.73092400
F	8.00552900	4.46470700	1.83097300
F	8.65743400	4.21702700	-0.22063800
F	8.27782300	2.47776500	1.01848800
C	7.20689100	1.61575900	-3.98116300
F	8.28563900	0.83390500	-4.01129400
F	7.61412600	2.86370300	-3.67305900
F	6.69106700	1.66247000	-5.22280900
H	4.50544500	1.15091200	-4.35374700
N	5.53702500	3.23713600	1.17403500
N	6.64564600	0.91437300	-1.74801100

(U)B3LYP-D3(BJ)/def2-SVP
Zero-point correction= 0.668362 (Hartree/Particle)
Thermal correction to Energy= 0.715747
Thermal correction to Enthalpy= 0.716692
Thermal correction to Gibbs Free Energy= 0.577145
Sum of electronic and zero-point Energies= -6325.479330
Sum of electronic and thermal Energies= -6325.431944
Sum of electronic and thermal Enthalpies= -6325.431000
Sum of electronic and thermal Free Energies= -6325.570546
HF= -6326.1476917
M06-2X/6-31G(d)-SMD(EA/DMA)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6324.571805
M06-2X/6-31G(d)//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6324.518832
Solvent correction = -0.0529735
(U)B3LYP-D3(BJ)/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP
HF = -6329.170182
M06/def2-TZVP//(U)B3LYP-D3(BJ)/def2-SVP

HF = -6327.331981

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