# ABSTRACT


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| Title of Dissertation: | EXPLORING MECHANISMS AND PREDICTING REACTIVITY OF TRANSITION METAL-CATALYZED AND PHOTOCATALYZED RADICAL AND POLAR ORGANIC TRANSFORMATIONS |
| | Robert Thompson Martin, Doctor of Philosophy, 2023 |
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The creation of protocols to form novel C-C and C-heteroatom bonds has been the primary goal of organic synthesis since its inception. Chemists have long harnessed both radical and polar reactivities, often as complementary paths to construct these bonds to yield more complex molecular architectures. However, compared to the development of synthetic protocols, development of mechanistic models and enriching of mechanistic understanding of many organic reactions has been limited. Computational studies into the mechanisms of organic transformations provide an avenue by which mechanisms of reactions can be better understood and new patterns of reactivity can be predicted. Herein, quantum-mechanical computational methods e.g., density functional theory (DFT) have been employed in the pursuit of understanding the mechanisms of a series of radical and polar reaction schemes. Specifically, DFT calculations were employed to understand the mechanism and origins of selectivity of two nickel(I)-catalyzed olefin functionalizations. These studies demonstrate a catalyst-control scheme by which selectivity can be induced by the steric properties of the catalyst (**Chapter 1**). Following this work, two

photocatalytic transformations which yield difluorinated products were studied thoroughly with computations. First, a synthesis of difluorinated lactone derivatives revealed a long-lived radical intermediate and motivated mechanistic experiments to isolate this radical. Next, a synthesis of difluorinated oxindole derivatives demonstrated the ability of arenethiols to act as photocatalysts (**Chapter 2**). Then, computations were used to rigorously explore a copper-catalyzed reductive cross-coupling of imine and allenamides. Specifically, computations were employed to explore the mechanism of the transformation and the origins of stereoselectivity and the divergent formation of urea and diamine products (**Chapter 3**). Finally, two computational investigations into the mechanisms of transformations catalyzed by first-row transition metals are detailed. In particular, a nickel-catalyzed hydroarylation of *gem*-difluoroalkenes is explored computationally to determine the order of steps in the reaction. In addition, the mechanism of a cobalt(I)-catalyzed allylic substitution is considered to ascertain the nature of the transformation as either radical or polar (**Chapter 4**). Given the complexity of the mechanisms of these transformations, computational studies provide an alternative route to acquire useful mechanistic understanding that can support or explain observed experiments and suggest further mechanistic experiments that could provide stronger evidence for a given mechanistic proposal.

# EXPLORING MECHANISMS AND PREDICTING REACTIVITY OF TRANSITION METAL-CATALYZED AND PHOTOCATALYZED RADICAL AND POLAR ORGANIC TRANSFORMATIONS

by

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*It was all a dream.* – Notorious B.I.G.

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# Chapter 1: Mechanistic Studies of Nickel(I)-Catalyzed Olefin Functionalization Reactions

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*Contributions*: Robert Martin led all computational efforts and performed all computational studies in this chapter.

## *1.1 Abstract*

Olefin functionalization has been a longstanding problem in the organic chemistry community. Recently, nickel has emerged as a powerful catalyst in, *inter alia*, synthesis and functionalization of olefins. Despite these recent successes, the understanding of the mechanisms for olefin functionalizations tends to be limited, and the factors that control the reactivity and selectivity of reactions with nickel are not well understood. One way to address this issue is to cooperatively use experimental/mechanistic studies and computational studies to study reactions of interest. Herein, I used quantum mechanical computations to elucidate the mechanisms of two nickel(I)-catalyzed olefin-functionalization reactions and explore the origins of selectivity in both reactions. Specifically, density functional theory (DFT) computations were employed to study the mechanism of a tandem Mizoroki-Heck functionalization/isomerization reaction. These studies provided support for a Ni(I)-alkoxide catalyst that can initiate a biphasic Ni(I)/Ni(III) catalytic chain mechanism wherein a Mizoroki-Heck-type coupling phase is followed by a non-radical "chain-walking" isomerization phase. Also, DFT calculations were employed to investigate the mechanism of a directing group-free catalytic dicarbofunctionalization of alkenes. This investigation revealed the relevance of the sterically hindered Ni(I) catalyst in controlling the

observed site-selectivity. Both investigations demonstrate a novel "catalyst-control" strategy for guiding regio- and stereoselectivity in transformations of alkenes.

*1.2 Introduction to Tandem Olefin Functionalization/Isomerization*

Developing protocols that afford stereochemically-defined acyclic tri- and tetrasubstituted alkenes is a longstanding goal in organic synthesis. These highly substituted C=C bonds (1-aryl(boryl)-1-methyl-substituted in particular) commonly reside in countless molecules of interest including organic materials and biologically active entities (**Figure 1.1A**), and are key intermediates for further derivatization[1,2] to a broader range of high-value compounds. Although several approaches for the preparation of tri- and tetrasubstituted olefins have been introduced[3–5], crucial drawbacks exist (**Figure 1.1B**). Reactions that convert carbonyl compounds[6–8] or alkynes[9–12] to tri- and tetrasubstituted olefins often involve lengthy synthetic routes, exhibit limited functional group compatibility, suffer from unsatisfactory regio- or stereoselectivity control and/or are not sufficiently general for applications in complex molecule synthesis. One problematic complication arises from the inappreciable energy difference between the *cis* and *trans* isomers of these highly substituted alkenes[13] (<0.4 kcal/mol; see **Appendix Figure A1.2.a1** for details), which precludes thermodynamic control from delivering products in synthetically useful *E:Z* ratios.

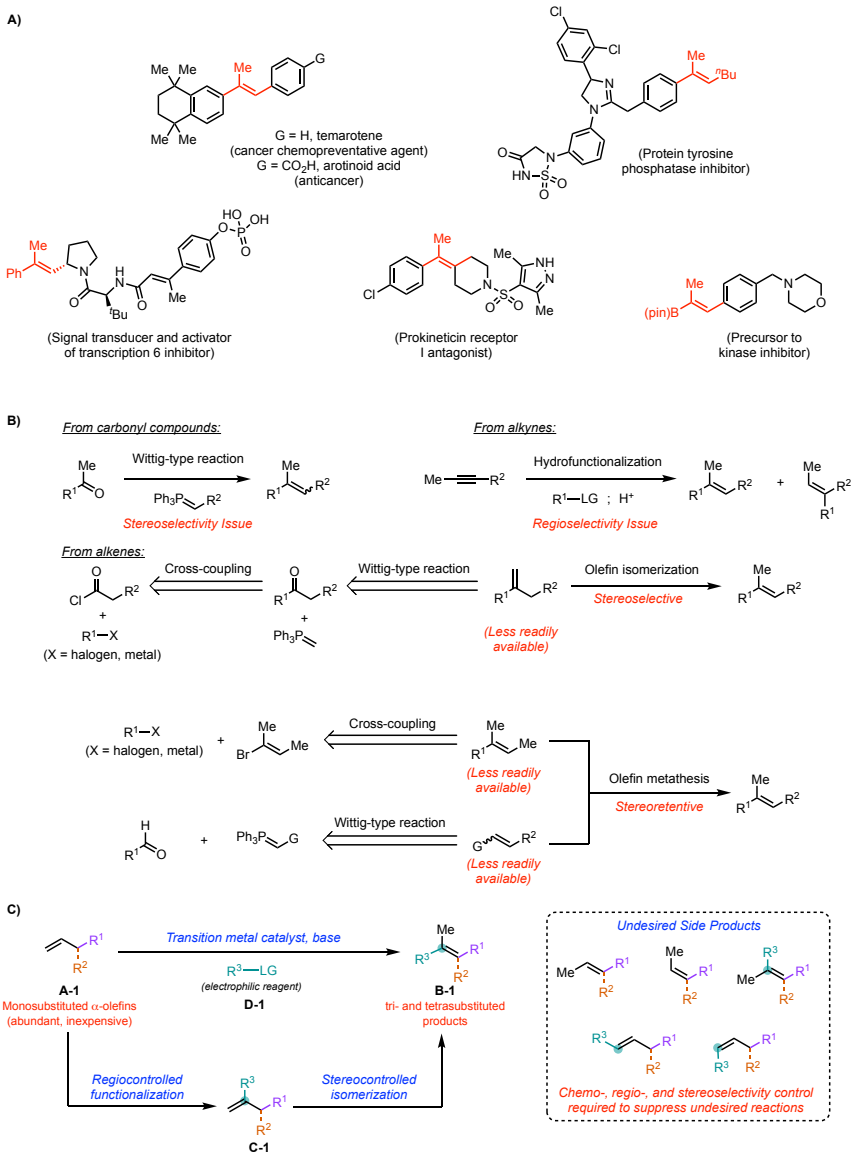



**Figure 1.1.** The importance of designing catalytic reactions that deliver stereodefined tri- and tetrasubstituted alkenes. A) Tri- and tetrasubstituted olefins are ubiquitous entities in biologically active compounds and synthetic intermediates. B) Common preparative routes to access trisubstituted alkenes. C) An attractive yet unexplored tandem process featuring a regioselective (net) olefin C–H functionalization followed by stereoselective C=C bond transposition.

Recent advances in catalytic olefin isomerization[14–17] as well as catalytic olefin metathesis[18,19] offer a distinct disconnection strategy starting from stable and more widely available alkenes as substrates, enabling access to certain highly substituted olefins with good control of *E/Z* selectivity (**Figure 1.1B**). However, these approaches are also plagued with

debilitating shortcomings. Isomerization reactions to trisubstituted olefins typically entail the use of presynthesized 1,1-disubstituted substrates that may limit broad use, particularly in cases where the starting materials are not easily accessible. On the other hand, stereoselective formation of trisubstituted C=C bonds by olefin metathesis relies on the use of trisubstituted substrates through stereoretentive processes, which for 1,1-disubstituted olefins lead to diminished *E:Z* ratios[18]. In addition, the second olefin cross-partner must be 1,2-disubstituted to minimize deleterious methylidene formation.[18] This requirement reduces the practicality of this approach, especially in cases where the cross-partner is not commercially available. Except for specific substrate-controlled cases,[20] olefin metathesis methods that selectively afford tetrasubstituted products are scarce, in part owing to the severe steric strain within the requisite metallacycle intermediates.

A general catalytic manifold that is complementary to the aforementioned systems and provides a myriad of heteroatom- and carbon-functionalized tri- and tetrasubstituted alkenes with exceptional stereoselectivity would be highly desirable. Previous reports of catalytic Mizoroki–Heck reactions of monosubstituted olefins with electrophilic sulfonates/halides[21–23] or boronic acids[24] delivered 1,1-disubstituted alkenes, whereas boryl-Heck transformations[25] of (*E)*-1,2-disubstituted styrenyl substrates (*(Z)* isomers are non-selective) with boryl halides offered access to trisubstituted alkenyl boronates with good *trans* selectivity. Notwithstanding these advances, a general strategy that has remained elusive is to directly transform abundant and easily accessible monosubstituted α-olefins (versus the more substituted variants that generally require more steps to be synthesized) to stereodefined tri- and tetrasubstituted products by cross-coupling with a suitable reagent. Such a process will facilitate synthesis of various classes of highly substituted C=C bonds that are otherwise difficult to obtain by other means.

Our approach to achieve this goal is to design a catalytic regime as illustrated in **Figure 1.1C**. We postulated that a suitable transition metal-based catalyst might first react with an electrophilic reagent **D-1** (for example, through oxidative addition or ligand substitution) to form an intermediate that subsequently undergoes branched-selective Heck-type functionalization[21–23] with terminal alkenes **A-1** to afford **C-1**. This is followed by a kinetically controlled stereoselective C–C double bond transposition to generate the desired product **B-1**. However, identifying an appropriate catalyst that is capable of promoting both steps in a tandem sequence is a formidable challenge, given that multiple levels of selectivity (chemo-, regio- and stereo-) have to be exquisitely controlled to minimize generation of side products arising from competitive isomerization of **A-1** as well as undesired isomeric products of **C-1** and **B-1**. Adding to these complications is the need for mild reaction conditions that tolerate diverse functional groups for broad applicability in chemical synthesis. Of the few instances of olefin functionalization/ isomerization that afforded trisubstituted enoates and enol ethers, an acid or base was presumably involved to drive C=C bond migration.

In collaboration with the Koh group, we report herein a nickel-catalyzed method that reliably transforms monosubstituted olefins to tri- and tetrasubstituted derivatives with remarkable control of regio- and stereoselectivity.

## *1.3 Results & Discussion: Olefin Functionalization/Isomerization Enables Stereoselective Alkene Synthesis.*

### 1.3.1 Optimization of reaction conditions and substrate scope.

Reaction screening experiments from the Koh group showed that the most effective catalyst for this transformation was **Ni-1**, a planar bis-μ-chloronickel(I) dimer featuring an NHC ligand, IPr (**Figure 1.2**).[26] This catalyst was able to readily furnish tri- and tetra-substituted

products from readily available monosubstituted alkene substrates with good yield (61-90%) and high selectivity towards *(E)* products (83:17–96:4 *E:Z*). The reaction was tolerant to numerous functionalities on the alkenes, including amides, esters, cyanides, and alcohols. They were also able to functionalize alkenes using various aryl and heteroaryl triflates.[27] This protocol was also successfully utilized in the synthesis of various biologically active compounds (such as those presented in **Figure 1.1** vide supra). These synthetic strategies were consistently more concise syntheses than those of previous reports.[28-34]

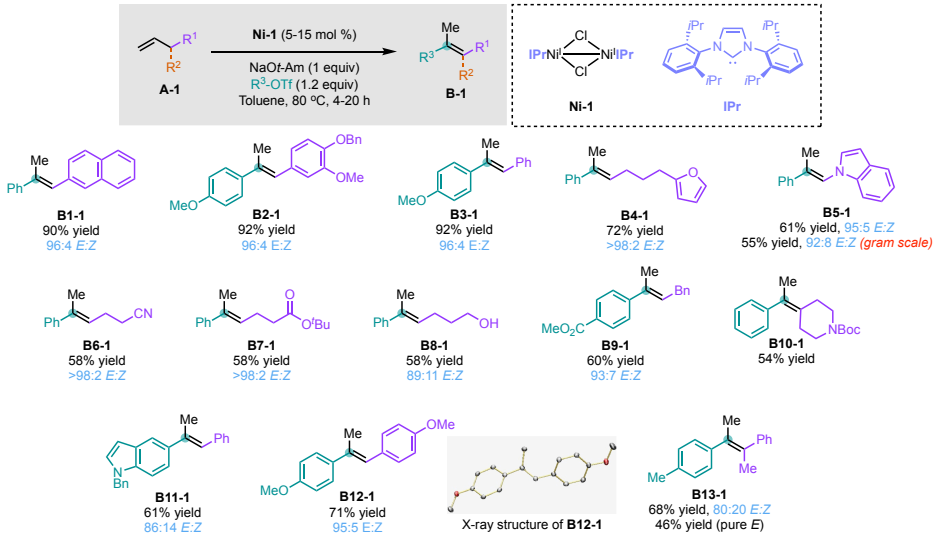



**Figure 1.2.** Representative substrate scope for the tandem functionalization/isomerization of alkenes performed by the Koh group. *E:Z* ratios were determined by $^{1}$H NMR analysis of unpurified mixtures; yields are for isolated and purified products.

### 1.3.2 Results of experimental mechanistic studies.

The remarkable enhancement in catalytic efficiency and selectivity with a Ni(I)-based catalyst prompted us to conduct a series of experimental and computational studies to shed light on the mechanism and origin of selectivity. Control studies revealed that 1,2-dialkyl-substituted olefins are incompetent substrates under the established conditions, suggesting that the present transformation probably proceeds through sequential functionalization to a 1,1-disubstituted alkene followed by isomerization. Given that **Ni-1** was previously shown to promote radical-based

alkene isomerizations,[15] it remains for us to elucidate whether olefin migration in our reaction system follows a similar radical pathway. Minimal cyclopropane ring rupture (<2%) was found in all cases, suggesting that hydrogen atom transfer via long-lived radical intermediates[35] is likely not involved.

These observations provided hints that C=C bond migration in our system could follow a pathway distinct from the "radical chain-walking" reported by Schoenebeck and coworkers.[15] Rather, a non-radical 1,3-hydrogen shift[36,37] through an allylnickel species might be operative during the course of olefin isomerization. More evidence to support our proposed non-radical 1,3-hydrogen shift mechanism could be derived from deuterium labeling and crossover studies. These studies suggested that a free nickel-hydride species is less likely to be involved in the C=C bond isomerization step. Instead, the observations are more consistent with an intramolecular Ni-promoted 1,3-hydrogen shift leading to the observed stereoselectivity. Electron paramagnetic resonance analysis of the reaction mixture by the Koh group further indicated the presence of paramagnetic organometallic species generated in the system.

**1.3.3 Mechanistic modeling with DFT.**

To gain further insights into the mechanism, unrestricted open-shell dispersion-corrected density functional theory (DFT) calculations (UB3LYP-D3, PBE0-D3 and UM06L) were used and, overall, supported a catalytic pathway as shown in **Figure 1.3** (see **Appendix A1.1.a** for full computational details). Specifically, solvent- or substrate-aided dissociation of **Ni-1** to the monomeric Ni(I) chloride species[15] is followed by a thermodynamically favorable ligand substitution with sodium *tert*-pentoxide to afford the catalytically active Ni(I)-alkoxide **I-1**. In the presence of an aryl triflate and monosubstituted alkene **A-1**, a branched-selective Mizoroki–Heck reaction proceeds through initial oxidative addition of **I-1** with the electrophile followed by regioselective arylnickelation and β-H elimination to deliver Ni(III)-hydride species **IV-1**. All

attempts to locate the energetically less favored linear-selective arylnickelation transition state were unsuccessful, presumably due to the inherent steric strain that substantially raised the energy. Finally, reductive elimination of **IV-1** facilitated by sodium *tert*-pentoxide base generates olefin-coordinated Ni(I)-alkoxide **V-1**. At this juncture, contrary to the radical-based isomerization detailed by Schoenebeck and coworkers,[15] computations support a stereoselective non-radical allyl isomerization sequence (see **Appendix A1.2** for further details and justification of this assertion). Specifically, Ni(I) **V** undergoes an inner-sphere *trans*-selective allylic C–H insertion (**Figure 1.4**) to furnish an $\eta^1$-allylnickel(III) intermediate **VI-1** that subsequently undergoes migration to yield **VII-1**. Finally, irreversible reductive elimination regenerates the catalytically active species **I-1** and releases the desired trisubstituted product **B-1**, overall −58.1 kcal/mol downhill in energy.

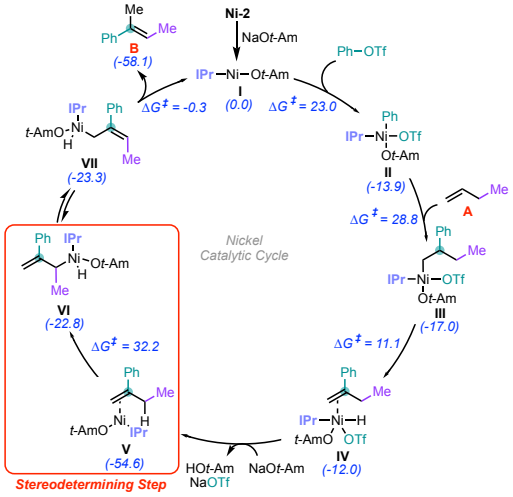



**Figure 1.3.** Energetics of the proposed Ni(I)-catalyzed mechanistic pathway for tandem Mizoroki-Heck functionalization/isomerization. All structures were optimized at the UB3LYP-D3/def2SVP-CPCM(toluene) level of theory and all free energies are reported in kcal/mol.

The proposed mechanistic model in **Figure 1.3** is also consistent with the observed stereochemical outcome. This is noteworthy because the discrepancy in energy between the two potential products, ***(E)*-B-1** and ***(Z)*-B-1**, is nowhere near large enough to explain the observed high *trans* selectivity. Instead, as seen in **Figure 1.4**, the difference in energy between the

diastereomeric transition states ***trans*-TS-V-VI-1** and ***cis*-TS-V-VI-1** correlates well with our stereoselectivity results. This difference is attributed to the shift in geometry of the *tert*-pentoxide that must occur to accommodate formation of the minor *cis* isomer. In the transition state leading to the *cis* isomer, the sizeable *tert*-pentoxide is forced down, pushing the bulky IPr ligand outwards, which raises the energy dramatically. Such steric repulsion is absent in the transition state leading to the major *trans* isomer. Distortion/interaction-activation strain analysis further suggest that the bulky *tert*-pentoxide group is important in inducing the selectivity of this reaction (see **Appendix Figure A1.2.a9** for further details). Taken together, these DFT results reveal the crucial roles played by the sterically encumbered *tert*-pentoxide and IPr ligand in inducing high stereoselectivity, a shift in C=C bond isomerization mechanism that arises from ligand substitution of Ni(I)-chloride with the bulky *tert*-pentoxide, as well as the need for high reaction temperatures to overcome the barrier for olefin migration (in accordance with our experimental observations).

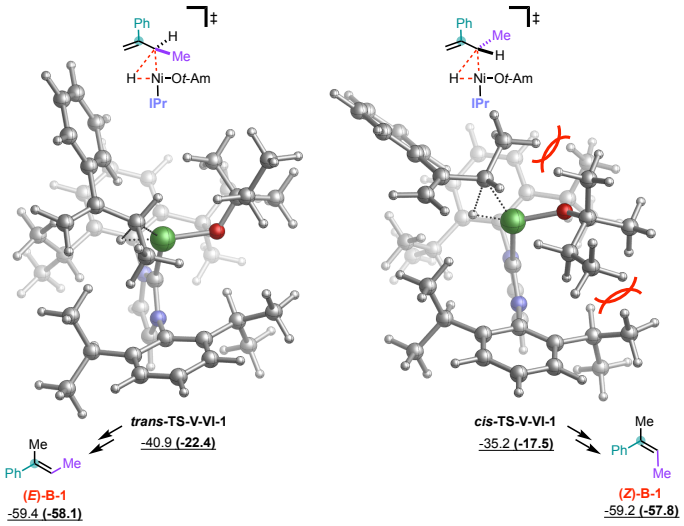



**Figure 1.4.** Key Ni(I)-catalyzed C=C bond migration transition state structures. including calculated enthalpies and (free energies) for each. All structures were optimized at the uB3LYP-D3/def2SVP-CPCM(toluene) level of theory and all enthalpies/energies are reported in kcal/mol.

An alternative Ni(0)/Ni(II) pathway for the tandem Heck reaction/isomerization, cannot be entirely ruled out. The allyl isomerization described herein could be promoted by a Ni(I) species

or, to a certain degree, by an *in situ*-formed Ni(0) species in the presence of base.[38] Computations were performed to assess the viability of a Ni(0)/Ni(II) pathway being operative in this transformation, the results of which are detailed in the **Appendix A1.2.a**. However, the results of these computations for the Ni(0)/Ni(II) pathway do not align with the observed selectivity or need for high temperatures to accomplish this reaction and the Ni(I)-catalyzed pathway shown above should be the more viable mechanistic pathway. Additionally, to probe the possibility of an adventitiously generated Ni(0) species[39], we relied on the propensity of NHC–Ni(0) complexes to promote vinylcyclopropane rearrangements to cyclopentenes.[40] Less than 5% olefin isomerization to cyclopropene was detected in all cases. Even though it cannot be completely excluded, these control experiments and computations indicate that any formation of Ni(0) species from **Ni-1** is probably not substantial under our established reaction conditions. Further computational results (see **Appendix A1.2.a**) also suggest that a Ni(0)/Ni(II) pathway is less feasible than the Ni(I)/Ni(III) pathway proposed here.[41-43]

*1.4 Introduction to Directing-Group-Free Catalytic Dicarbofunctionalization*

Multicomponent catalytic processes that can form multiple carbon–carbon bonds in a single step under mild conditions are highly sought-after for generating molecular complexity in chemical synthesis, particularly if the catalysts and substrates are inexpensive.[44] One such class of reactions involves the transition-metal-catalyzed installation of carbogenic units across readily available alkene feedstocks to access functionalized $sp^3$-hybridized carbon frameworks.[45–51] These entities are found within countless natural products, drug molecules and other important compounds of interest.[52,53] A central challenge associated with these transformations is the ability to control the regioselectivity of olefin addition,[49,54] especially in situations when the two newly introduced motifs possess similar electronic and/or steric attributes. This problem is further

exacerbated with unactivated alkyl-substituted C=C bonds[55] which, by virtue of their diminished electronic and steric bias, are innately less reactive. Consequently, inseparable product mixtures arising from poor regiochemical control and other competing reactions are inevitable.[56,57] To this end, two primary strategies have been adopted for promoting efficient and site-selective dicarbofunctionalizations across aliphatic olefins, both of which entail contrived substrate modifications[58,59] (**Figure 1.5A**): (1) substrate control in which intramolecularity drives carbometallation to form a cyclic intermediate and (2) auxiliary control with a strategically positioned directing group that coordinates and stabilizes the metal center in the putative organometallic species.

In the context of three-component 1,2-diarylation, various chelating groups have been developed to direct additions across unactivated C–C π bonds, using catalytic amounts of a transition-metal complex in conjunction with a haloarene and an arylmetal(boron) reagent (**Figure 1.5B**).[60-63] Despite these remarkable advances, conceiving a general approach to carry out regioselective dicarbofunctionalization that is compatible with both unactivated and activated alkenes, without relying on substrate modifications, is in crucial demand.[58,64] To achieve this, I hypothesized that catalyst control could be exploited as a new strategy in reaction design to overcome substrate reactivity and selectivity limitations for diarylation (**Figure 1.5C**). If successful, this would significantly enhance the way in which many biologically active molecules are prepared, by removing the requirement for pre-installation and removal of pendant-directing auxiliaries, which would otherwise incur additional reaction steps and costs.[65,66]

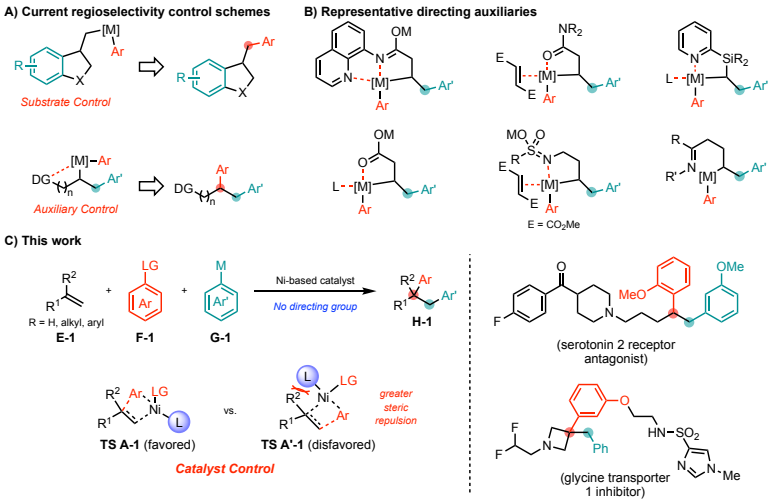



**Figure 1.5.** The significance and challenges of designing a catalyst-controlled blueprint for olefin dicarbofunctionalization. A) Current schemes for controlling the regioselectivity of cross-coupling reactions. B) Representative examples of directing group auxiliaries developed to promote site-selective 1,2-diarylation. C) Catalyst control as a novel strategy for directing group-free dicarbofunctionalization.

Rather than relying on directing-group effects,[59] we postulated that the preferential branched addition of the **Ar** group is likely to be caused by the elevated steric repulsions between the olefin substituents and **L** in the energetically less favored transition state **TS A′**. At. Based on this mechanistic proposal, the projected sense of regioselectivity is opposite to those disclosed previously[56,57] (compare with **Figure 1.5A/B**). To selectively obtain the alternative regioisomer of **H-1'**, the aryl moieties of **F** and **G** could be simply switched. In addition, the versatility of replacing **F** and **G** with different combinations of electrophiles and nucleophiles means that a broader assortment of dicarbofunctionalization adducts beyond diarylated molecules may be potentially generated.

However, implementation of this catalyst-controlled blueprint presents onerous challenges on several fronts. First, the catalyst must be sufficiently sizeable to induce high regiocontrol, yet sufficiently active to promote aryl additions to unactivated alkenes. With the sterically more demanding 1,1-disubstituted olefins, reaction efficiency may be further reduced as observed in

previous reports.[61,63] Second, in the absence of a chelating auxiliary to occupy a vacant metal site,[67] adventitious β-H elimination to afford Heck-type side products is possible. Thus, the ligand **L** must be adequately large to preclude any agostic $C_\beta$–H bond coordination. Third, transmetalation and reductive elimination steps in the mechanism must outcompete β-H elimination and/or undesired hydroarylation pathways arising from reactions with trace moisture.[68]

## *1.5 Results & Discussion: Directing-Group-Free Catalytic Dicarbofunctionalization of Unactivated Alkenes*

### 1.5.1 Experimental results.

Following reaction optimization, the Koh group reported the directing-group-free catalytic dicarbofunctionalization reaction shown in **Figure 1.6** below. The diarylation reaction was found to be most effective with the bis-μ-chloronickel(I) dimer with an IPr (NHC) ligand **Ni-1**.[26] The transformation was found to be effective with a wide array of alkene substrates and is compatible with various functional groups including protected amines, protected alcohols, heteroaryl groups, amides, etc.[70] The Koh group also found that bis-diarylation was possible (as in **H7-1**). Further experiments with alternative organometallic reagents (**G-1** with either M = MgBr or M = ZnCl) found these to be viable substrates as well. This reactivity was able to be effectively utilized in the synthesis of biologically relevant molecules.[71-74] Notably, simply switching the identities of the aryl Grignard reagent and the aryl triflate would allow for induction of the opposite regiochemistry, allowing for different permutations of diarylated regioisomers to be readily synthesized.[75]

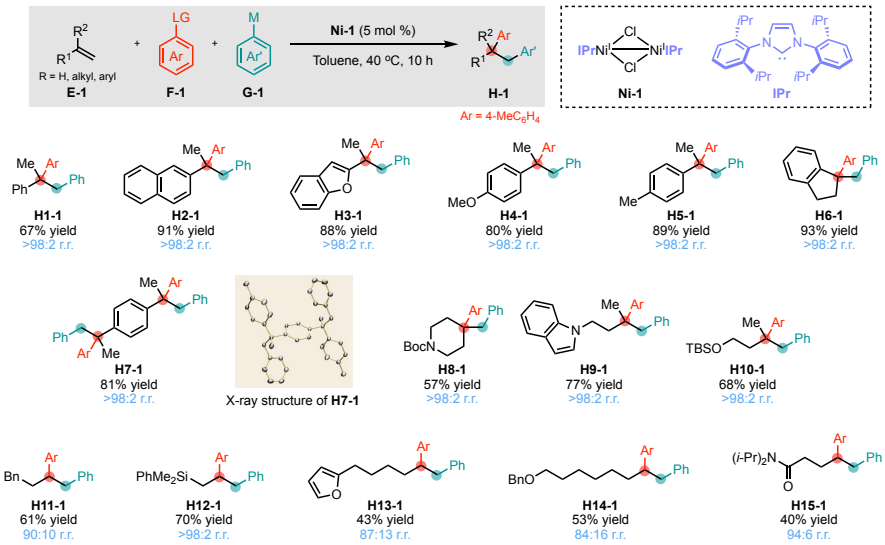



**Figure 1.6.** Representative examples of substrate scope for site-selective directing group-free dicarbofunctionalization. Experiments from the Koh group. Regioisomeric ratios were determined by gas chromatography analysis of unpurified mixtures; yields are for isolated and purified products.

### 1.5.2 Mechanistic evaluation with experiments and DFT.

The mechanistic underpinnings influencing the efficiency and regioselectivity of diarylation are further deliberated in **Figure 1.7**. With respect to the results shown in **Figure 1.6**, the alternative regioisomer (**H1-1′**) was never detected in the remarkably regioselective diarylation of **E-1** and biaryl cross-coupling of **F-1** and **G-1** was a common side reaction. This suggests that formation of a hypothetical biarylnickel species **vi-1** by transmetalation of **ii-1** with the arylmetal reagent is plausible in our system. However, in such a scenario, addition of **vi-1** to **E-1** is unlikely to be site-selective because both aryl units are insufficiently distinct (electronically and sterically) to favor preferential generation of **iv-1** or its regioisomer. Rather, **vi** presumably undergoes facile reductive elimination to give biaryl by-product **J-1** as seen in a previous report[76] and supported by quantum mechanical calculations.

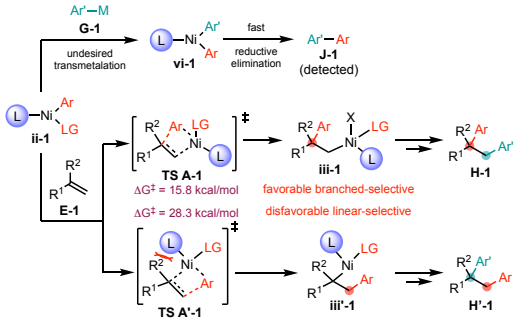



**Figure 1.7**. Potential divergent reactivity pathways resulting from oxidative addition of **F-1** to **Ni-1**. **TS A-1** and **TS A'-1** were optimized at UB3LYP-D3/def2svp-CPCM(toluene) level of theory.

Unrestricted, dispersion-corrected density functional theory (DFT) calculations lend further credence to the proposed Ni(I)-catalyst-controlled mechanistic model based on steric arguments (**Figure 1.7, Figure 1.8**) (see **Appendix A1.1.b** for full computational details). Specifically, as shown in **Figure 1.8**, substrate- or solvent-assisted formation of Ni(I) chloride species **i-1** from the dimeric **Ni-1** pre-catalyst[15,26,69] is followed by oxidative addition with the triflate to afford **ii-1**. Compound **ii-1** will then undergo a branched-selective 1,2-migratory insertion (via **TS A-1**) across the alkene substrate to generate **iii-1**. Notably, the opposite linear-selective insertion (via **TS A′-1**) is significantly less favored than branched-selective insertion ($\Delta\Delta G^{\ddagger}$ = +10.0 kcal/mol), presumably due to severe steric repulsions between the alkene substituents and the sizeable IPr ligand bound to the Ni center in **TS A′-1**, which can be avoided by addition of the nickel to the less substituted end of the C=C bond. Indeed, the structure of **TS A′-1** is significantly distorted compared to that of **TS A-1**, which is likely to be as a consequence of this steric hindrance. Following branched-selective arylnickelation, irreversible transmetalation with the organometallic reagent will lead to species **iv-1**. Compound **iv-1** is primed to undergo reductive elimination to furnish the desired product **H16-1** with high regioselectivity and to regenerate the catalytically active Ni(I) species **i-1**. Additionally, we were unable to locate the biarylnickel species **vi-1** and all attempts led to formation of the corresponding biaryl by-product

**J-1**. This result supports the earlier notion that **vi-1** prefers to undergo reductive elimination instead of olefin addition.

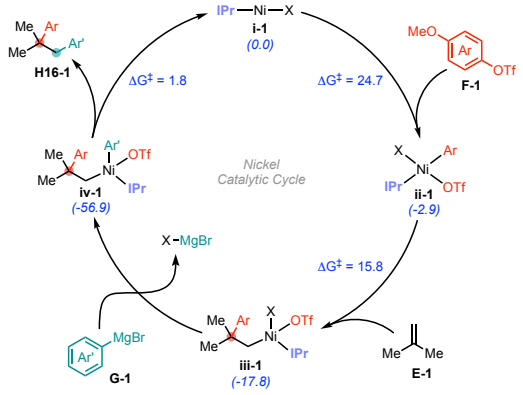



**Figure 1.8.** Energetics of proposed mechanistic pathway for site-selective diarylation of 2-methylpropene (model system). All structures were optimized at UB3LYP-D3/def2svp-CPCM(toluene) level of theory and energies are reported in kcal/mol

## *1.6 Conclusions*

In conclusion, we have developed two nickel(I)-catalyzed olefin functionalization systems. Quantum mechanical calculations were employed to study the mechanisms of these transformations and elucidate the origins of selectivity for each. In the tandem Mizoroki-Heck/isomerization reaction, the computations support a Ni(I)/Ni(III) pathway initiated by a Ni(I)-alkoxide wherein the cross-coupling and isomerization steps are sequential. For the dicarbofunctionalization of unactivated alkenes, the computations support a Ni(I)/Ni(III) pathway that takes advantage of the bulky IPr ligand on the nickel to induce the observed regioselectivity, which is in accordance with the experimental observations. In both cases, the computations demonstrate the ability of properties of the catalyst to control the outcome of a reaction, which provides a novel framework for further development of highly selective olefin functionalization reactions.

# Chapter 2: Mechanistic Studies of Photoactivation for Synthesis of Difluoro-Substituted Products

Excerpts from this chapter were published in: a) Dhungana, R. K.; Granados, A.; Ciccone, V.; **Martin, R. T.**; Majhi, J.; Sharique, M.; Gutierrez, O.; Molander, G. A. *ACS Catal.* **2022**, *12*, 15750-15757. b) Matsuo, B.; Mahji, J.; Granados, A.; Sharique, M.; **Martin, R. T.**; Gutierrez, O.; Molander, G. A. *Chem. Sci.* **2023**,*14*, 2379-2385.

*Contributions:* Robert Martin led all computational efforts and performed all computational studies in this chapter.

## *2.1 Abstract*

Photochemical reaction schemes have become a subject of great interest in the organic chemistry community, owing to their utility in synthesizing various functional groups. In parallel to this trend, the incorporation of fluorine into biologically relevant molecules has also seen significant interest owing to the ability of fluorine to drastically affect the properties of pharmaceuticals. Recently, in collaboration with the Molander group, I have used quantum mechanical computations to explore the mechanisms of two transformations that yield difluorinated products. Specifically, I have investigated the mechanism for the photoinduced synthesis of fluorinated lactone derivatives from cinnamyl alcohols. Herein, I used density functional theory (DFT) and time-dependent DFT to identify a unique radical-polar-radical sequential mechanism which helped guide mechanistic study experiments performed by the Molander group. My computations supported a sequential Giese addition-lactonization-halogen atom transfer process that was further substantiated by experimental results. DFT calculations were further employed in the study of a transition metal-free C-F bond activation to yield difluorinated oxindole derivatives. My DFT calculations support the proposed mechanism wherein an organophotocatalyst can induce single electron transfer in ethyl difluorobromoacetate, which then

effectuates a spin-center shift. Following this process Giese addition, ring closure, and hydrogen-atom transfer rapidly yield the desired difluorinated oxindole derivatives.

*2.2 Introduction to Trifunctionalization of Cinnamyl Alcohols*

Polar and radical reaction schemes are effective and powerful tools for synthetic organic chemistry because they provide complementary paths to the expansion of molecular diversity. Specifically, the sequential manifestation of radical and polar reactivity in a one-pot transformation represents a step-economical process in organic synthesis. In this context, radical/polar crossover (RPC) chemistry is a vibrant area of investigation in photoredox catalysis (**Figure 2.1**).[77] These transformations rely on the initial formation of a radical via single-electron transfer (SET) from a photocatalyst or via an electron donor/acceptor complex. The radical generated thus undergoes a typical radical addition reaction to an alkene, generating a translocated radical. Subsequent single electron reduction of this radical, generating a carbanion, or oxidation of the radical, creating a carbocation, followed by polar reactions with an electrophile or nucleophile, respectively, completes the RPC process. The novel features of RPC reactions have inspired the synthetic community to develop conceptually new transformations, providing efficient access to complex organic molecules via the construction of multiple new bonds.[78] Herein, we describe the first example of a novel radical–polar–radical transformation in one pot to prepare functionalized lactones from readily available cinnamyl alcohols via Giese addition/lactonization/halogen-atom transfer (XAT) processes (**Figure 2.1**).

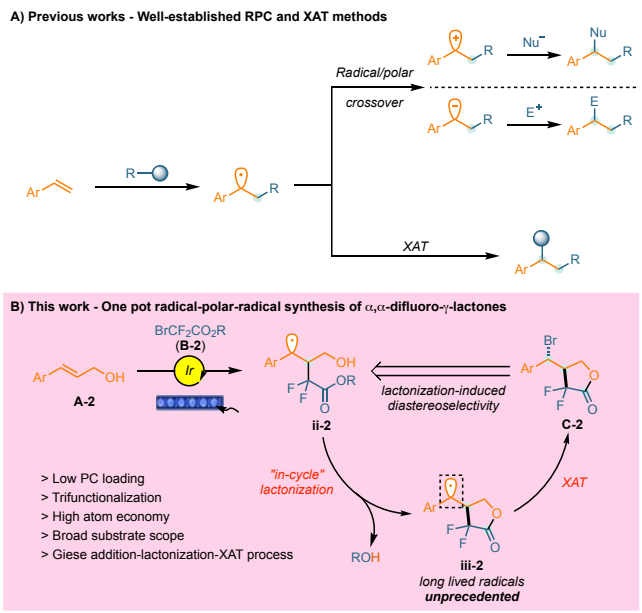



**Figure 2.1.** Background for the functionalization of alkenes and a novel Giese addition-lactonization-XAT protocol for synthesis of α,α-difluoro-γ-lactones.

Difunctionalization of alkenes is a versatile and powerful strategy for expanding molecular diversity and structural complexity of organic molecules, incorporating various functional groups concurrently across a carbon–carbon double bond from readily available feedstocks.[77,78]

The difunctionalization of double bonds can be achieved by the intermolecular addition of two groups onto the double bond, with subsequent cyclization of embedded functional groups providing a notable increase in molecular complexity.[79] The formation of heterocycles in this manner is particularly interesting given their broad applicability in medicinal chemistry and agrochemistry,[80] photoinduced methods have proven to be an excellent tool for the construction of such complex organic backbones.[81] In this context, the difunctionalization of alkenes provides the expedited generation of molecular complexity from simple chemical feedstocks with excellent atom economy. A process to access multifunctional compounds (e.g., brominated α,α-difluoro-γ-lactones) from simple feedstocks, would represent a unique approach to such highly elaborated platforms. Owing to their abundance in natural and pharmaceutical products, remarkable

biological function, and unique chemical architecture, lactones are particularly desirable targets for organic synthesis.[82] The venerable Yamaguchi lactonization,[83] Boden–Keck lactonization,[84] and Corey–Nicolaou macrolactonization,[85] in addition to the hydroxy ester lactonization in acidic or basic media,[82c] represent important traditional methods for the construction of lactones. Syntheses of lactones have been reported using both transition metal-catalyzed and organo-catalyzed methods,[86] as well as through photoinduced processes.[87] The chemical synthesis of α,α-difluoro-γ-lactones in particular has been explored using tin reagents,[88] and recently via visible-light irradiation from methyl fluorosulfonyldifluoroacetate[87h] and chlorodifluoroacetic anhydride.[87i]

Fluorination of the backbone of a therapeutic molecule imparts unique characteristics, such as improved binding selectivity and enhanced metabolic stability. Fluorination can also influence the lipophilicity of drug-like molecules, allowing for improved drug uptake and metabolism.[89] Of importance to the research described herein, the presence of the *gem*-difluoro functional motif has grown because of its oxidative stability and pharmacological properties as a bioisostere of carbonyl or sulfonyl groups and a modulator of lipophilicity.[90] Given the increasing popularity of the *gem*-difluoroalkyl group[91] in organic molecules, ethyl bromodifluoroacetate, Chen's reagent, and Hu's reagent[91a] have become broadly applied reagents for the introduction of this structural motif.

In collaboration with the Molander group, we report a photochemical trifunctionalization method for the synthesis of α,α-difluoro-β-(bromo((hetero)aryl)methyl)-γ-lactones from cinnamyl alcohols as feedstocks via well-orchestrated Giese addition/lactonization/XAT processes in a single flask (**Figure 2.1**). To the best of our knowledge, the construction of such brominated α,α-difluoro-γ-lactones through the sequential formation of C–$CF_2$, C–O, and C–Br bonds has never been previously explored. I performed dispersion-corrected density functional theory (DFT)

calculations (UωB97XD and UB3LYP-D3) to explore the mechanism of this transformation and predict the reactivity of the system to provide insights into useful experiments for mechanistic study (see the Supporting Information for full computational details).

## *2.3 Results & Discussion: Trifunctionalization of Cinnamyl Alcohols Provides Access to Brominated α,α-Difluoro-γ-lactones via a Photoinduced Radical–Polar–Radical Mechanism*

### 2.3.1 Initial reaction optimization.

Initial reaction optimization results from the Molander group demonstrated that a wide scope of cinnamyl alcohols could be employed with ethyl bromodifluoroacetate to form α,α-difluoro-γ-lactones (**Figure 2.2**). This transformation proceeds with good yield (up to 76%) and moderate diastereoselectivity (up to 9:1) and is tolerant of many different functionalities on the aryl group of the cinnamyl alcohol. This transformation exhibited a high process mass intensity (PMI), suggesting that the transformation is highly sustainable.[92] Photochemical quantum yield (Φ) experiments suggested that the reaction may undergo a radical chain pathway (Φ = 2.5, thus indicating a feasible short radical chain mechanism).[93] To scout for radical formation, 2,2,6,6-tetramethyl-1-piperidinyloxyl (TEMPO) was added in the reaction of **A1-2** and **B-2**. In this case, the formation of the difluorolactone product (**C1-2**) was inhibited when 5 equivalents of TEMPO were used, and the ethyl difluoroacetate-TEMPO adduct (**D-2**) was detected by gas chromatography/mass spectrometry (GCMS).

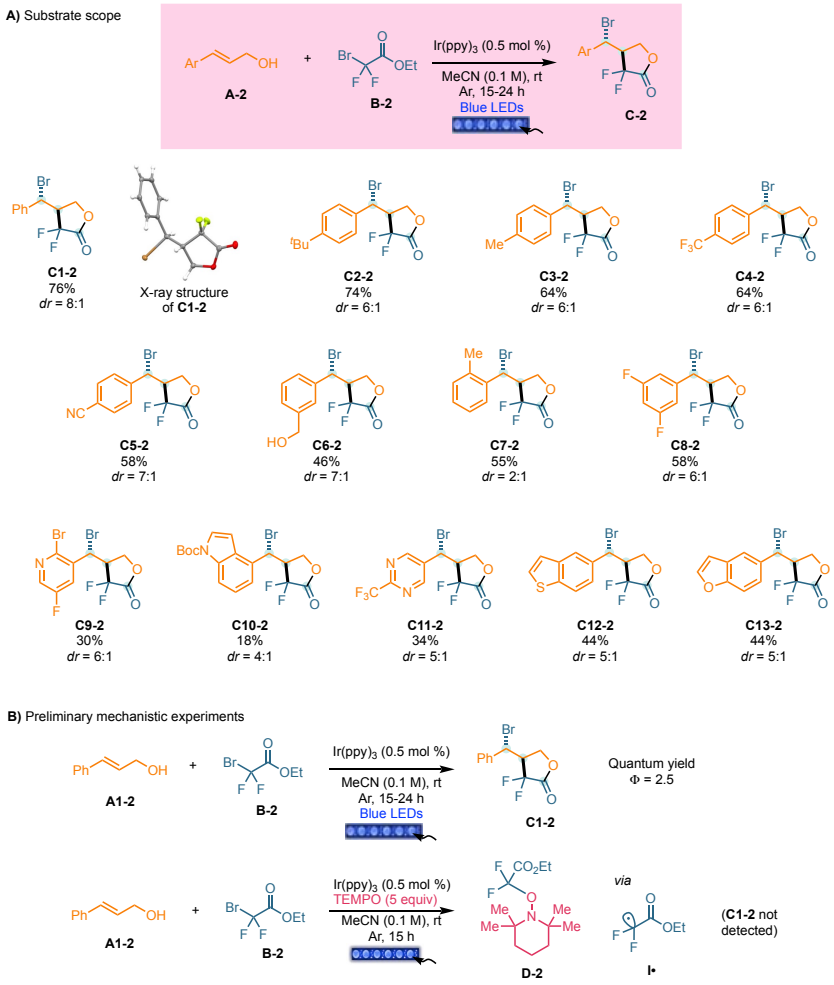



**Figure 2.2.** Preparation of α,α-difluoro-γ-lactones from photoactivation of cinnamyl alcohols and ethyldifbromofluoroacetate. A) Representative α,α-difluoro-γ-lactone products. Reaction conditions: cinnamyl alcohol 1 (0.5 mmol), 2 (1 mmol, 2 equiv), $Ir(ppy)_3$ (0.5 mol %) in MeCN (5.0 mL, 0.1 M) for 15-24 h irradiation with blue LED strips ($\lambda_{max}$ = 456 nm) under argon atmosphere. B) Preliminary mechanistic experiments to scope for radical formation.

### 2.3.2 Mechanistic investigation with DFT and experiments.

Based on these experimental results and previous work,[94,95] I developed the mechanistic proposal shown in **Figure 2.3** below.

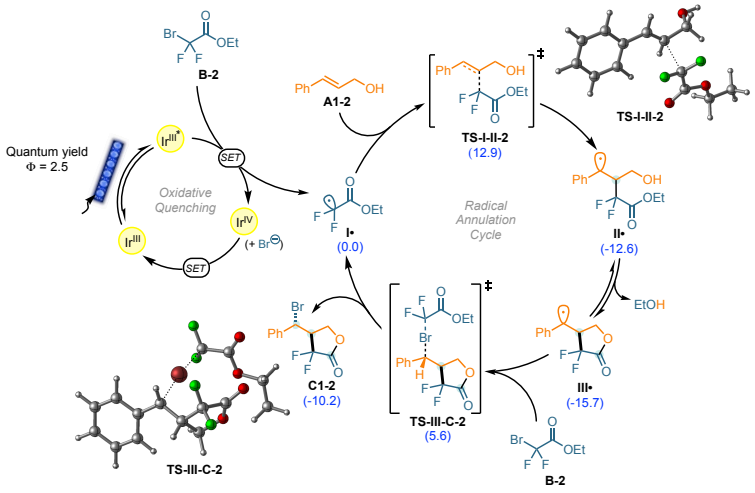



**Figure 2.3.** Proposed mechanism for the photoinduced preparation of α,α-difluoro-γ-lactones (**C1-2**) from cinnamyl alcohols (**A1-2**). Free energies reported in kcal/mol at UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory.

Upon photoexcitation, the generated Ir(III)* rapidly promotes SET to form a bromide anion and a difluoro radical intermediate **I**·. In turn, my DFT calculations revealed that **I**· can then undergo *rapid irreversible and regioselective Giese addition* to the homoallylic alcohol (**A1-2**) with an overall barrier of only ~13 kcal/mol (via TS-I-II), leading to **II**·. To determine the order of lactonization and XAT processes, I proposed that the Molander group perform another radical trap experiment with TEMPO by adding TEMPO after the reaction had already run for 1 hour. Detection of the **II**-TEMPO adduct would provide confirmation that **II**· is a long-lived intermediate that can accumulate during the reaction. The **II**-TEMPO adduct (**E1-2**) was detected by GCMS, suggesting the unprecedented result that **II**· is a persistent radical species (**Figure 2.4**).

DFT computations suggest **II**· can rapidly undergo "on-cycle" lactonization to form a thermodynamically more favorable "on-cycle" radical intermediate **III**·. To probe the feasibility of this lactonization (relative to XAT by **II**·), we proposed that control experiments should be run using alternative radical precursors that may be less amenable to lactonization (**Figure 2.4**). When carboxylic acid **B2-2** was employed as a radical precursor, we observed the formation of the

desired lactone (**C1-2**) in 55% yield and a 7:1 dr without the formation of the uncyclized difunctionalized carboxylic acid product **F1-2**. However, the reaction with the radical precursor **B3-2** yielded both lactone **C1-2** and the uncyclized trifunctionalized ester **G1-2**. Presumably, using sterically hindered **B3-2**, the nucleophilic acyl substitution process is less efficient because of the slower kinetics for an acyclic adduct **H1-2** to undergo lactonization, leading to appreciable formation of an "off-cycle" uncyclized product **G1-2**. Moreover, when using **B3-2** as a radical precursor and after the addition of TEMPO after 1 h, we were able to trap the uncyclized **H1-2**.

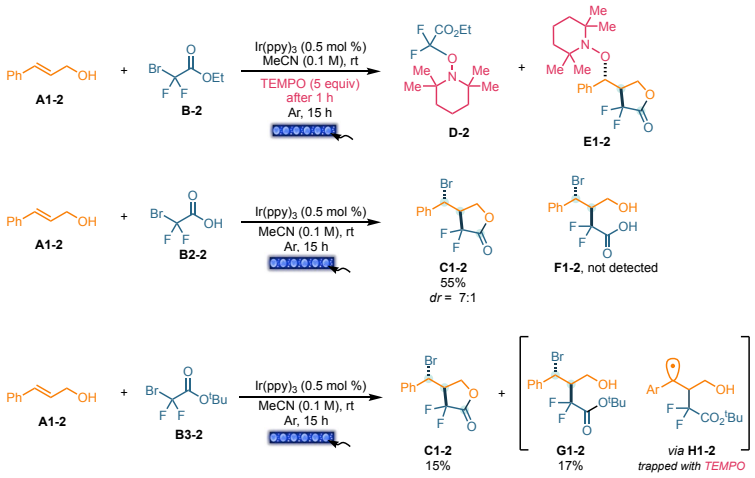



**Figure 2.4.** Experiments for validation of proposed mechanism. Yields reported as determined (by the Molander group) by $^{1}$H-NMR.

Finally, **III**· can undergo diastereoselective XAT[96] with **B-2** to regenerate the radical species **I**· and form the cyclic product (**C1-2**). Notably, although the product **C1-2** is uphill in energy from the lactone radical intermediate **III**·, the Giese addition of the concurrently formed radical **I**· to the cinnamyl alcohol (**A1-2**) serves as a driving force, as reformation of the stabilized benzylic radical **II**· is energetically favorable. Full computational details can be found in **Appendix A.2.2.a**.

*2.4 Introduction to Transition Metal-Free C-F Bond Activation*

Challenging synthetic organic transformations have driven the development of new protocols to diversify and broaden existing methods. New technologies and activation modes have dramatically changed how chemical space is being explored. Among the various challenges in the field, the selective activation of a single C–F bond in polyfluorinated substrates is has become a desirable transformation.[97-99] The inherent interest in accessing C-F bond-containing molecules is attributed to the fact that these bonds are prevalent in biologically active compounds. Fluorinated molecules have proved to be key in drug discovery programs because they can dramatically change the properties of drug candidates by improving stability, permeability, and, consequently, the efficacy of molecules discovered therein.[100,101] It is not a coincidence that fluorinated molecules are highly represented in many currently marketed drugs. Consequently, continuous efforts have been made to prepare and derivatize such molecules. A central challenge in this synthetic field remains the high bond dissociation energy of C–F bonds, which imposes limitations for selective bond cleavage and further functionalization in polyfluorinated substrates.

Considering modern approaches to this challenge, electrochemical and photochemical methods have emerged as extremely useful technologies, allowing for selective C–F bond activation in various classes of compounds,[99,102] including fluoroarenes,[103-109] trifluoromethylated arenes[110-113] and -alkenes,[114-119] *gem*-difluoroalkenes,[120-125] and others, such as trifluoromethyl esters, -amides,[126-129] and -ketones[130] under mild reaction conditions.

In this arena, photoinduced metal-free protocols represent a highly attractive approach to C-F activation, providing valuable structures without trace metals; a feature that is especially relevant in the industrial sector. Small organic conjugated molecules have been shown to exhibit interesting properties as photocatalytic species, successfully allowing C-F bond activation. Some

examples include the use of pyrenes[131] and phenoxazines[15] in catalytic hydrodefluorination of polyfluoroarenes and trifluoromethylarenes, respectively; the exploration of phosphinophenolates[128] in defluoroalkylation and hydrodefluorination of trifluoromethylated substrates [e.g., esters, acetamides, and (hetereo)arenes]; in addition to the well-known applications of dicyanobenzenes as potent organophotocatalysts.[112,129,132]

Last year, the Molander group disclosed a metal-free and mechanistically novel approach to install *gem*-difluoromethylene groups from trifluoroacetates and -acetamides onto (un)activated alkenes.[126] The method was designed to be promoted by a hydrogen atom transfer (HAT) step via combination of diaryl ketone, thiol, and sodium formate. In collaboration with the Molander group, we focused on developing a metal-free preparation of difluorinated oxindole derivatives via a cascade reaction between *gem*-difluoromethylene radicals and *N*-arylmethacrylamides, exploring the photoreactive nature of thiols as photocatalysts.

Aryl acrylamides are useful precursors to build more complex structures containing the oxindole moiety, known to exhibit extraordinary activities as drugs as well as being present in many active natural products.[133-135] They have been explored in cascade-type transformations where the sequence of addition to the alkene moiety followed by cyclization and rearomatization leads to interesting and valuable compounds from a medicinal point of view. Our approach would represent a complementary and alternative route to access these privileged motifs under milder conditions, extending the chemical space covered by previous advances in the field, which have demonstrated the use of trifluoromethylated arenes[113] and -ketones[130] as *gem*-difluoromethylene radical sources. In these examples, activation of the C–F bond was achieved by employing a combination of Ir-catalysts and Lewis acids to facilitate the fluoride elimination (**Figure 2.5A**).

Previous approaches to installing *gem*-difluoroacetates for the preparation of valuable difluorinated oxindoles make use of harsh conditions in the presence of metal-based catalysts, oxidants, and/or high temperatures, and are restricted regarding the structural diversification of the fluorinated moiety (**Figure 2.5B**).[136-139] Recently, a seminal Giese addition protocol using trifluoromethylated compounds was also reported by the Shang group, supporting the application of thiolate species as reductants and HAT catalysts. An efficient hydrodefluorination of trifluoroacetates, -arenes, and -amides and the coupling with a range of alkenes was reported (**Figure 2.5C**).[127] In another vein, Chiba and co-workers explored the powerful ability of excited-thiol anions to promote the single-electron reduction of aryl halides with reduction potentials as low as −2.4 V vs SCE;[140,141] while Hamashima explored thiobenzoic acid as single-electron reducing and efficient HAT agent to promote regioselective Cα–H arylation reactions.[142] All of these precedents demonstrate the rich applicability of sulfur anions as potential photocatalysts.[143]

Seeking alternative methods that would provide easy access to *gem*-difluoromethyl radicals under metal-free and milder conditions, we recognized that benzenethiols play a key role as photocatalysts under blue and purple light irradiation and, in the presence of sodium formate,[126-128,132,144,145] directly leads to selective mono C-F bond cleavage in trifluoroacetates. Herein, we report a transition metal-free, mild, and operationally simple method to overcome the limitations associated with the preparation of fluorinated oxindole molecules by single C-F bond activation (**Figure 2.5D**). I employed dispersion-correct density functional theory (DFT) computations (UB3LYP-D3, UωB97XD) to explore the mechanism and reactivity of this system. (See **Appendix A2.2.b** for full computational details).

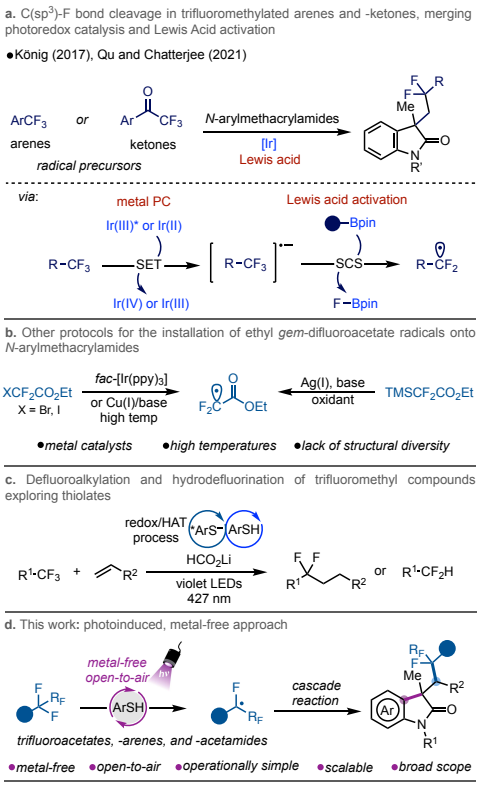



**Figure 2.5.** Classical and proposed approaches for preparation of difluoroalkylated compounds.

## *2.5 Results & Discussion: Transition Metal-Free Photochemical C–F Activation for the Preparation of Difluorinated-Oxindole Derivatives*

### 2.5.1 Experimental results.

Initial experimental results from the Molander group demonstrated that arenethiols can be employed as organophotocatalysts for activation of C-F bonds (**Figure 2.6**). In particular, the group reported that 4-methoxybenzenethiol can serve as a catalyst for activation of various trifluoromethylated compounds in conjunction with *N*-methylacrylamide to yield difluorinated-oxindole derivatives. This protocol is able to produce the target fluorinated molecules in open-to-air conditions and is tolerant of various functionalities on the *N*-arylacrylamide. The trifluoromethylated compound can also be varied. This transformation is able to produce many

classes of oxindole derivatives, including spirocyclic compounds (e.g., **L8-2** and **L9-2**), which are often challenging targets for organic synthesis.[134,146]

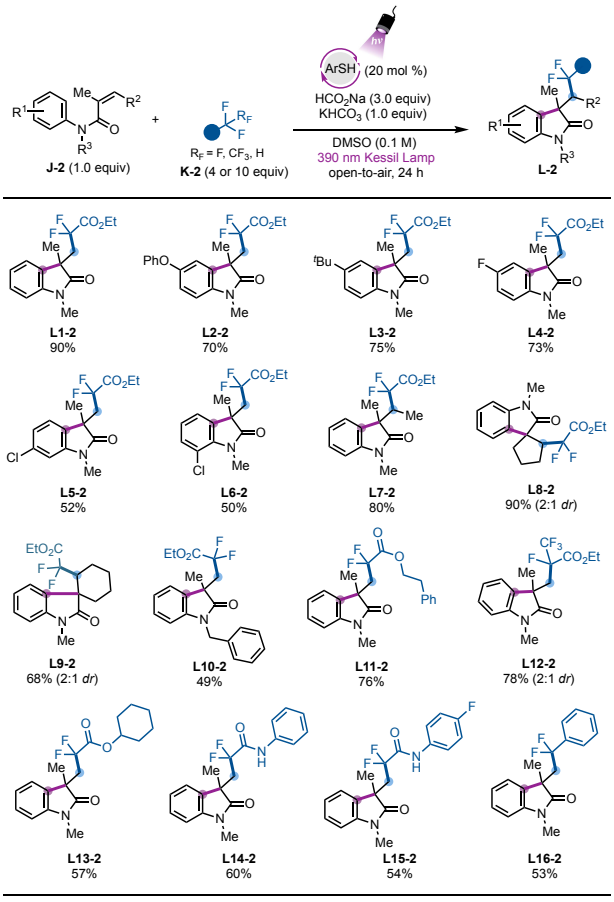



**Figure 2.6.** Representative examples of difluorinated oxindole derivatives. Reaction conditions: *N*-arylacrylamide 1 (0.5 mmol, 1 equiv), trifluoromethylated compound (10 equiv for **L1-2** through **L10-2**, 4 equiv for **L11-2** through **L16-2**), ArSH (0.20 equiv), $HCO_2Na$ (3.0 equiv) and $KHCO_3$ (1.0 equiv) in DMSO (0.1 M) under purple Kessil light irradiation and open-to-air. ArSH = 4-methoxybenzenethiol. Experiments performed by the Molander group.

### 2.5.2 Mechanistic investigation with DFT.

A proposed mechanism for this transformation is outlined in **Figure 2.7** below.

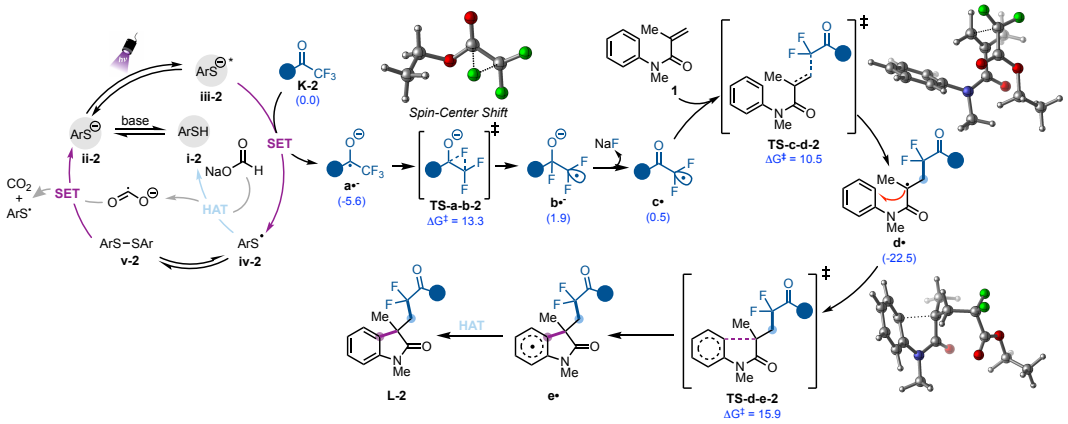



**Figure 2.7.** Proposed mechanism for the metal-free defluorinative alkylation strategy. Free energies of relevant species reported in kcal/mol at UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO) level of theory.

As shown in **Figure 2.7**, the proposed mechanism initiates with the formation of the thiolate species **ii-2** from deprotonation of the thiol **i-2** in the presence of base. The thiolate **ii-2** is then promoted to the excited anion (**iii-2**) under purple light irradiation. Given the strong ability of the latter to act as a reductant ($E_{red}$ = −3.3 V vs SCE),[127] the initial defluorinative step to form the radical anion species **a•⁻** should take place via single electron reduction of the ethyl trifluoroacetate **K-2** ($E_{red}$ = −2.0 V vs SCE), which was supported by quenching experiments.[126] In the thiolate catalytic cycle, the thiyl radical **iv-2** formed is prone to undergo dimerization, and it is in equilibrium with the disulfide **v-2**. Regeneration of the precatalyst **i-2** can then take place via HAT between **iv-2** and sodium formate. In this step, the reductant $CO_2$•⁻ is formed, which can also contribute to the generation of the active thiolate species **ii** by promoting the reductive cleavage of the S-S bond in **v-2**. Each of these processes is energetically feasible (see **Appendix Figure A2.2.b1** for full computational details). Additionally, the quantum yield (Φ) value for the transformation was found to be 0.35, which suggests that a chain process is possibly not operative. Thus, the formate radical anion is unlikely to be contributing to the reduction of **K-2**.[126,129,132,147,149]

From this point, the formed C-centered radical anion species **a•⁻** undergoes a spin-center shift (SCS)[148,149] to form the electrophilic *gem*-difluoromethyl radical intermediate **c•**, which was also observed as a TEMPO adduct in control experiments. DFT computations suggest that the SCS proceeds through a stepwise 1,2-F migration pathway (**TS-a-b-2**), wherein the fluorine on the terminal carbon shifts to the carbonyl carbon. This process is energetically feasible ($\Delta G^{\ddagger}$ = 13.3 kcal/mol). Following the 1,2-F migration, the fluoride is released as an anion (via coordination with sodium from sodium formate) which forms the carbon centered radical **c•**.[149] In turn, alkyl radical **c•** then undergoes *regioselective and irreversible Giese addition* to the olefin moiety of the *N*-arylmethacrylamide (**J-2**) to form radical species **d•**. Finally, a facile radical cyclization and HAT could take place to provide the difluorinated oxindole **L-2**. The hydrogen can be abstracted by radical intermediate **c•**, which is being formed in excess in the reaction medium. Alternatively, the single electron oxidation of **e•** by the thiyl radical **iv-2** could provide the corresponding carbocation intermediate, which after proton loss furnishes the final difluorinated compound **L-2**. The HAT process via either radical or carbocation would rearomatize the system and, as such, is very energetically favorable and irreversible (see **Appendix Figures A2.2.b3** and **A2.2.b4** for further details).

*2.6 Conclusions*

Herein we have reported the photoinduced synthesis of difluoro-substituted molecules. In particular, a transition metal-catalyzed photocatalyzed transformation yielded lactone derivatives and an organophotocatalyzed transformation yielded oxindole derivatives. These results demonstrate the applicability of mechanistic studies using DFT to both radical and polar chemical transformations. Specifically, DFT can be employed in studying reactions that can undergo both 1-electron and 2-electron transfer processes. The DFT results for the lactone derivative synthesis

also showcase the ability of DFT to not just validate experiments, but to predict reactivity of a system and to guide experimental mechanistic studies.

# Chapter 3: Access to Chiral Diamine Derivatives through Stereoselective Cu-Catalyzed Reductive Coupling of Imines and Allenamides

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*Contributions:* Robert Martin led all computational efforts and performed all computational studies in this chapter.

## *3.1 Abstract*

Chiral 1,2-diamino compounds are important building blocks in organic chemistry for biological applications and as asymmetric inducers in stereoselective synthesis that are challenging to prepare in a straightforward and stereoselective manner. Herein, we disclose a cost-effective and readily available Cu-catalyzed system for the reductive coupling of a chiral allenamide with *N*-alkyl substituted aldimines to access chiral 1,2-diamino synthons as single stereoisomers in high yields. Mechanistic investigations by density functional theory calculations identified the mechanism of this transformation Distortion/interaction-activation strain analysis and non-covalent interaction analysis revealed the relevance of non-covalent interactions in guiding the diastereoselectivity of this reaction. We also explored the relevance of the *t*-BuOH additive in inducing selectivity towards diamine or urea formation. Further, the addition to the imine was shown to be reversible, which has implications toward development of catalyst-controlled stereoselective variants of the identified reductive coupling of imines and allenamides.

## *3.2 Introduction*

Chiral vicinal diamines are valuable and important motifs in organic chemistry that are exploited by both nature and the pharmaceutical industry for their biological activities,[150,151] and in stereoselective organic synthesis as powerful chiral inducers through application as organocatalysts,[152] chiral ligands[153] for transition metal-catalyzed reactions, and as chiral

auxiliaries.[154] For example, a variety of biologically active pharmaceuticals and natural products are given in **Figure 3.1** possessing either the chiral 1,2-diamino-fragment or its corresponding urea form.[151] Representative therapeutics being developed for the treatment of important human diseases include antibiotics (penicillin,[151e] jogyamycin[151j]), anticancer compounds (cisplatin derivatives,[155] LP99[151c]), HIV protease inhibitors (NBD-11021[151d]), NK1-antagonists[156] (CP-99,994;[151a] Sch425078[151g]) for central-nervous-system (CNS) related diseases and rheumatoid arthritis, and influenza (tamiflu).[151b]

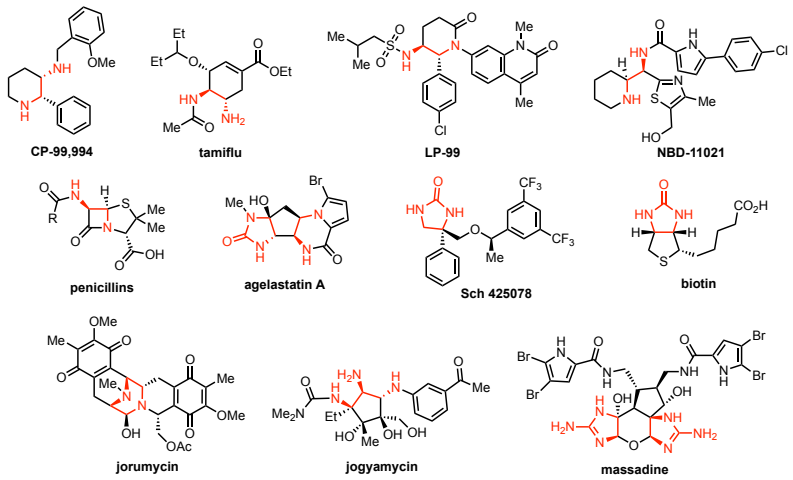



**Figure 3.1.** Selected examples of chiral 1,2-diamine- and urea-derived biologically active molecules.

Due to the biological and synthetic value of chiral 1,2-diamines, stereoselective methods for their preparation are an important endeavor in organic chemistry.[150a-d,157] Potential synthetic options to access the chiral vicinal diamine moiety can be envisioned to occur either by formation of the two C− N bonds starting from unsaturated hydrocarbons (**Figure 3.2A**) or through direct C−C bond formation between C1 and C2 of the 1,2-diamine from two *N*-substituted reagents (**Figure 3.2B**).[150a-d,157] Using a C−N bond forming approach (**Figure 3.2A**), diamination may be achieved by forming both C−N bonds at the same time,[157,158] or sequentially through either aziridination[159] followed by ring-opening with an amine nucleophile[150a-d,160] or through

aminohydroxylation[161] followed by alcohol activation and amine substitution.[150a–d] While direct catalytic 1,2-diamination of **b-3** represents an ideal strategy for diamine synthesis, the amino-groups added across the π-system are typically identical leading to the formation of diamines with identical substituents (i.e., $R^3 = R^4$ in **a-3**),[157,158] and a recent approach employing electrochemistry[158b] suffers from potentially forming high-energy/explosive diazocompounds[162] en route to the desired diamines. Further, the aziridination/ring opening strategy can suffer from poor stereoselectivity in the aziridination step and regiochemistry issues in the subsequent opening step, while the aminohydroxylation route requires regiocontrol in the aminohydroxylation step followed by additional transformations to convert **d-3** to the desired diamine. Alternative synthesis of **a-3** through C−C bond formation can be achieved through aza-pinacol coupling of two imines,[163] nitro-Mannich,[164] or glycine-Mannich[165] reactions (**Figure 3.2B**). Typical aza-pinacol coupling protocols only afford symmetrical diamines through homocoupling of a single imine; however, recent photoredox strategies[163h–l] enabling the generation of α- aminoradicals[166] from amines have enabled cross-selective coupling of imines and N-methylamines.[163j–l] Furthermore, nucleophilic additions to imines using α-aminoanion derivatives[167] from nitroalkanes (**f-3**)[164] or protected glycines (**g-3**)[165] offer another entry into the diamine core **a-3**.

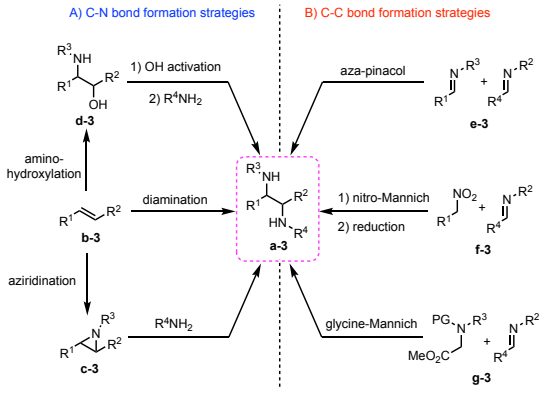



**Figure 3.2.** Synthetic strategies towards the synthesis of 1,2-diamines

Regarding chiral amine synthesis, asymmetric allylation of imines using allyl organometallic nucleophiles by direct addition or through catalyst control has been an area of intense research in organic chemistry (**Figure 3.3A**).[168] The chiral allylamine products are highly valuable in the context of the synthesis of complex amine-containing organic compounds because of the high versatility of the olefin functional group present within the product. Substituted allylorganometallic reagents (e.g., **h-3**) allow for increased molecular complexity by introducing two stereocenters in the allyl addition reaction (e.g., **Figure 3.3B**). Therefore, we envisioned that use of an amino-substituted allyl reagent **h-3** in addition reactions with imine electrophiles would be a powerful strategy to prepare 1,2-diamines (**a-3**) with differential substitution patterns on nitrogen and containing an olefin motif for further functional group manipulations. Surprisingly, only a single example of such a strategy for the preparation of 1,2-diamines has been reported, which employs a lithiated derivative of **h-3** (M = Li) with chiral *tert*-butanesulfinimide-derived aldimines affording products in moderate yields with mixtures of branched and linear allylation products.[169] In contrast, amino-substituted allyl reagents **h-3** have been used in reactions employing carbonyl electrophiles to provide 1,2-aminoalcohols (**Figure 3.3C**).[170–172] Recently, the Krische[171] group and the Sieber group[172] have developed reductive coupling[173,174] procedures for the catalytic generation of amino-substituted allyl reagents **h-3** and have studied their reactions with carbonyl electrophiles. These techniques represent orthogonal methodologies whereby the Krische[171a] system employs a chiral Ir-catalyst and processes aldehyde electrophiles using an achiral allenamide, while our work utilizes a Cu-catalyst and a chiral allenamide (**A-3**) for reactions using ketone electrophiles.[172] Based on our success in the stereoselective Cu-catalyzed reductive coupling of ketones and chiral allenamides to afford branched chiral 1,2-aminoalcohols[172a] or the corresponding linear products,[172b] and the lack of literature data for imine

allylation reaction utilizing aminosubstituted allylic nucleophiles, we began to investigate the reaction of allenamide **A-3** with imine electrophiles **B-3** for the stereoselective synthesis of chiral 1,2-diamine synthons **C-3** (**Figure 3.3D**). The results of these studies leading to the identification of a practical and highly stereoselective synthesis of diamine synthons **C-3** using Cu-catalyzed reductive coupling are disclosed herein. Further, I employed density functional theory (DFT) calculations to explore the mechanism of this transformation and to elucidate the factors affecting selectivity towards diamine vs. urea synthesis.

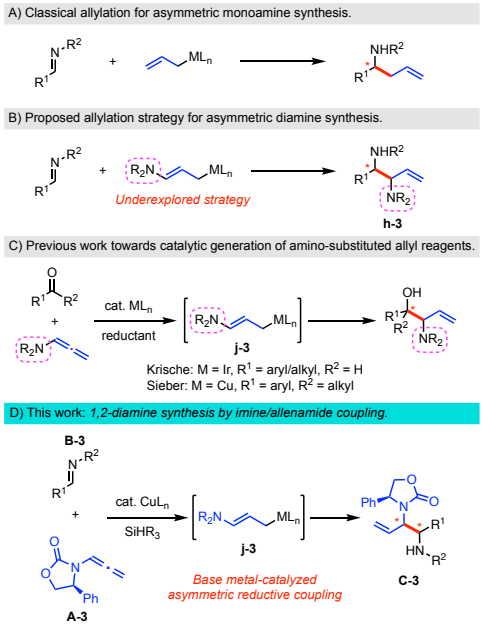



**Figure 3.3.** Classical strategies for amine/diamine synthesis and proposed allylation strategy towards the synthesis of 1,2-diamines.

## *3.3 Results & Discussion*

### 3.3.1 Experimental Results.

To investigate the proposed Cu-catalyzed reductive coupling of imines and allenamides, initial studies examined the ligand effect when employing DMB-protected imine **B-3** with chiral allenamide **A-3** in the reaction. The phenyl-derived Evans oxazolidinone of allenamide **A1-3** was specifically targeted due to its low-cost and high-availability,[175] (as were the copper pre-catalyst

and $PCy_3$ ligand[176]) and because it allows for more deprotection options of the desired diamine products over other alkyl-substituted oxazolidinones (i.e., hydrogenolysis). The DMB-group of the aldimine was employed due to its acid lability to allow for chemoselective differentiation of the two amine protecting groups in the final products. The initial reaction study afforded both diamine (**C-3**) and urea products (**D-3**), presumably resulting from migration of the carbamate carbonyl in the diamine products. Notably, addition of *t*-BuOH to the reaction led to the exclusive formation of diamine products (**C-3**) in excellent yield and diastereoselectivity. As a result, substrate scope experiments for this Cu-catalyzed reductive coupling reaction were performed both using *t*-BuOH as additive to provide branched diamino-derived products **C-3** (**Figure 3.4**) and without the *t*-BuOH additive to yield urea products **D-3** (**Figure 3.5**). In general, a wide variety of imines could be employed in the reaction under both conditions in good to excellent yields. Electron-deficient and electron-rich aryl groups both performed well in the reaction. Heterocyclic imines and C-substituted arenes were also well tolerated.

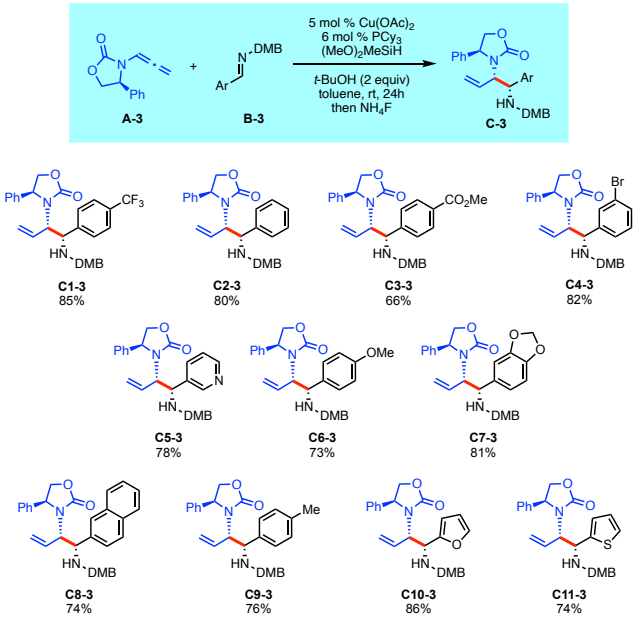



**Figure 3.4.** Representative examples of reductive cross-coupling of imines and allenamides to yield diamine products (**C-3**).

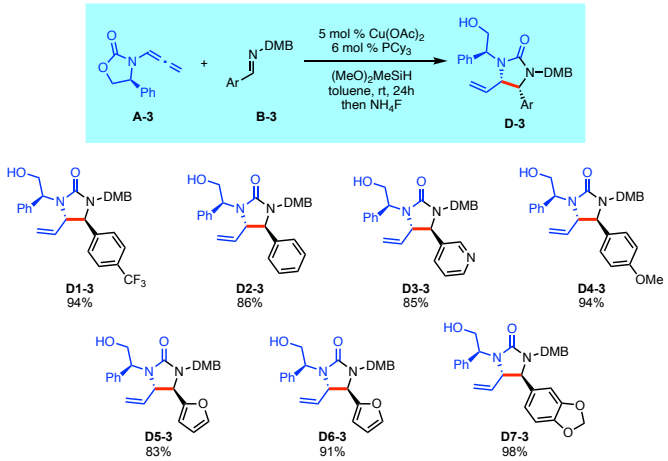



**Figure 3.5.** Representative examples of reductive cross-coupling of imines and allenamides to yield urea products (**D-3**).

In all cases, a single diastereomer of product was obtained as determined by $^1$H NMR spectroscopy of the unpurified reaction mixture. In all cases, a single diastereomer (the *(S,S,S)*-diastereomer) of product was obtained as determined by analysis of the unpurified reaction mixture by $^1$H NMR spectroscopy. Stereochemical assignment of the products obtained in the Cu-catalyzed reductive coupling reaction as the *(S,S,S)*-diastereomer was determined unequivocally by X-ray crystallography of the HCl-salt of one diamine product).

### 3.3.2 Mechanistic Proposal.

An initial working hypothesis to understand the difference in product selectivity between the formation of urea **D-3** in the absence of *t*-BuOH versus the exclusive formation of diamino derivative **C-3** when *t*-BuOH was used as an additive is given in **Figure 3.6**. Regioselective hydrocupration of allenamide **A-3** by the LCuH[172,174c] catalyst **i-3** initially is expected to afford substituted linear allylcopper reagent **ii-3** that may undergo *E/Z* isomerization through σ−π−σ equilibration prior to reaction with the imine electrophile. Then, diastereoselective reaction of intermediate **ii-3** with imine **B-3** provides Cu-amide intermediate **iii-3**. To afford diamine product **C-3** from **iii-3**, direct silylation of the amine by the silane must occur to regenerate the LCuH catalyst **i-3**; however, this step is expected to be slow due to the strength of the N−Si bond (BDE

≈ 104 kcal/mol).[177] Due to the strong basicity of the N-anion in **iii-3**, intramolecular attack of the oxazolidinone carbonyl may occur competitively to provide **iv-3** containing an O−Cu bond that should more easily silylate due to the high bond strength of the O−Si bond (BDE ≈ 190 kcal/mol)[178] affording urea **v-3** (which can be reprotonated with $NH_4F$ to form the urea product **D-3**) and regenerating the LCuH catalyst (**i-3**). Alternatively, when *t*-BuOH is present, protonation of the Cu−N bond of **iii-3** by *t*-BuOH to afford product **C-3** directly and generate LCu-O*t*Bu is thermodynamically favorable based on the pKa values for a secondary amine (pyrrolidine pka∼44 in DMSO)[179] vs *t*-BuOH (pka∼32 in DMSO)[180] and supported by DFT calculations (vide infra). The LCu-O*t*Bu intermediate can then undergo silylation to regenerate the LCuH catalyst **i-3**. The role of alcohol additives to facilitate catalyst turnover by protonation of Cu−N intermediates has been documented previously.[174c,181] Sterically hindered alcohols such as *t*-BuOH have been shown to be preferred since the rate of competitive protonation of the Cu−H catalyst is reduced with bulky alcohols.[181]

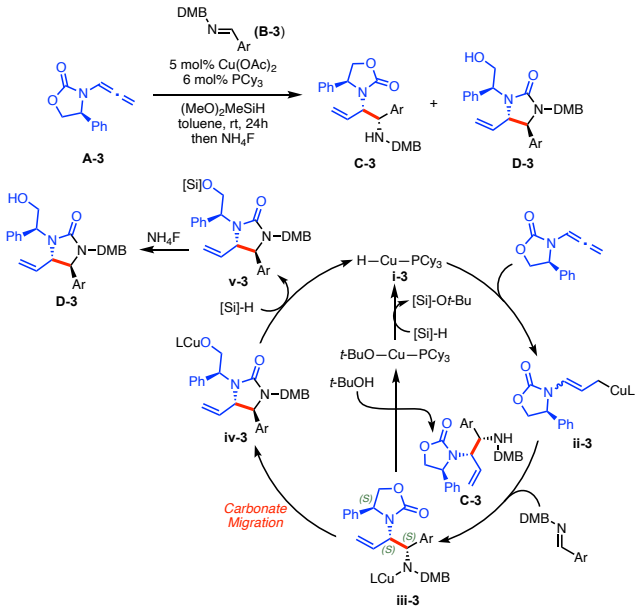



**Figure 3.6.** Proposed catalytic cycle for synthesis of diamine (**C-3**) and urea (**D-3**) products.

### 3.3.3 Mechanistic Modeling by DFT Analysis.

To shed light onto the mechanism and origin of diastereoselectivity, we used dispersion-corrected DFT calculations (see **Appendix A3.2** for full computational details). Specifically, we performed extensive conformational analysis on all intermediates and transition states using the B3LYP-D3 functional and a def2-SVP basis set[182] with toluene as the solvent using the CPCM solvation model[183] as implemented in Gaussian16. Further, to refine the energetics and compare methods, single-point calculations using the M06-L functional,[184] as well as a larger basis set (def2-TZVPP) with B3LYP-D3, which yielded similar energetic profiles, were subsequently performed. For simplicity, only B3LYP-D3/def2-SVP optimization energetics will be discussed in the text. Structures were visualized using CYLview Version 1.0.561.[185]

As shown in **Figure 3.7**, initial investigations were conducted by first analyzing the hydrocupration of allenamide **A-3** with ($PCy_3$)CuH as catalyst. Following coordination of the copper and allenamide π-bond, the energetically favored hydrocupration proceeds via **TS−i-ii-3** (barrier of 10.4 kcal/mol with respect to separate **A-3** and LCuH structures) to form the branched allylcopper species **ii-3**. Presumably this transition state benefits from lack of steric hindrance between the ligand and the chiral auxiliary, which were present in the alternative transition states. Specifically, alternate hydrocupration transition states leading to linear allylcopper species (**TS−i-iii-3** ***cis*** and **TS−i-iii-3** ***trans***) were found to be much higher in energy by ~3 kcal/mol for **TS−i-iii-3** ***trans*** and by >7 kcal/mol for all other pathways and were therefore not productive.

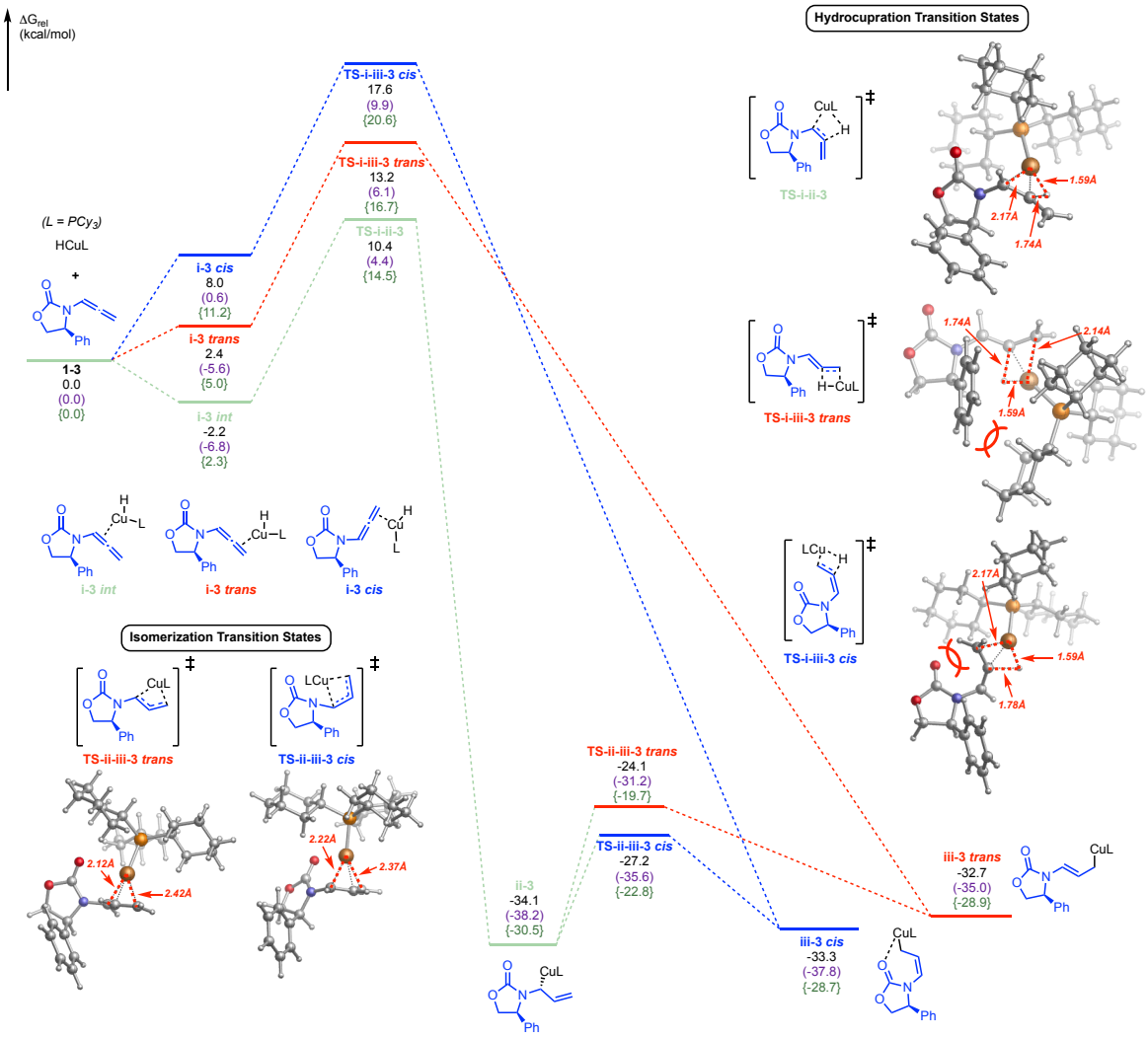



**Figure 3.7.** Structures and relative free energies (in kcal/mol, with respect to separate LCuH catalyst and reactants) of possible hydrocupration pathways. Optimizations performed at B3LYP-D3/def2SVP-CPCM(toluene), M06-L/def2SVP-gas//B3LYP-D3/def2SVP-CPCM(toluene) (in parentheses) and B3LYP-D3/def2TZVPP-gas//B3LYP-D3/def2SVP-CPCM(toluene) {in braces} levels of theory.

In turn, the branched allylcopper intermediate is expected to undergo isomerization to linear allylcopper species by σ–π–σ isomerization. Recently, Buchwald and co-workers reported branched-linear allylcopper isomerizations for a system with a bidentate phosphine ligand[174c] as well as with a CuH-catalyzed allylation of ketones and dienes.[186] In our case, it was calculated that the branched allylcopper intermediate **ii-3** can readily isomerize (barrier of only 6.9 and 10.0 kcal/mol via **TS−ii-iii-3** ***cis*** or **TS−ii-iii-3** ***trans***, respectively) to form the nearly isoenergetic *cis*

or *trans* linear allylcopper intermediates (**iii-3 *cis*** and **iii-3 *trans***). Intermediate **iii-3 *cis*** was slightly favorable compared to intermediate **iii-3 *trans*** (by 0.6 kcal/mol), as was the *cis* isomerization transition state (**TS−i-iii-3 *cis*** was favored by 3.1 kcal/mol), presumably due to coordination between the oxazolidinone and the copper (Cu−O bond distance = 2.37 Å). However, upon coordination of the imine to the copper, the *trans* conformation (**iii′-3 *trans***) becomes significantly more favored (as seen in **Figure 3.7**), likely due to unfavorable steric hindrance between the imine and the oxazolidinone in the **iii′-3 *cis*** conformation (see **Appendix 3.2** for further details).

Next, we focused on the key C−C bond formation steps. As shown in **Figure 3.8** and **Figure 3.9**, after performing extensive conformational analysis on the subsequent diastereomeric C−C bond forming transition states with the allylcopper intermediates and the imine substrate (see **Appendix A3.2** for further details), the most favorable pathway for diastereoselective C−C bond formation was identified to proceed from the *trans* linear intermediate **iii′-3 *trans*** through a Zimmerman−Traxler transition state **TS-iii′-iv-3 *trans (S,S,S)*** (barrier of only 7.4 kcal/mol from complexed **iii′-3 *trans*** intermediate) to branched addition product **iv-3 *(S,S,S)***. Further, in agreement with experiment, the competing diastereomeric transition state **TS-iii′-iv-3 *trans (R,R,S)*** which would lead to the opposite diastereomer was determined to be much higher in energy. Notably, all C−C bond formation steps from **iii′-3 *trans*** are reversible, as the branched addition products **iv-3 *(S,S,S)*** and **iv-3 *(R,R,S)*** were each uphill in energy (by ~2 kcal/mol and ~6 kcal/mol respectively), which can have implications for rational catalyst and reaction design (vide infra).

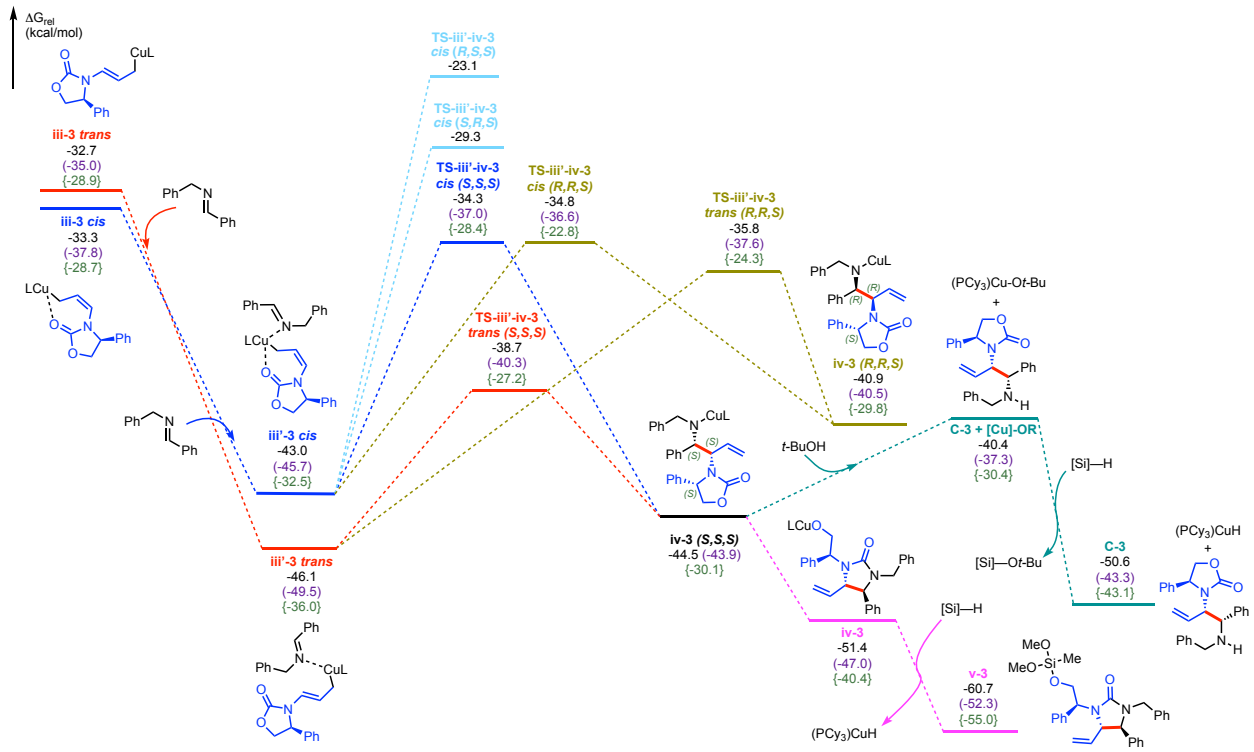



**Figure 3.8.** Relative free energies (in kcal/mol, with respect to separate LCuH catalyst and reactants) for proposed mechanistic pathway. Optimizations performed at B3LYP-D3/def2SVP-CPCM(toluene), M06-L/def2SVP-gas//B3LYP-D3/def2SVP-CPCM(toluene) (in parentheses) and B3LYP-D3/def2TZVPP-gas//B3LYP-D3/def2SVP-CPCM(toluene) {in braces} levels of theory.

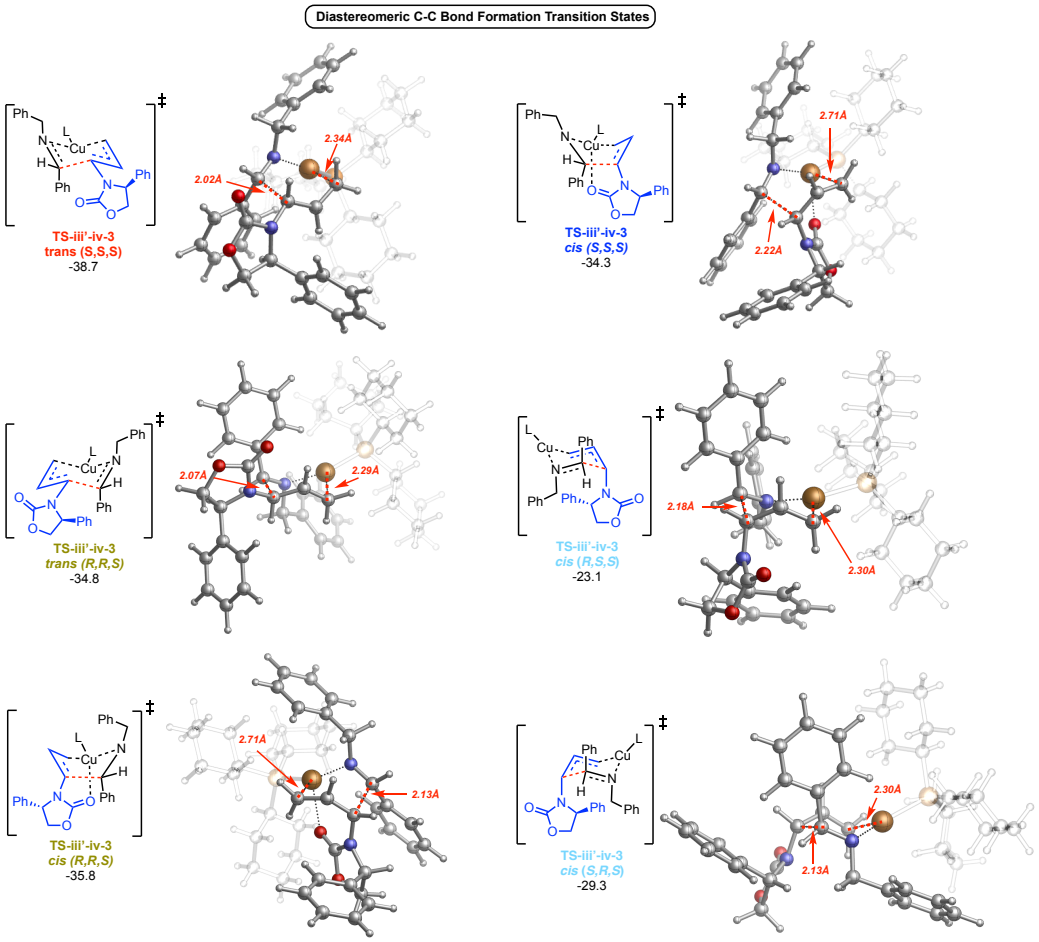



**Figure 3.9.** Structures of diastereomeric C-C bond formation transition states. Optimized structures of transition states visualized with CYLview are shown (with $PCy_3$ ligand faded out for clarity). Energies (in kcal/mol) reported at B3LYP-D3/def2SVP-CPCM(toluene) level of theory.

To gain insights into the origin of diastereoselectivity, we performed distortion/interaction-activation strain and NCI analysis (**Figure 3.10**). Overall, comparing the structures of the lowest energy competing diastereomeric transition states **TS-iii′-iv-3** ***trans (S,S,S)*** and **TS-iii′-iv-3** ***trans (R,R,S)*** reveals that the structures of these transition states were remarkably similar, with key C−C and C−Cu bond distances differing by no more than 0.05 Å. However, the orientation of the chiral auxiliary is different, as the **TS-iii′-iv-3** ***trans (S,S,S)*** transition state has the oxazolidinone moiety of the enamide group of the substituted Cu(allyl) ligand in an s-*trans* conformation while **TS-iii′-iv-3** ***trans (R,R,S)*** has this group in an s-*cis* conformation that, as shown in **Figure 3.11**, leads to a 2.2 kcal/mol energy destabilization. Furthermore, the ground state structures of chiral

oxazolidinone-derived enamides are known to favor an s-*trans* conformation.[187] In addition, distortion/interaction-activation strain analysis[188] (**Figure 3.10A**) showed that the distortion energy of the **TS-iii′-iv-3** ***trans (S,S,S)*** transition state was higher than that of the corresponding **TS-iii′-iv-3** ***trans (R,R,S)*** transition state (by 3.9 kcal/mol). However, the *(S,S,S)* system benefited from much stronger interaction energy (by 8.5 kcal/mol). Overall, this favorable interaction between the imine and allylcopper makes the **TS-iii′-iv-3** ***trans (S,S,S)*** the favorable diastereomeric transition state. Finally, noncovalent interaction (NCI) analysis (performed using Multiwfn[189] software and visualized using VMD[190] software) further supports the presence of favorable interactions in the **TS-iii′-iv-3** ***trans (S,S,S)*** transition state (**Figure 3.10B**). Specifically, in both transition states, there appeared to be favorable C−H···π interactions between the ligand and the benzyl group of the imine (highlighted inside the blue circle). However, comparing the areas in red circles, the **TS-iii′-iv-3** ***trans (S,S,S)*** system had stronger noncovalent interactions between the oxazolidinone group and the phenyl ring on the imine. This suggests that noncovalent interactions (i.e., between the oxazolidinone moiety and the protecting group) are critical for control of diastereoselectivity. Taken together, these results suggest that both the conformational preference for the s-*trans* geometry about the *N*-enamide group of the substituted Cu(allyl) ligand and favorable noncovalent interactions between the oxazolidinone group and the imine are the major contributing factors for diastereocontrol in these reactions.

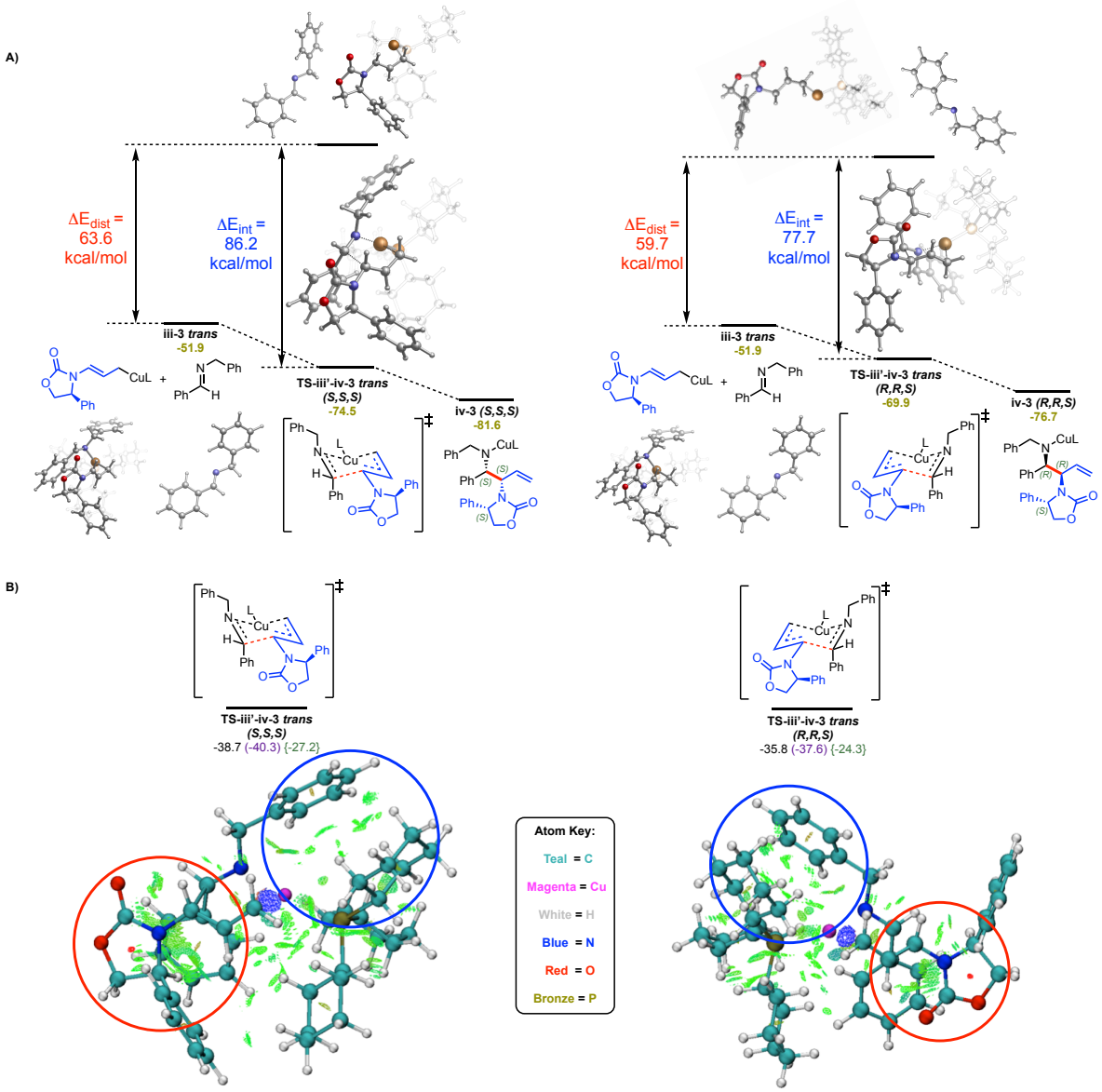



**Figure 3.10.** Analysis of key diastereomeric C-C bond formation transition states. A) Distortion/interaction-activation strain analysis. Electronic energies reported at B3LYP-D3/def2SVP-CPCM(toluene) level of theory. B) Non-Covalent Interaction analysis. Color code for the atoms is shown.

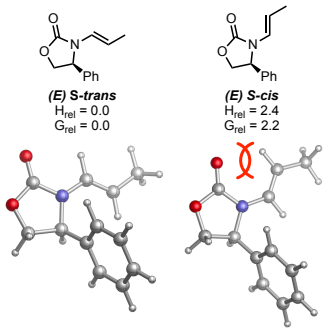



**Figure 3.11.** Energetic comparison of s-*trans* and s-*cis* conformations of an *(E)* allylic system with chiral oxazolidinone, with steric hindrance causing allylic strain highlighted. Structures optimized using B3LYP-D3/def2SVP-CPCM(toluene) ($H_{rel}$ and $G_{rel}$ shown in kcal/mol).

Following C−C bond formation, intermediate **iv-3** serves as a fork between two reaction pathways depending on whether there is *t*-BuOH present (as supported by experiments; vide supra). Specifically, in the presence of *t*-BuOH, the alcohol can act as a proton source to protonate the Cu−N bond and yield branched product **C-3**, while the alkoxide binds to the copper. From this, the silane reagent can exchange hydride for the alkoxide group, reforming the catalyst. While this protonation of the amine moiety and concomitant release of the *t*-BuO-CuL was calculated to be initially energetically unfavorable (uphill by ∼4 kcal/mol), the exchange of hydride for the alkoxide was thermodynamically favorable (downhill by ∼10 kcal/mol), rendering this overall process energetically feasible. In the absence of *t*-BuOH, a thermodynamically favorable rearrangement of intermediate **iv-3** can yield the Cu-alkoxide urea intermediate **iv-3** (∼7 kcal/mol exergonic), which can then readily undergo transmetalation with silane to reform the LCuH catalyst and furnish the silylated product of urea **D-3**. This mechanistic model is consistent with experimental findings that the presence of *t*-BuOH has a profound effect on the product selectivity (but not diastereoselectivity) of the reaction toward either of the products (vide supra).

As previously noted, computational modeling of the imine addition predicts this step should be reversible. This phenomenon has important impacts for future developments of catalyst controlled enantioselective reactions utilizing a chiral catalyst in conjunction with an achiral

allenamide. In this regard, reaction of achiral allenamide **A2-3** with imine **B-3** using *(S,S)*-Ph-BPE as a chiral ligand was examined with and without *t*-BuOH as the additive (**Figure 3.11**). Again, branched product **E-3** was formed as a single diastereomer when *t*-BuOH was present in the reaction, and urea **F-3** was formed as a single diastereomer in the absence of *t*-BuOH. Separate conversion of **E-3** to **F-3** using *n*-BuLi confirmed that the same relative stereochemistry was formed in both reactions. Importantly, **E-3** and **F-3** were formed in different enantiopurities (57:43 vs 80:20 er, respectively), *supporting a reversible imine addition step in these reactions*. For example, if imine addition were irreversible, reaction of **A2-3** with a chiral catalyst to afford the analogous intermediate to **iii-3** (**Figure 3.6**) must be enantiodetermining and requires that urea product **F-3** formed from rearrangement of the intermediate **iii-3** derivative to have identical enantiopurity to that of **E-3**. However, when a chiral ligand is employed, rearrangement of the two enantiomers of intermediate **iii-3** may occur at different rates because the transition states will be diastereomeric due to the chirality on the ligand. Therefore, the carbamate migration step may also be enantiodetermining if the imine addition step becomes reversible enabling different enantiomeric ratios to be obtained for a **E-3**-selective vs. a **F-3**-selective process, as was observed.

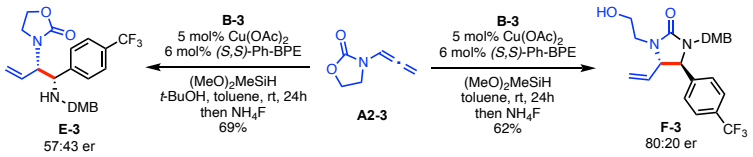



**Figure 3.11**. Mechanistic implications relevant to designing catalyst-controlled enantioinduction.

## *3.4 Conclusions*

In conclusion, a highly stereoselective method for the reductive coupling of imines with a chiral allenamide was developed as a convenient strategy for the asymmetric synthesis of valuable 1,2-diamino and urea synthons. Use of *tert*-butanol as an additive was shown to aid in the amine

release and catalyst regeneration to avoid the formation of urea products that are exclusively obtained in the absence of this additive. Mechanistic investigations by density functional theory calculations identified the mechanism for stereoselection in these processes as determined from the relative transition state barriers of *N*-substituted allylcopper complexes to the imine electrophile. This C−C bond forming addition step was shown to be reversible by calculation and was experimentally supported by the catalytic asymmetric reaction of a chiral catalyst with an achiral allenamide. These mechanistic insights are important for the development of future asymmetric catalyst-controlled procedures and are currently under further investigation in these laboratories.

# Chapter 4: Mechanistic Studies of First-Row Earth-Abundant Transition Metal-Catalyzed Reactions

*This chapter contains unpublished data.*

*Contributions:* Robert Martin performed all computational studies in Chapter 4.3. Robert Martin performed the computational studies in Chapter 4.5 in collaboration with Zhihui Song.

## *4.1 Abstract*

For decades, transition metal catalysts based on precious metals have proven to be effective and efficient for a variety of organic transformations. However, these catalysts bear many disadvantages, including high price, toxicity, and limited availability, among others. In recent years, Earth-abundant first-row transition metals have seen growing attention and numerous transformations have been explored with these catalysts. Herein, I have employed density functional theory (DFT) computations to explore two transformations that employ first-row transition metal catalysts: one with nickel, and one with cobalt. For the nickel transformation, I present the preliminary results of a mechanistic investigation into the nickel-catalyzed hydroarylation of *gem*-difluoroalkenes. Here, I have determined the likely order of steps for this reaction is different from that previously proposed for an analogous reaction of non-fluorinated alkenes. Specifically, my calculations suggest that C-H bond formation should precede C-C bond formation in this reaction. I am also exploring the mechanism of a cobalt(I)-catalyzed substitution reaction of allylic carbonates with dimethylmalonate. Here, I have used DFT to rule out the feasibility of a radical pathway for the mechanism. Instead, my computations also suggest that a polar (2-electron transfer) pathway is more energetically feasible. Further DFT studies into the mechanisms of these transformations are ongoing.

*4.2 Introduction to Nickel-Catalyzed Hydroarylation of gem-Difluoroalkenes*

The synthesis of fluorinated molecules has become a particular interest to organic chemists in recent years.[191-194] Fluorinated molecules have a wide range of applications in medicine, agrochemistry, fine chemicals, and materials, among other fields.[195,196] *gem*-Difluoroalkanes in particular exist widely in many of these fields,[197-200] but they are particularly important in pharmaceuticals.[192,195,196] As bioisosteres of groups like alcohols and thiols, *gem*-difluoroalkanes are a unique moiety that has received significant attention in the synthetic community.[195,201-203] One potential source for *gem*-difluoroalkanes is functionalization of *gem*-difluoroalkenes. Like other fluorinated molecules, *gem*-difluoroalkenes can exhibit unique steric and electronic properties[203-245], which make their use in synthesis very interesting from a mechanistic perspective. However, synthesis of these compounds has faced difficulties, particularly from side reactions with the substrates and catalysts and with control of the catalytic cycle to achieve desired selectivity (**Figure 4.1A**).[196,199]

Considerable effort has been expended in the field of alkene hydrocarbofunctionalization to be able to simultaneously form C-C and C-H bonds regioselectively with a wide variety of substrates.[206-209] To this end, the Koh group has recently reported a nickel-catalyzed branched-selective hydroarylation of alkenes (**Figure 4.1B**).[206] This protocol can accomplish hydroarylation with up to 95% yields and >99:1 regioselectivity. Initial mechanistic studies indicated that the likely mechanism for this transformation was a sequential carbonickelation-hydride transfer. Specifically, following oxidative addition of the aryl halide to the nickel, C-C bond formation precedes H-atom abstraction and reductive elimination. This order of steps is noteworthy as it is contrary to previous reports of hydrometallation processes.[210]

Following this report, the Koh group began investigating the reactivity of *gem*-difluoroalkenes towards this hydroarylation (**Figure 4.1C**). They have found evidence that the mechanism of this transformation differs from that of the non-fluorinated system. To this end, we would like to investigate the mechanism of this transformation computationally to explore whether the fluorinated substrates can affect the order of C-H and C-C bond formation steps. Initial computational evidence suggests that the mechanism of this transformation proceeds through a different order of steps, with H-atom transfer and C-H bond formation preceding carbonickelation and C-C bond formation. The preliminary results of this study are presented herein.

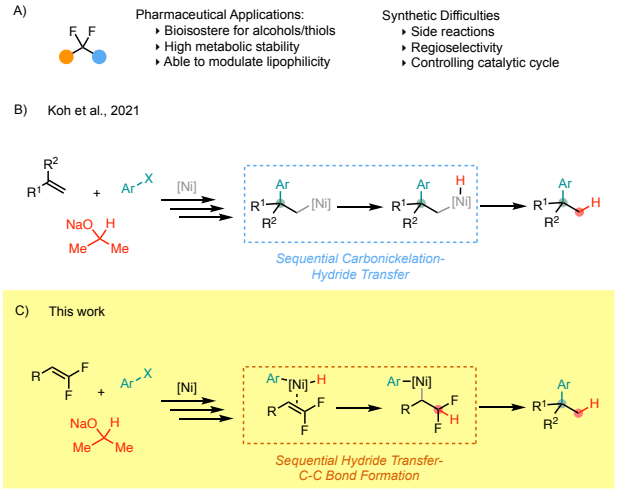



**Figure 4.1.** Motivation for developing and exploring the mechanism of a hydroarylation protocol for *gem*-difluoroalkenes. A) Unique properties of organofluorines. B) Recent hydorarylation of alkenes from Koh et al.[206] C) Nickel-catalyzed site-selective hydroarylation of *gem*-difluoroalkenes.

## *4.3 Results & Discussion: Nickel-Catalyzed Hydroarylation of gem-Difluoroalkenes*

### 4.3.1 Experimental results.

Recently, the Koh group has reported a three-component hydroarylation of difluoroalkenes (**Figure 4.2**). This transformation utilizes a nickel(0) catalyst with the *N*-heterocyclic carbene ligand IPr, along with an alkoxide base (sodium 1-phenylethan-1-olate, **C-4**) and an aryl halide (**B-4**). The halide and a hydride from the alkoxide can then be coupled with *gem*-difluoroalkenes

with high yield and excellent regioselectivity towards branched addition of the aryl group. This protocol is summarized in **Figure 4.2** below. Experiments are underway to determine the scope of substrates that can undergo this transformation and the optimal reaction conditions. Initial mechanistic studies suggest that **C-4** is the most effective alkoxide base to use for this transformation.

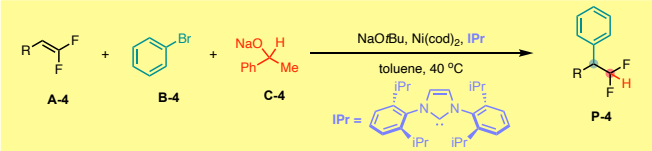



**Figure 4.2.** Optimized reaction conditions for nickel-catalyzed three-component hydroarylation of *gem*-difluoroalkenes.

### 4.3.2 Mechanistic study with DFT.

A proposed mechanism for this reaction is shown in **Figure 4.3** below (see full computational details in **Appendix A4.2.a.** I have employed density functional theory (DFT) computations to study the mechanism of this transformation for a model system (R = Me). My results have indicated that the mechanism of this reaction can proceed through oxidative addition of the aryl halide to the nickel(0) catalyst **a-4** to form the nickel(II) halide species **b-4**. This oxidative addition is exergonic and has a low barrier ($\Delta G^{\ddagger}$ = 2.1 kcal/mol). Following oxidative addition, the H atom from the alkoxide **C-4** can be abstracted by the nickel to form the nickel(II)-hydride species **c-4**. Addition of *gem*-difluoroalkene **A-4** can induce migratory insertion of the H atom to yield the nickel(II)-alkyl complex **iv-4**, before reductive elimination forms the product and reforms the catalyst **A-4**. Each of these processes is exergonic and has a relatively low barrier that can be readily overcome under the given reaction conditions.

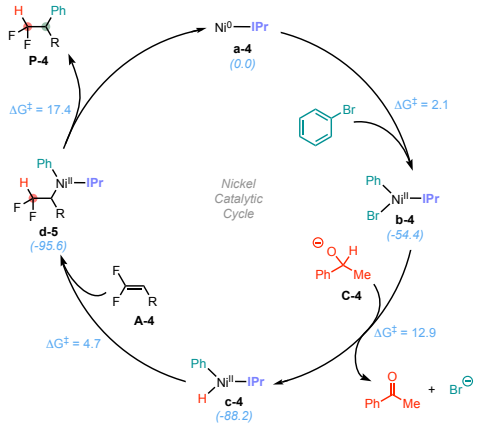



**Figure 4.3.** Proposed mechanistic pathway for three-component hydroarylation of *gem*-difluoroalkenes. All structures optimized at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory and free energies are reported in kcal/mol.

One important distinction that must be made between this work and previous proposals[244] is that the migratory insertion of the H atom (from intermediate **c-4**) should precede insertion of the aryl group. I investigated whether this order of steps was reasonable based on my computations. As seen in **Figure 4.4** below, although the products of both C-C bond formation (**k-4**) and C-H bond formation (**e-4**) are similar in energy, the C-C bond formation pathway is significantly less energetically favorable than C-H bond formation ($\Delta\Delta G^{\ddagger}$ = 18.8 kcal/mol). This suggests that C-H bond formation should forego C-C bond formation during the course of the reaction.

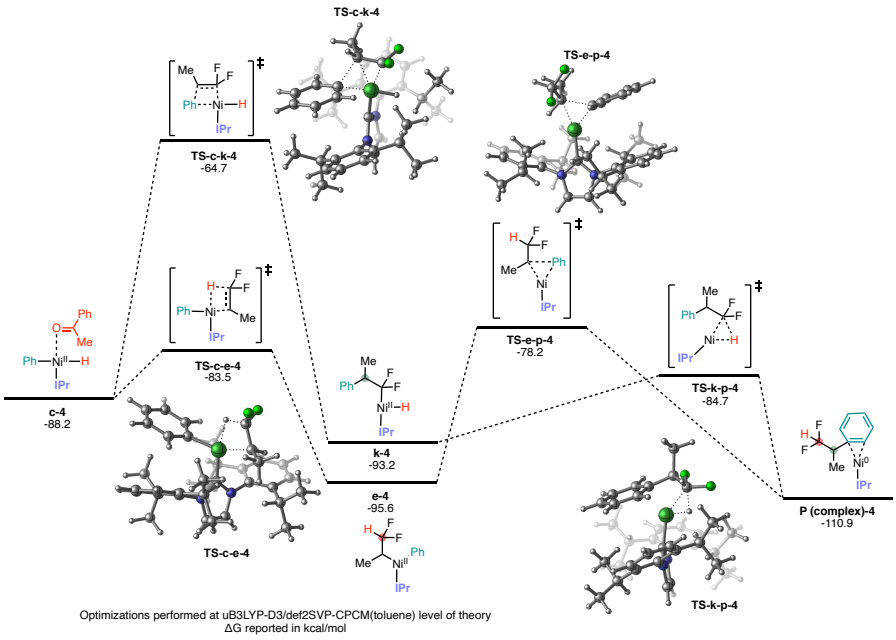



**Figure 4.4.** Energetics for competing migratory insertion pathways. All structures optimized at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory and free energies are reported in kcal/mol.

Further computational investigations are underway into more details of this transformation's mechanism. One avenue of research is computationally probing the effects of the alkoxide base (**C-4**) on reactivity. Additionally, comparison of this mechanism to the mechanism of hydroarylation of non-fluorinated alkenes is underway.

## *4.4 Introduction to Cobalt(I)-Catalyzed Allylic Substitution*

Transition metal-catalyzed allylic substitution reactions have long been powerful synthetic methods that are used to produce various products of interest (**Figure 4.5A**).[211,212] These reactions are extremely versatile and can be utilized to construct a wide variety of C-C and C-heteroatom bonds.[211,213,214] Palladium has emerged as the preeminent metal of choice to conduct many of these reactions.[211a,b,e,215-217] However, one major difficulty faced by many of these protocols is regioselectivity. Specifically, many allylic substitutions catalyzed by palladium, such as the classic Tsuji-Trost reaction, are strongly selective towards linear addition, often for steric reasons.[211a] As

such, many reaction protocols have been developed using alternative precious metals (including rhodium,[218] iridium,[219] and ruthenium,[220] among others[220]) to provide access to many biologically relevant molecules. However, these protocols continue to struggle with formation of quaternary centers as well as with low reactivity. These transformations are also not as attractive from a cost or green chemistry perspective as those that are be catalyzed by earth-abundant transition metals.[213] Many results utilizing first-row transition metals (including copper,[221] nickel,[222] iron,[223] and others) have been explored recently, although cobalt remains one metal that is generally underdeveloped, particularly from a mechanistic perspective.[211d,213,214,224,225]

Recent reports from the groups of Matsunaga,[224] Li,[213] and Meng[225] demonstrate that cobalt can catalyze allylic substitution with a variety of nucleophiles under reducing conditions (**Figure 4.5B**). In both cases, cobalt(I) has been implicated as the likely active catalyst for activation of the allyl carbonate. For the work by Matsunaga et al.,[224] they find that a cobalt-catalyzed allylic substitution can be achieved with an organic photocatalyst. They argue that a cobalt(II) pre-catalyst can be activated by a photocatalyst (undergoing SET) to form a cobalt(I) species that is catalytically active. This transformation has good tolerance for various functionalities, but is limited to secondary allylic carbonates. For the work from Li et al.,[213] the authors can induce enantioselectivity with a chiral ligand and a cobalt(I) catalyst. They assert that the active cobalt(I) catalyst is formed from the reaction of an inactive cobalt(II) pre-catalyst with $NaBH_4$ and EtOH. This work provides an exciting avenue for inducing stereoselectivity in branched-selective allylic substitution, which has historically been very difficult. However, the work has limited substrate scope and produces little mechanistic evidence for the formation of cobalt(I). Meng et al.[225] were similarly able to induce enantioselectivity in a prenylation of aldehydes. They were able to demonstrate that this prenylation can be catalyzed by a cobalt(I) catalyst with an oxazoline-

phosphine-ligand ((N,P)-ligand) that enables the formation of radical intermediates. However, the effect of using a bisphosphine ligand was not explored.

We would like to address the limited understanding of the mechanisms and expand the scope of cobalt(I)-catalyzed allylic substitutions. As such, in collaboration with the Casitas group (University of Marburg), I have employed density functional theory (DFT) computations to explore the mechanism of an allylic substitution reaction catalyzed by a cobalt(I) species with a bisphosphine ligand (**Figure 4.5C)**. The preliminary results of this study are disclosed herein.

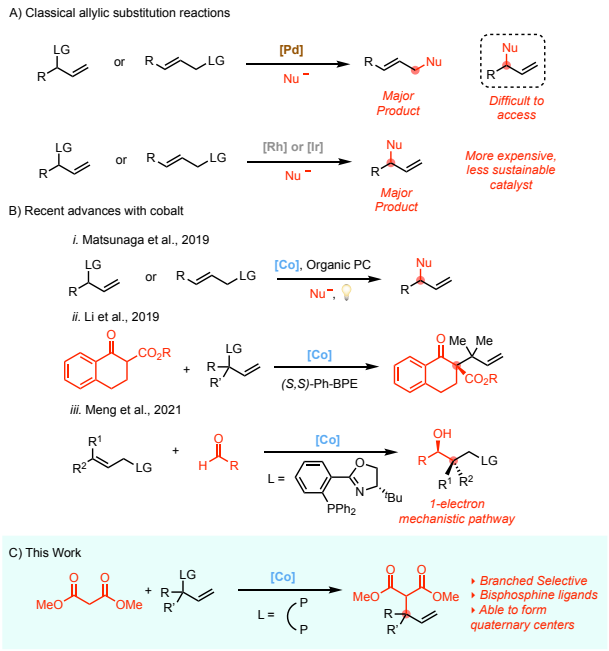



**Figure 4.5.** Transition metal-catalyzed allylic substitution reactions. A) Typical allylic substitution reaction paradigms with precious metals. B) Recent advances in allylic substitution reactions with cobalt(I) catalysts. C) Cobalt(I)-catalyzed allylic substitution of carbonates with malonates.

*4.5 Results & Discussion: Cobalt(I)-Catalyzed Allylic Substitution*

Recently, the Casitas group has reported an allylic substitution reaction of allylic carbonates (**E-4**) with malonic ester (**D-4**) catalyzed by a cobalt(I) complex. This reaction proceeds with high regioselectivity towards branched products. A selection of products of this reaction are summarized in **Figure 4.6** below. This transformation was achieved using various bisphosphine

ligands on the cobalt catalyst, including 1,3-Bis(diphenylphosphino)propane (**dppp**) and 1,2-Bis(diphenylphosphino)ethene (**dppen**), among others.

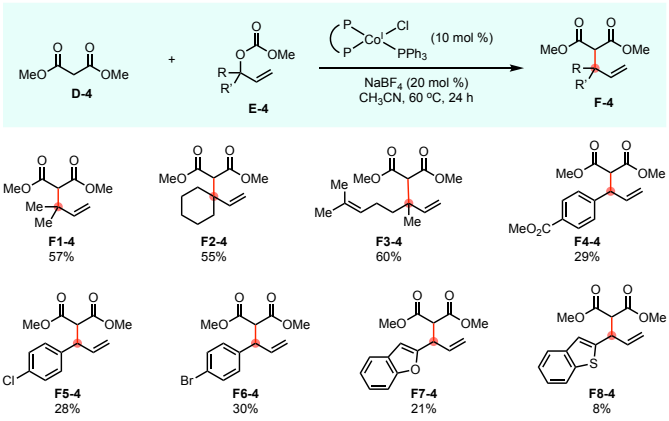



**Figure 4.6.** Cobalt(I)-catalyzed allylic substitution products. Yields reported as determined by $^{1}$H-NMR by the Casitas group. These reactions were performed with the bisphosphine ligand 1,3-bis(diphenylphosphino)propane (**dppp**), although other bisphospine ligands were employed and yielded similar results.

### 4.5.1 DFT study of one-electron mechanistic pathway.

To better understand the mechanism of this transformation, I performed density functional theory (DFT) computations on the system for formation of **F1-4**. Prior to investigating the mechanism, I performed (in collaboration with Dr. Zhihui Song) a screening of potential methods to utilize. The results of this screening are summarized in **Appendix Figures A4.2.b2** and **A4.2.b3**. We decided to focus on the two most effective bisphosphine ligand systems for all calculations: **dppp** and **dppen**.

Our initial mechanistic proposal, based on prior work from Meng et al.,[225] was that this reaction may proceed via a 1-electron pathway, such as the pathway shown in **Figure 4.7** below. In this pathway, the cationic cobalt(I) catalyst **i-4** could undergo either outer-sphere oxidative addition (**TS-i-vi-4**) with the allylic carbonate to form the carbonate radical/cobalt-allyl complex **vi-4**, or inner-sphere oxidative addition (**TS-i-vi-4**) with the allylic carbonate to form **ii-4**, followed by dissociation of the carbonate to form **vi-4**. The carbonate radical can then exchange an H atom

with the malonate, forming the malonate radical. The malonate radical can then add to the cobalt-allyl complex (via **TS-vi-F-4**) to yield the product. My DFT calculations revealed that the inner-sphere oxidative addition pathway is significantly more energetically favored, but dissociation to **vi-4** is energetically unfavorable. This may be due to the relative stability of the Co-O bond (Co-O bond dissociation energy ~ 88 kcal/mol[177]) and lack of stabilization of the carbonate radical present in **vi-4**. Additionally, computations from Dr. Zhihui Song revealed that the reductive elimination step is even higher in energy. These findings suggest that this 1-electron pathway is not energetically feasible.

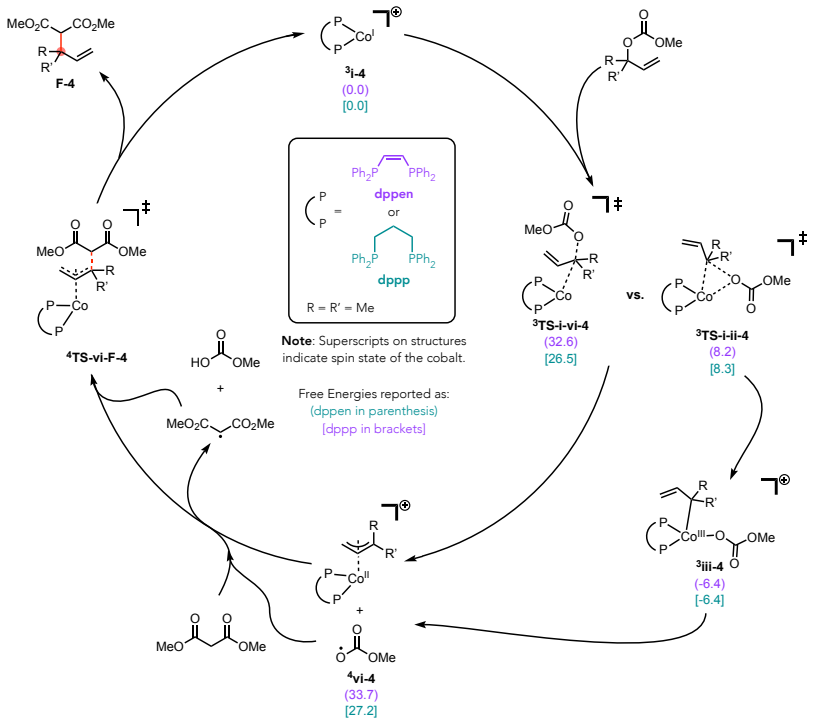



**Figure 4.7.** Proposed 1-electron reaction pathway for cobalt(I)-catalyzed allylic substitution reaction. All structures optimized at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory. Only intermediate (triplet/quartet) spin state energies are shown, as all low (singlet/doublet) spin state energies were significantly higher.

### 4.5.2 DFT study of two-electron mechanistic pathway.

These results inspired us to consider an alternative 2-electron mechanistic pathway. Such a pathway is summarized in **Figure 4.8** below. In this pathway, following oxidative addition to

form the Co(III) complex **ii-4**, the malonate can add directly to the cobalt to form **iii-4**. This can lead directly to formation of the C-C bond (**TS-iii-iv-4**) to form the product **F-4** (bound to the cobalt as **iv-4**). Subsequent dissociation of the product and of the carbonate anion should reform the catalyst **i-4** and allow for continuation of the catalytic cycle.

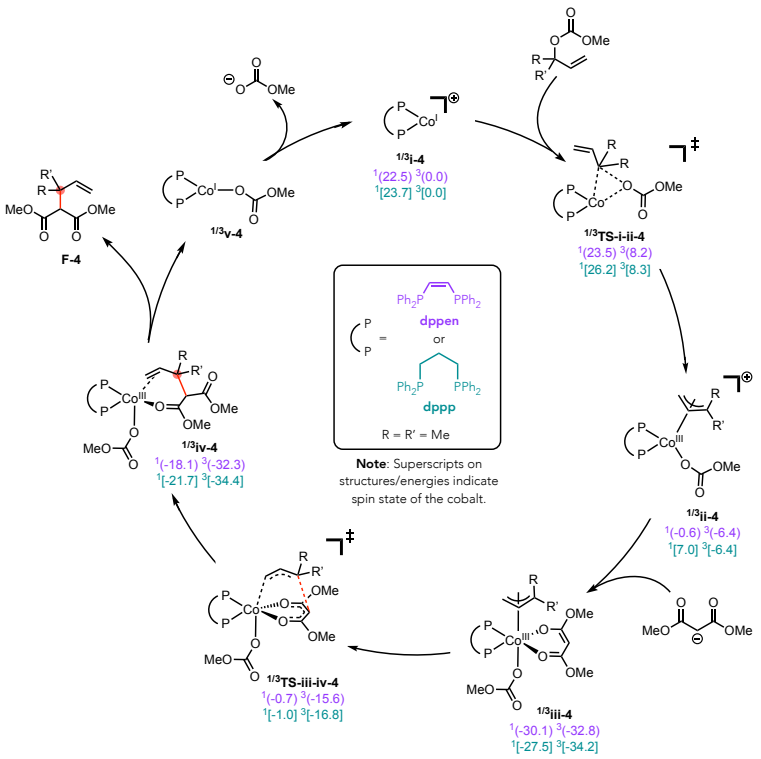



**Figure 4.8.** Proposed 2-electron reaction pathway for cobalt(I)-catalyzed allylic substitution reaction. Optimizations performed at UB3LYP-D3/def2SVP-CPCM(acetonitrile) level of theory, ΔG reported in kcal/mol. Both low and intermediate spin state energies are shown (superscript next to energies indicate spin state). Energies are reported for cobalt with **dppen** ligand, followed by for cobalt with **dppp** ligand.

I explored this pathway computationally for both **dppen** and **dppp** ligands full computational details are found in **Appendix A4.2.b**). These energetic pathways are significantly more feasible than those of the 1-electron pathway described above. In the case of both ligands, following formation of **ii-4**, coordination of the malonate is energetically favorable, and subsequent C-C bond formation is energetically feasible, although it is reversible. However, it is possible that dissociation of the product and the carbonate anion could be irreversible. Further

studies are currently being conducted on the dissociation step to determine whether it is energetically feasible. If this dissociation is not feasible, it is possible that the reaction could continue through further productive cycles with **v-4** as the catalytically active species, rather than **i-4**. Additional efforts are underway to explore an alternative 2-electron mechanism wherein the malonate undergoes ligand exchange with the carbonate following formation of **ii-4**, rather than adding to the cobalt directly. Additional investigations are underway into an enantioselective variant of this reaction to understand the origin of enantioselectivity.

### *4.6 Conclusions*

Here, we have reported two first-row transition metal-catalyzed transformations. I have employed DFT calculations to explore the mechanisms of these transformations. My calculations showed that for the nickel-catalyzed hydroarylation, the order of steps was contrary to previous reports of an analogous reaction with non-fluorinated alkenes. For the cobalt-catalyzed allylic substitution, my computations revealed that a 1-electron pathway for the reaction is likely unfeasible and that a 2-electron transfer pathway is more likely. These studies once again demonstrate the utility of DFT for mechanism elucidation in both radical and polar reactions. Further work is ongoing in each study. In the nickel-catalyzed reaction, further calculations are in progress to help us understand the effects of the fluorine and side reactions. For the cobalt-catalyzed reaction, further calculations are underway to fully study the 2-electron pathway and to understand the effects of ligands on the catalyst.

# Chapter 5: Conclusions and Future Directions

Developments in recent years of computational studies of organic transformations have provided an avenue by which mechanisms of these reactions can be more thoroughly explored and better understood. This mechanistic understanding allows for novel patterns and modes of reactivity can be predicted and developed. My graduate studies have been devoted to exploring a wide variety of organic transformations using quantum mechanical computations.

My work with nickel(I)-catalyzed olefin functionalizations (**Chapter 1**) demonstrate the ability of sterically hindered nickel(I) catalysts to guide the stereo- and regioselectivity of various transformations. My mechanistic studies of photocatalytic transformations (**Chapter 2**) revealed the importance of both radical and polar reactivity modes in photocatalysis and how these modes can be used concurrently to perform organic transformations. My work with the copper-catalyzed reductive coupling in **Chapter 3** yielded mechanistic understanding of the regio-, stereo-, and chemoselectivity of the cross-coupling. The computations I performed on the nickel and cobalt-catalyzed transformations shown in **Chapter 4** revealed how relatively small changes in the reaction system (e.g. using fluorinated alkenes or using bisphosphine ligands instead of oxazoline-phosphine ligands) can result in drastic changes to the reactivity and mechanism of the transformation. My computational results were able to not only provide mechanistic insights, but also support proposed experiments for mechanistic verification.

Each of these computational studies provide mechanistic insights that are relevant for not only these particular transformations, but for development of future organic reactions. Further development of mechanistic understanding will no doubt be accomplished through cooperation and collaboration between experimental and computational chemists. Collaborations between these previously disparate groups, including those reported in this thesis, have already

demonstrated the power that synergizing these techniques can have on expanding the scope of methodologies for construction of C-C and C-heteroatom bonds. Further developments in the accuracy and reliability of computational methods and development of computational techniques to understand dynamical behavior in reaction systems or incorporate machine learning into ligand and catalyst design are likely to help accelerate reaction discovery.

Further computational efforts are already underway to deepen our mechanistic understanding for the systems discussed herein to and apply this understanding into new reaction avenues. I expect that the rapid development of computational techniques and data-driven modeling will hasten the expansion of our understanding of these and other reactions and allow for design of novel catalytic systems. I plan to continue employing computational tools to develop mechanistic understanding of various transition metal-catalyzed and photocatalyzed organic transformations.

*And it's crazy, it seems it'll never let up/But please, you got to keep ya head up.* – Tupac Shakur

# Appendices

## Appendix 1: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 1 (Mechanistic Studies of Nickel(I)-Catalyzed Olefin Functionalization Reactions)

### A1.1 Computational Methods

*A1.1.a Computational Methods in the Study of Olefin Functionalization/Isomerization Enables Stereoselective Alkene Synthesis.*

All optimizations of intermediates and transition states were calculated using unrestricted B3LYP/def2-SVP[226,227] level of the theory, with dispersion correction ("empiricaldispersion=gd3" keyword[228]) in implicit solvent (toluene) using CPCM as the solvation model[229] with the "guess=mix" keyword and with a Fine grid size, as implemented in Gaussian16.[230] Frequency calculations, at the same level of theory, were used to obtain thermal corrections (at 298K) and to characterize optimized structures as transition states (if only a single imaginary frequency was found) or intermediates (if no imaginary frequencies were found). Single point energy calculations in implicit solvent using UM06-L/def2-TZVPP[184] and PBE0-D3/def2-TZVPP[231] with an ultrafine grid size were also performed to compare energetics. All 3-D structures were generated using CYLview 1.0.[185] Exhaustive conformational searches were performed for all structures to elucidate the lowest energy profiles for each potential reaction pathway.

*A1.1.b Computational Methods in the Study of Directing-Group-Free Catalytic Dicarbofunctionalization of Unactivated Alkenes.*

All optimizations of intermediates and transition states were calculated using unrestricted B3LYP/def2-SVP[226,227] level of theory, with dispersion correction (using the "empiricaldispersion=gd3" keyword[228]) in implicit solvent (toluene) using CPCM as the solvation model[229] with the "guess=mix" and "nosymm" keywords as implemented in Gaussian16 Revision C.01.[230] Frequency calculations (at the same level of theory) were used to obtain thermal

corrections (at 298K) and to characterize all optimized structures as either transition states (containing only one imaginary frequency) or intermediates (containing no imaginary frequencies). To refine energetics and for method comparison, single point energy calculations were performed in implicit solvent (CPCM(toluene)) using UM06-L/def2-TZVPP[184] and PBE0-D3/def2-TZVPP[231] levels of theory. All 3-D structures were generated using CYLview.[185] Non-Covalent Interaction (NCI) Analysis[232] was performed using the Multiwfn software[189] using checkpoint files generated from the frequency calculations described above and the results of this NCI analysis were visualized using VMD software.[190] Exhaustive conformational searches were performed for all structures to elucidate the lowest energy profiles for each potential reaction pathway.

## A1.2 Supplementary Figures

### *A1.2.a Supplementary Figures in the Study of Olefin Functionalization/Isomerization Enables Stereoselective Alkene Synthesis.*

As discussed in the manuscript, the energy differences between *(E)* and *(Z)* isomers of tri- and tetrasubstituted alkenes can be extremely small and therefore rule against thermodynamic control. Consider the examples shown in **Figure A1.2.a1** below. In such cases as this, the inappreciable energy difference makes selectivity for one isomer difficult to achieve.

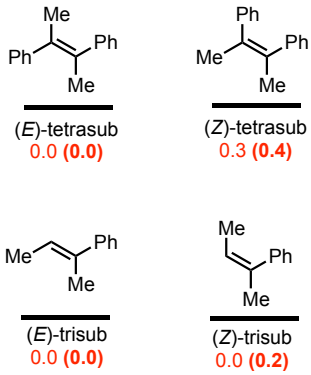



**Figure A1.2.a1.** Examples of energy differences between *(E)* and *(Z)* isomers of tri- and tetrasubstituted alkenes. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔH (ΔG; in parenthesis) reported in kcal/mol.

Preliminary experimental evidence suggested that the reaction of interest was unlikely to proceed via a Ni(0)/Ni(II) pathway. In order to computationally determine which path was more likely, we compared the energy for the disproportionation of the Ni(I) dimer (**Ni-1**) to form a Ni(0) and a Ni(II) species with cleavage of the dimer to form 2 equivalents of the Ni(I) species **Cat**. These results can be seen in **Figure A1.2.a2** below. This comparison suggests that disproportionation to a Ni(0) and Ni(II) species is completely unfeasible as the energy barrier is in excess of 75 kcal/mol. However, cleavage to form the Ni(I) **Cat** species is energetically feasible with a significantly lower barrier of 19.5 kcal/mol.

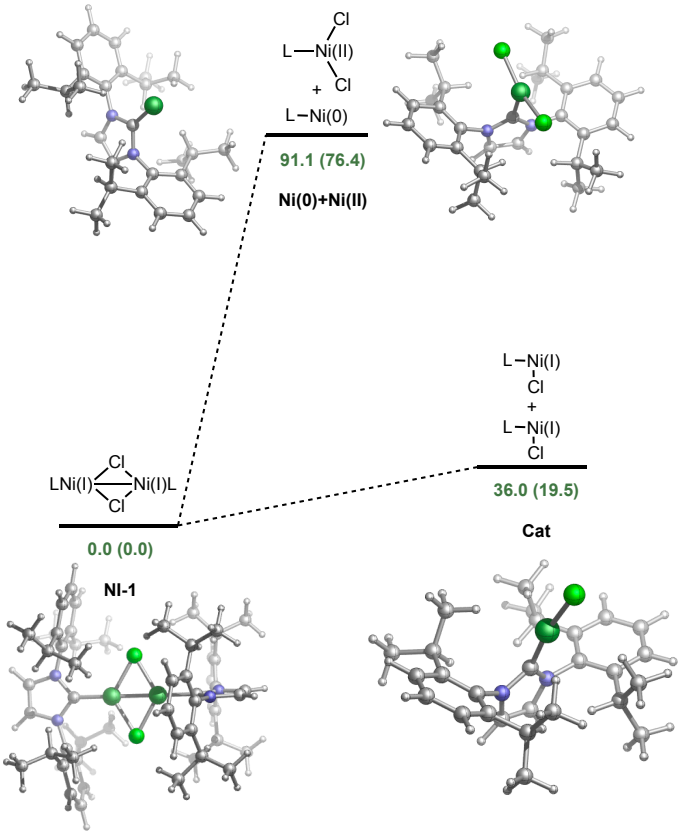



**Figure A1.2.a2**. Potential energy surface for options to cleave Ni(I) dimer **Ni-1**. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, $H_{rel}$ ($G_{rel}$; in parenthesis) reported in kcal/mol.

To further support the claim of a Ni(I)-catalyzed mechanistic pathway, we also computationally investigated the Ni(0)/Ni(II) Heck reactivity profile, which can be seen in **Figure A1.2.a3** below.

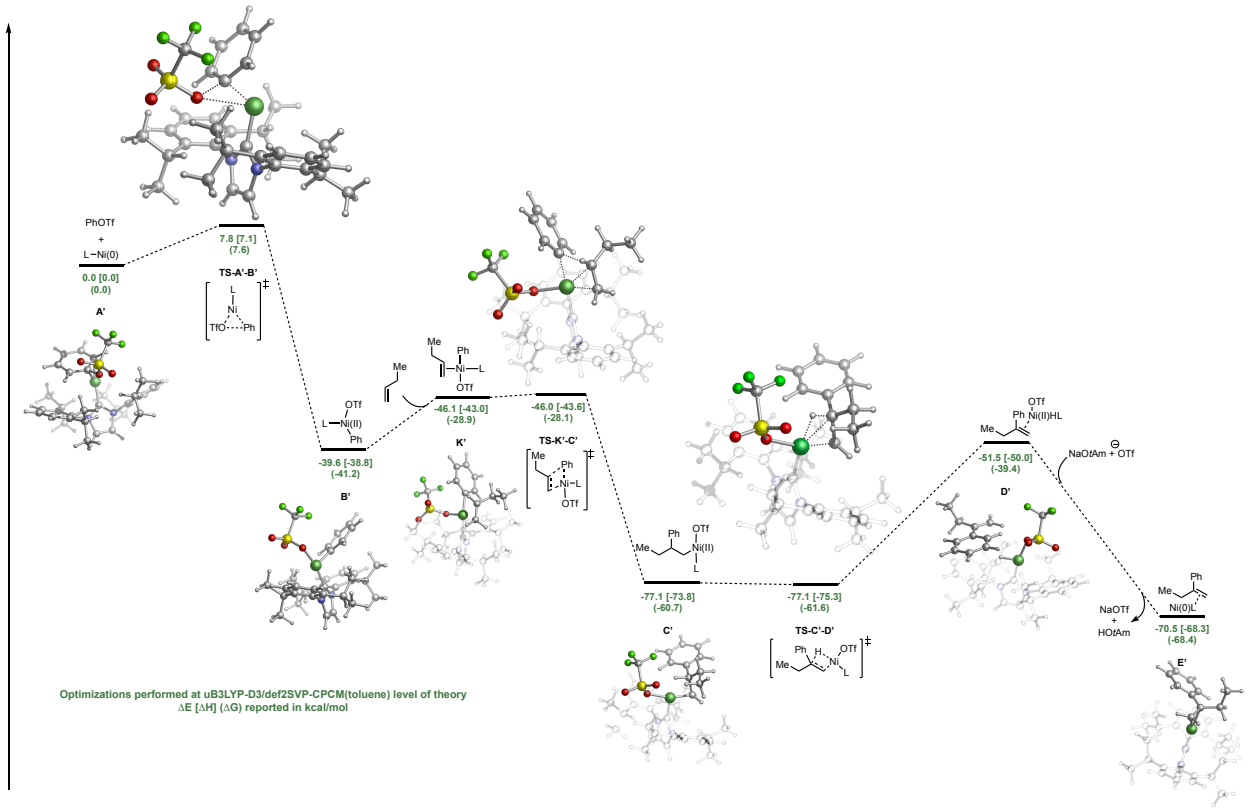



**Figure A1.2.a3.** Potential energy surface for Ni(0)-catalyzed Mizoroki-Heck reaction. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔE [ΔH; in brackets] (ΔG; in parenthesis) reported in kcal/mol.

Most of the barriers for the Ni(0)-catalyzed Heck reaction are fairly low, suggesting that this rection should be able to proceed readily at room temperature. The experimental observation of the need for higher reaction temperatures to complete this reaction using the Ni(I) dimer suggests that this pathway would not predominate.

As such, a Ni(I)-catalyzed pathway was proposed to explain both the Mizoroki-Heck-like reaction (to couple the Ph-OTf with the initial alkene) as well as the chain-walking isomerization. Additionally, the observed superiority in efficiency and selectivity with the Ni(I) dimer **Ni-1** compared to Ni(0) and Ni(II) complexes intimated that a different catalytically active species should be considered for this reaction.

Details of the computations for the Ni(I)-catalyzed Mizoroki-Heck like reaction can be seen below in **Figure A1.2.a4**.

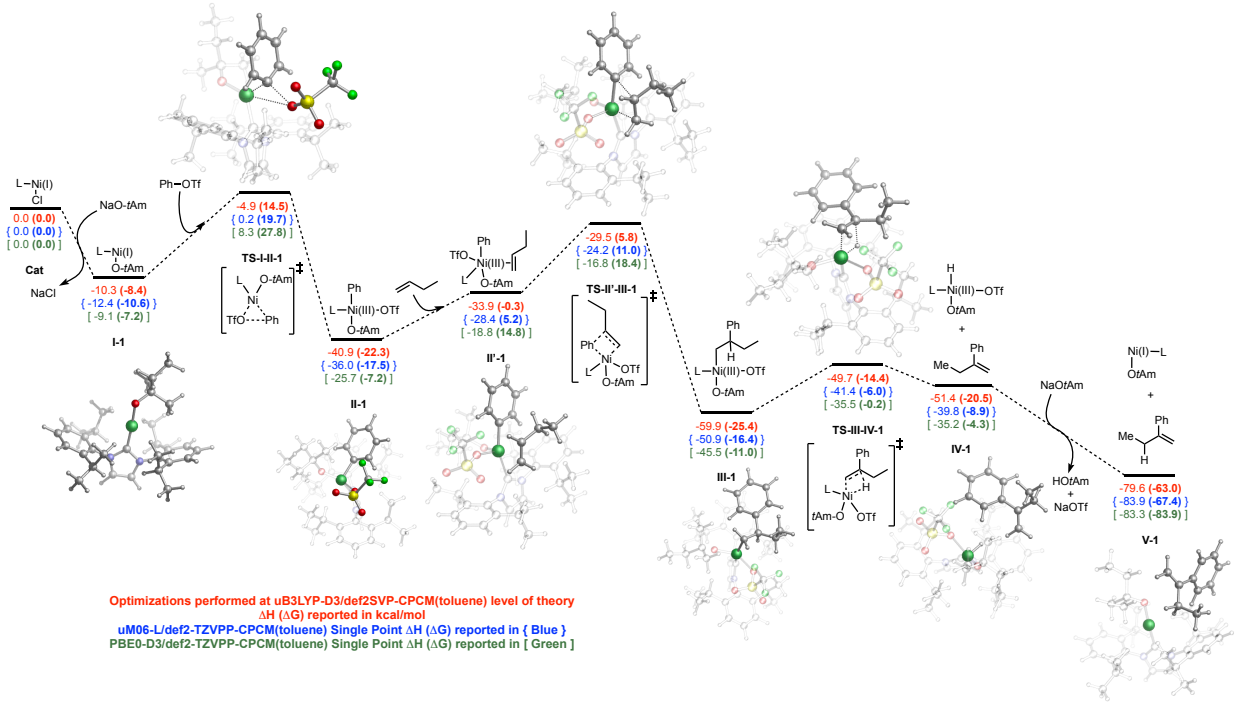



**Figure A1.2.a4.** Downhill potential energy surface leading from initial Cl-Ni(I)-IPr catalyst (**Cat**) to key chain-walking intermediate (**V**). Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔH (ΔG; in parenthesis) reported in kcal/mol. Single point enthalpies and free energies are also shown.

Notably, from these calculations, it is clear that if the precatalyst "**Cat**" can be formed from the initial Ni(I) dimer (**Ni-1**), then the formation of the catalytically active species **I-1** can be readily achieved. This species can then readily perform the Mizoroki-Heck like reaction to couple the Ph from the PhOTf to the initial unsubstituted alkene to form a disubstituted alkene. In this process, the catalytically active **I-1** can be reformed so that it can perform a "Chain-Walking" isomerization (detailed in **Figure A1.2.a5** below). All transition states are reasonable at the temperature that the reaction is performed (80 ºC). This process is thermodynamically favorable (ΔH = -79.6 kcal/mol, ΔG = -63.0 kcal/mol) and irreversible beyond the alkene insertion step (**TS-II'-III-1**).

We also performed DFT calculations to determine the energetics of a potential Ni(0)/Ni(II) pathway for the isomerization from terminal to internal alkene. These results are summarized in the energy diagram shown in **Figure A1.2.a5** below.

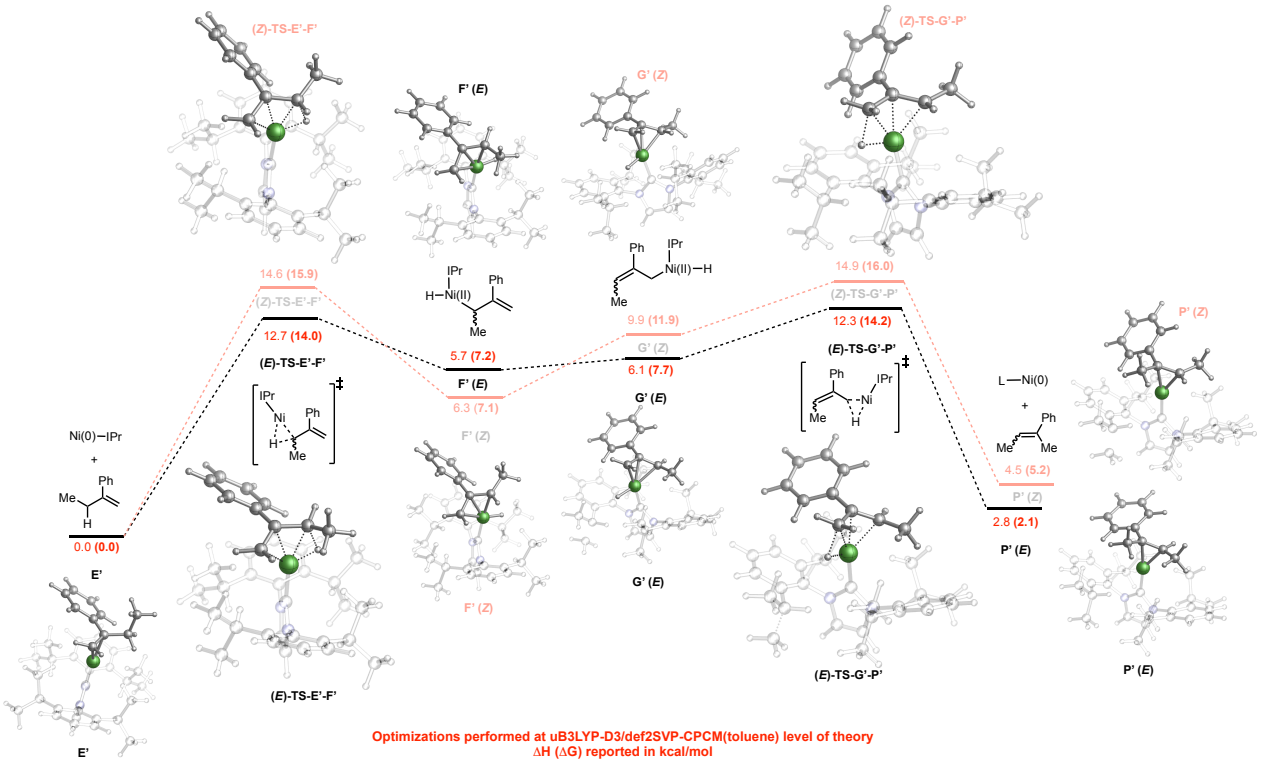



**Figure A1.2.a5.** Potential energy surface for Ni(0)-catalyzed "Chain-walking" showing isomerization from unsubstituted to tri-substituted alkene. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔH (ΔG; in parenthesis) reported in kcal/mol.

There are a few notable observations from these results. In this Ni(0)/Ni(II) pathway, the highest energy barrier is ~16 kcal/mol. This suggests that the isomerization should proceed readily at room temperature. If the Ni(0) species is being formed *in situ*, then the isomerization should occur readily at room temperature. However, experimental evidence shows that the reaction conditions require elevated temperature in order to perform the tandem Mizoroki-Heck/isomerization detailed in this manuscript. This suggests that it is unlikely that the Ni(0) species is the predominant pathway by which the isomerization occurs.

Additionally, the isomerization should be easily reversible, as the barrier back from the products is low (~ 12 kcal/mol). As such, since the products can easily revert to the unsubstituted alkene and isomerize to the alternative stereochemistry, *one would expect the distribution of the products to align with the relative thermodynamic stability* of the products. The difference in energy between the products is ~0.3 kcal/mol (using the optimization methods shown above), which should correspond to an E:Z product ratio of ~1.5:1. However, the observed selectivity of the reaction is significantly higher than this. This would suggest that the Ni(0)/Ni(II) pathway should not be the predominant pathway for the isomerization.

On the other hand, the Ni(I)/Ni(III) pathway (seen in **Figure A1.2.a6** below) seems to be more in line with experimental observations. There are many features of this isomerization pathway that are notable and relevant for the selectivity of this reaction. Firstly, it is clear that the difference in enthalpy and energy between the (*E*) and (*Z*) products ($\Delta H$ = 0.2 kcal/mol, $\Delta G$ = 0.3 kcal/mol) is not sufficient to explain the observed (*E*) selectivity of this reaction (which ranges from 83% to >98% (*E*) selectivity). Additionally, the isomerization barrier is significantly higher (33.4 kcal/mol) and is not easily reversible. As such, *the selectivity should align more with a kinetic pathway*, where the heights of the transition state barriers is the major controlling factor. the difference in energy between the reductive elimination transition states (**TS-VII-B-1**) is also too small to justify the (*E*) selectivity. Overall, these calculations are more consistent with **TS-V-VI-1** as the selectivity determining transition state. The difference in energy between (*E*) and (*Z*) transition states (4.8 kcal/mol) is more in line with observed preference for (*E*) over (*Z*) products, suggesting that this pathway may be the predominant pathway.

While the Ni(0)/Ni(II) pathway cannot be fully ruled out, these computational data suggest that the Ni(I)/Ni(III) pathway is more in accordance with the observed experimental results.

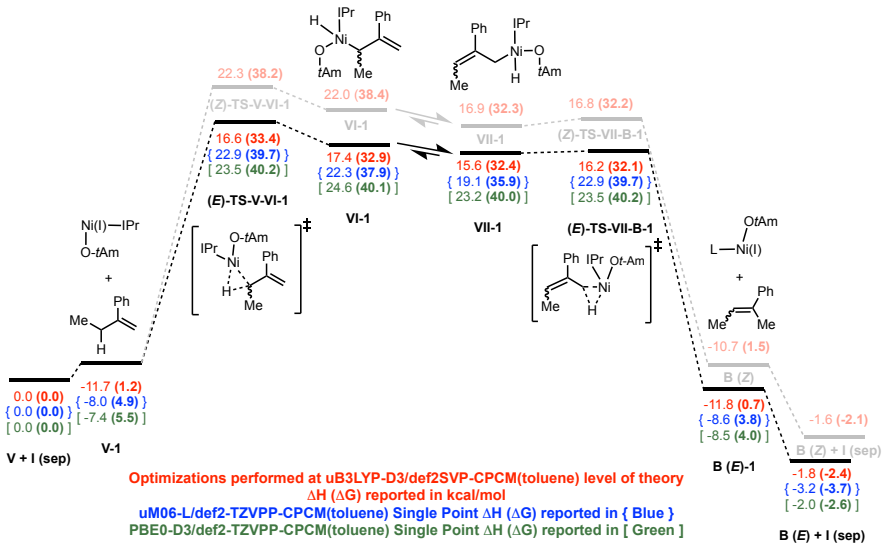



**Figure A1.2.a6** Potential energy surface for inner-sphere "Chain-walking" showing isomerization from unsubstituted to tri-substituted alkene. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔH (ΔG; in parenthesis) reported in kcal/mol. Single point enthalpy and energy calculations are also presented.

This Ni(I)-catalyzed chain-walking mechanism, while superficially similar to that recently detailed by Schoenebeck et al.,[15] appears to be operating under a different pathway than the radical pathway Schoenebeck et al. propose. The evidence for this conclusion can be seen in **Figure A1.2.a7** below. Spin densities and charges do not seem to be changing over the course of the chain-walking. This would seem to imply that the nickel is remaining Ni(I) throughout the reaction, suggesting that no radical on the nickel is formed during the chain-walking. Additionally, based on the bond lengths (labeled in **Figure A1.2.a7**), the nickel seems to be σ-bound to the carbon(s) in all intermediates in the chain-walking pathway. Schoenebeck argues for the formation of a nickel π-allyl complex followed by an H-atom abstraction to create a π-bound nickel, followed by H-atom addition to form the migration product. At no point during Schoenebeck's mechanism is the nickel σ-bound to the alkene. This suggests that the mechanism detailed here is different from that of Schoenebeck. In the mechanism detailed here, there is not enough space for the nickel to be π-bound due to steric hindrance from the O*t*-Am and IPr. This steric hindrance from the O*t*-Am

seems to be the key to differentiating this mechanism as observed experimentally. Non-covalent interaction (NCI) analysis on the transition states shows significantly more interactions between the O*t*-Am and IPr ligands in both (*E*) and (*Z*) isomers of **TS-V-VI-1** (See **Figure A1.2.a8**). The chlorine atom in Schoenebeck's catalyst is not hindering at all, so the π-complex can form readily. Additionally, experimental evidence using radical clocks suggests that a radical pathway is not the major pathway for this reaction. Based on the experimental and computational evidence, it seems clear that the mechanism of the transformation detailed in this report is fundamentally different from the "radical relocation" chain-walking proposed by Schoenebeck.

As seen in the structures of **VI-1** and **VII-1** in **Figure A1.2.a7**, the Ni−H bond length is relatively small (1.45 - 1.49 Å), indicating that this C−H migration and insertion takes place in an inner-sphere manner. Additionally, the Ni−C bond length for these structures does not change drastically (2.00 - 2.04 Å), indicating that the allyl system remains σ-bound to the nickel through the isomerization and is likely not dissociating during isomerization. Without the dissociation, this isomerization and insertion should be occurring via an inner-sphere mechanism. These computations suggest that 1,3-H shift is inner-sphere and proceeds via a stepwise C–H migration and insertion via discrete Ni-σ intermediates

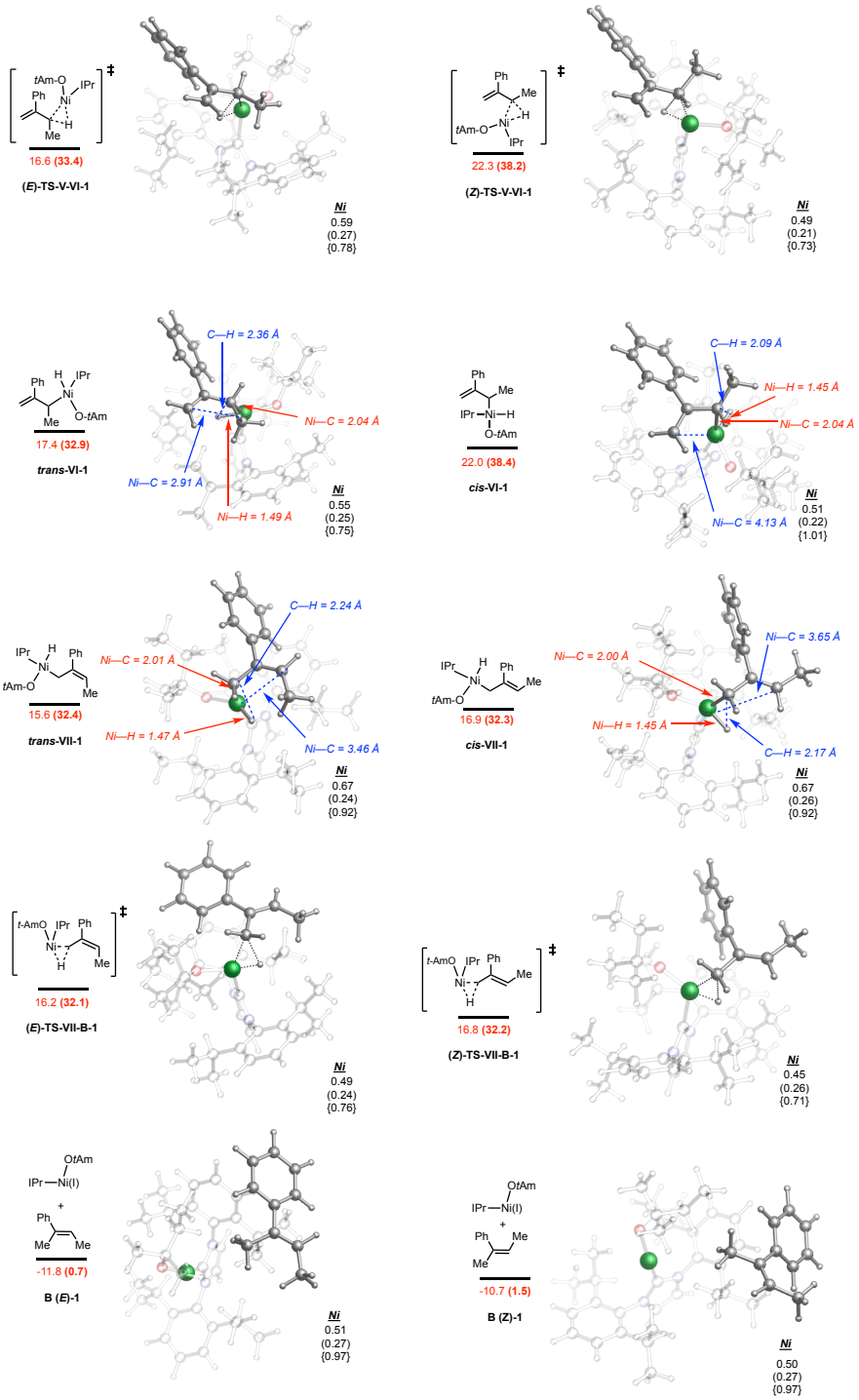



**Figure A1.2.a7.** Progress of inner-sphere chain-walking isomerization mechanism. Charges and spin density on Nickel shown: APT charge (Mulliken Charge in parentheses) {Spin Density in brackets}. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔH (ΔG; in parenthesis) reported in kcal/mol.

While it is clear that **TS-V-VI-1** is the stereodetermining step, it is not clear what the source of the difference in energy between the (*E*) and (*Z*) isomers is. In order to elucidate this source, non-covalent interaction (NCI) analysis[270] was performed on both transition states using the Multfiwfn software[189], the results of which are shown in **Figure A1.2.a8** (visualized using VMD software[190]). It can be seen (green interactions inside the red circles) that there are significantly more interactions between the O*t*-Am and the IPr ligand in the (*Z*) isomer than in the (*E*) isomer. The O*t*-Am being pushed downwards by the methyl on the alkene forcing it closer to the IPr likely causes these interactions to be more pronounced in the (*Z*) isomer. This suggests that one potential cause for the stereoselectivity being introduced in this step is due to the interactions between the O*t*-Am and the IPr ligand.

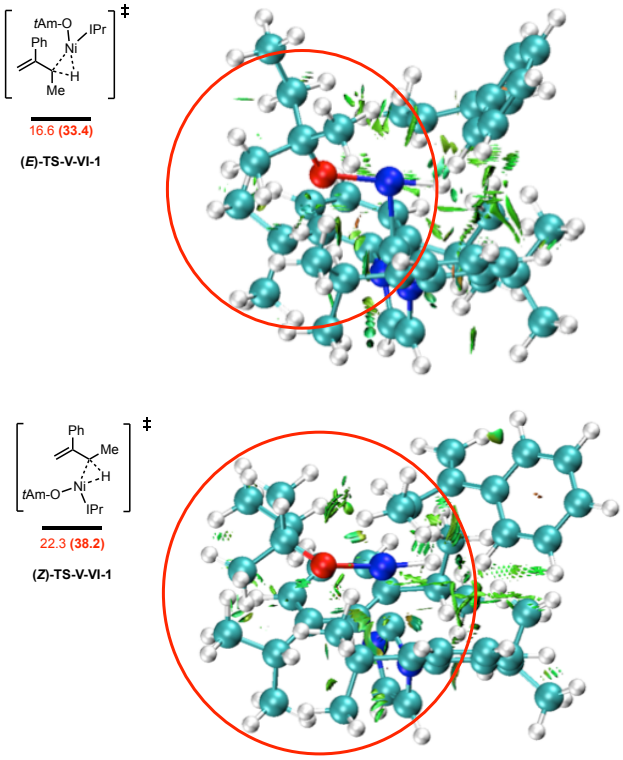



**Figure A1.2.a8.** Non-covalent interaction (NCI) analysis of stereodetermining transition state (**TS-V-VI**) isomers. Interactions can be seen as green patches between atoms.

In order to account for the observed energy difference between (*E*) and (*Z*) isomers of **TS-V-VI-1**, distortion/interaction-activation strain analysis was performed.[188] The results of this analysis are detailed in **Figure A1.2.a9** below. Both (*E*) and (*Z*) systems have similar distortion energies, meaning it is equally difficult to distort the geometries required for both transition states. However, the (*E*) system has significantly larger interaction stabilization than the (*Z*) system (79.8 kcal/mol vs. 73.5 kcal/mol). As such, if the system can accommodate the energy required to distort the geometries of the starting materials, the interactions for the (*E*) transition state help lower the energy of this system significantly more than the (*Z*). This favorable interaction energy encourages the reaction to yield the (*E*) isomer of **VI-1**, which can then readily proceed downhill in energy to the (*E*) product **B-1**.

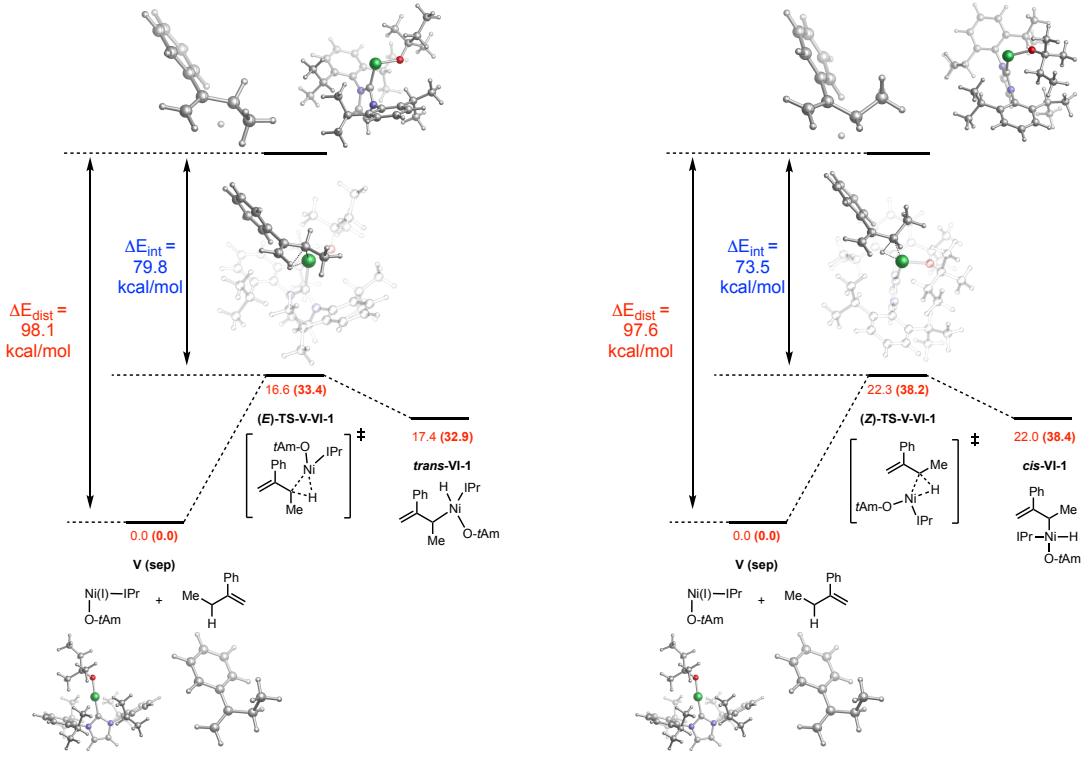



**Figure A1.2.a9:** Distortion-Interaction analysis for the stereodetermining steps: **(*E*)-** and **(*Z*)-TS-V-VI**. Energies calculated using uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory.

*A1.2.b Supplementary Figures in the Study of Directing-Group-Free Catalytic Dicarbofunctionalization of Unactivated Alkenes.*

Preliminary experimental evidence (discussed in the manuscript) suggested that the catalytically active species in this reaction is a Ni(I) species. As such, in accordance with Schoenebeck et al.'s previous work with the **Ni-1** dimer,[15] we propose that the reaction is catalyzed by the Ni(I)-chloro species **i-1** seen in **Figure A1.2.b1** below. The dissociation of the dimeric **Ni-1** into the catalytically active **i-1** is energetically feasible with the experimental conditions described in this manuscript.

The energetics of the pathway from Ni(I)-chloro species (**i-1**) to product **H16-1** are outlined in **Figure A1.2.b1** below. Oxidative addition via **TS-i-ii-1** ($\Delta G^{\ddagger}$ = +24.7 kcal/mol) will lead to Ni(III) species **ii-1**. In turn, this species can then coordinate to the alkene and undergo branched-selective migratory insertion (via **TS-A-1**, $\Delta G^{\ddagger}$ = +15.8 kcal/mol) to form alkyl nickel species **iii**. Finally, this species will undergo irreversible transmetalation with the Grignard reagent (not calculated) to form the biarylnickel species **iv**. Reductive elimination (**TS-iv-H16-1**, $\Delta G^{\ddagger}$ = +1.8 kcal/mol) can swiftly follow, irreversibly forming the product **H16-1**. Notably, all steps in this process are energetically feasible and irreversible beyond the transmetalation.

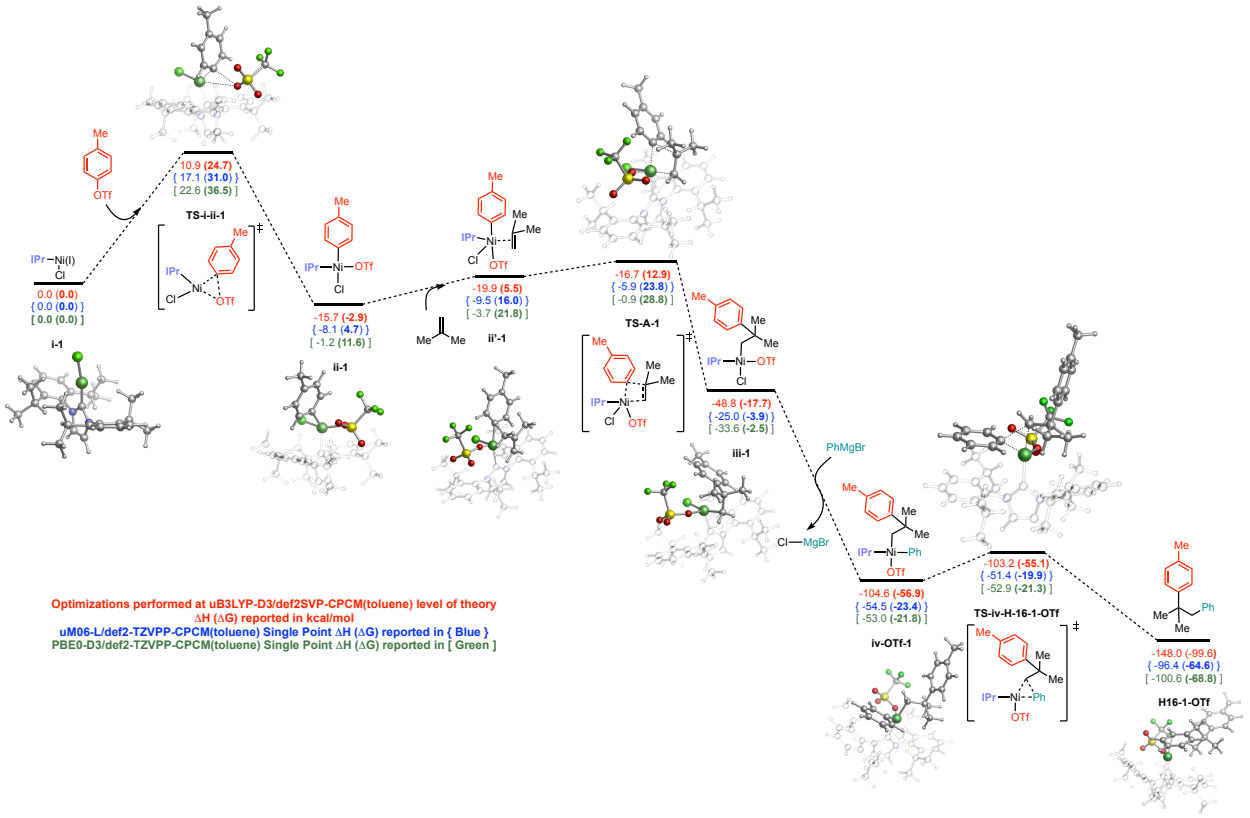



**Figure A1.2.b1.** Reaction coordinate leading to the desired product. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, $H_{rel}$ ($G_{rel}$; in parenthesis) reported in kcal/mol.

Following our investigation into the energetics of the mechanism, we were interested in the origin of the regioselectivity of the difunctionalization. Namely, we sought to compare the transition states for the favorable branched-selective (**TS-A-branched-1**) vs. the disfavorable linear-selective (**TS-A'-linear-1**) carbonickelation and to understand the origin of the large difference in energy between these two transition states. The details of this investigation are shown in **Figure A1.2.b2** below.

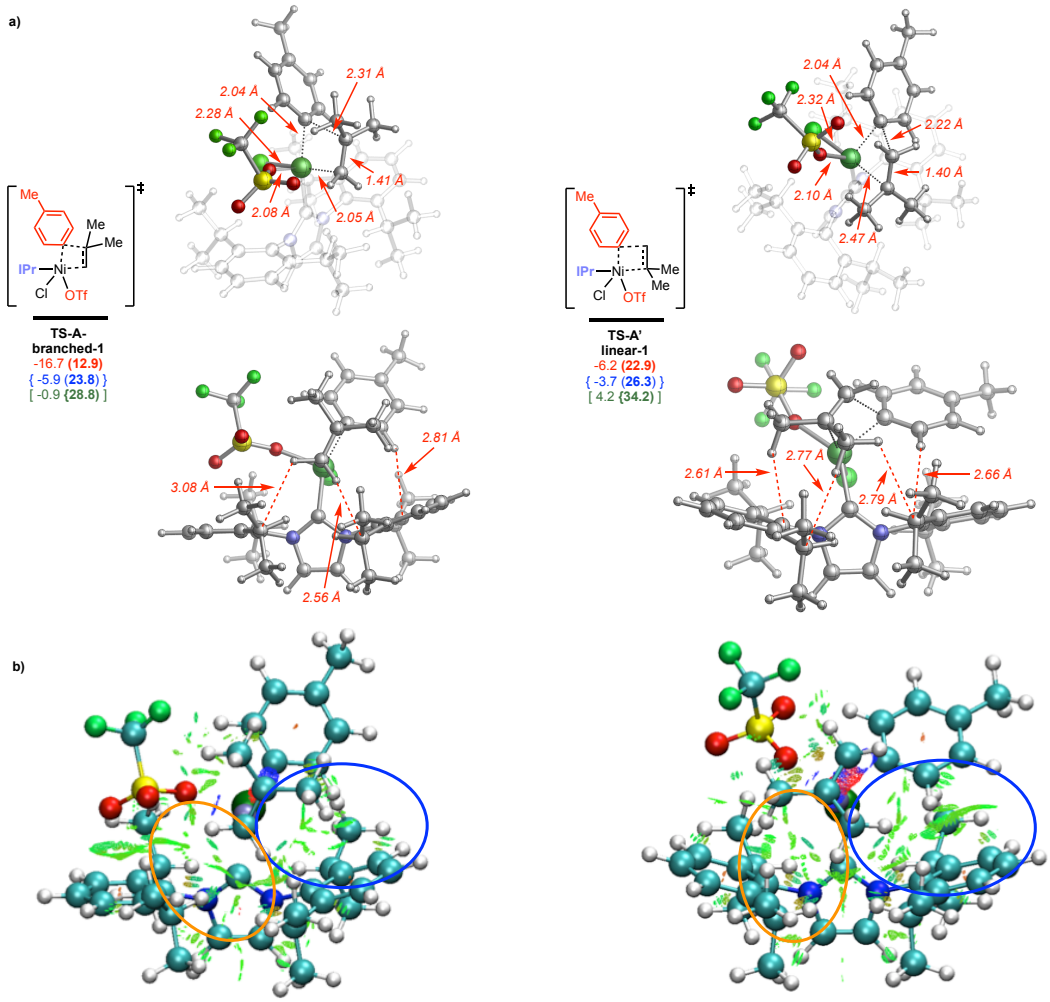



**Figure A1.2.b2.** a) Structures and energies of regioselective transition states for branched and linear carbonickelation. Side-on and front-on views are presented. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, $H_{rel}$ ($G_{rel}$; in parenthesis) reported in kcal/mol. b) NCI analysis of transition state structures for branched and linear carbonickelation. Non-covalent interactions labeled in orange (left) and blue (right) circles.

From these results, the structure of the linear-selective transition state can be seen to be highly distorted from the geometry of the branched-selective transition state (**Figure A1.2.b2a**). The distances between the ligand and the alkene are shorter in the linear-selective transition state, which is likely causing steric hindrance. Additionally, the distance between the aryl group and the ligand is shorter in the linear-selective transition state, further contributing to steric hindrance in this transition state. The geometry of the linear-selective transition state appears to have distorted to accommodate for the methyl groups on the alkene being pushed as far from the ligand as

possible as well as the aryl group being pushed away from the ligand. NCI analysis[232] (**Figure A1.2.b2b**) further supports that this distortion of geometry is likely a result of steric hindrance from the ligand. As seen in the blue and orange circles, there are more non-covalent interactions between the alkene and the ligand as well as between the aryl group and the ligand. These results suggest that steric effects between the ligand and the alkene and aryl groups are the major controlling factor affecting the regioselectivity of this reaction as the ligand is causing steric strain in the linear-selective transition state from being forced closer to the alkene and aryl group.

We also compared the energetics of the transmetalation to determine whether the chloride or the triflate would be more likely to undergo transmetalation. These results are summarized in **Figure A1.2.b3** below. While the energetics of these two alternatives are similar, the transmetalation of the chloride is slightly energetically favored ($\Delta\Delta G$ = 4.8 kcal/mol). As such, we used the nickel triflate version of species **iv-1** to undergo reductive elimination (via **TS-iv-H16-1-OTf**) to form product **H16-1-OTf**.

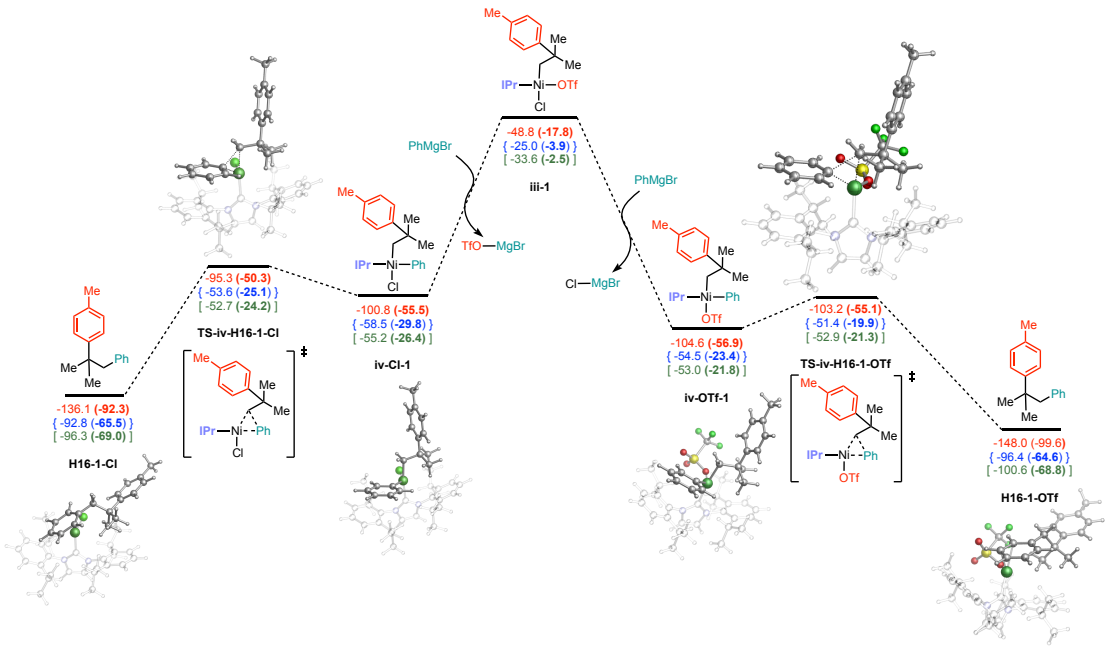



**Figure A1.2.b3.** Comparison of transmetalation of intermediate **iii-1** for exchange of either triflate or chloride. Optimizations performed at uB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, $H_{rel}$ ($G_{rel}$; in parenthesis) reported in kcal/mol.

## A1.3 Coordinates & Energies

### *A1.3.a Coordinates & Energies in the Study of Olefin Functionalization/Isomerization Enables Stereoselective Alkene Synthesis.*

**Ni-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 1.147844 (Hartree/Particle)
Thermal correction to Energy= 1.215398
Thermal correction to Enthalpy= 1.216342
Thermal correction to Gibbs Free Energy= 1.044471
Sum of electronic and zero-point Energies= -6254.234955
Sum of electronic and thermal Energies= -6254.167401
Sum of electronic and thermal Enthalpies= -6254.166457
Sum of electronic and thermal Free Energies= -6254.338328

| | | | |
|---|---|---|---|
| Ni | 1.19214300 | -0.54612400 | 0.18031500 |
| Ni | -1.33659400 | -0.22167800 | 0.82235700 |
| Cl | -0.23853500 | -2.32640800 | 0.49305500 |
| C | 2.97834700 | 0.08030800 | -0.04861000 |
| C | 4.95271100 | 1.21327500 | -0.20555600 |
| C | 5.20871500 | 0.05115500 | 0.45061500 |
| C | -3.10455000 | -0.14908400 | 0.13115800 |
| C | -5.17948700 | -0.56370800 | -0.72123000 |
| C | -5.10839300 | 0.77121400 | -0.46630700 |
| N | 3.99730600 | -0.62355100 | 0.53116900 |
| N | 3.58884300 | 1.21831200 | -0.49421700 |
| N | -3.84029900 | 1.00215100 | 0.05271500 |
| N | -3.95176200 | -1.10354600 | -0.35090000 |
| H | 6.12906800 | -0.35876800 | 0.85584400 |
| H | 5.60855500 | 2.02350700 | -0.50777200 |
| H | -5.83252800 | 1.56904500 | -0.60272300 |
| H | -5.97832400 | -1.17566900 | -1.12982900 |
| C | 3.82252100 | -1.91988600 | 1.12961900 |
| C | 4.07728400 | -3.06011700 | 0.33985900 |
| C | 3.39571900 | -2.00454400 | 2.47034900 |
| C | 3.96000600 | -4.31516500 | 0.95263800 |
| C | 3.30355300 | -3.28269200 | 3.03923400 |
| C | 3.59527700 | -4.42520700 | 2.29480400 |
| H | 4.14165500 | -5.22018000 | 0.36976300 |
| H | 2.98470800 | -3.38532500 | 4.07830500 |
| H | 3.51484400 | -5.41214100 | 2.75773800 |
| C | 2.95937900 | 2.26577600 | -1.25316700 |
| C | 2.57699300 | 3.45622100 | -0.59876700 |
| C | 2.80472100 | 2.07881900 | -2.64322700 |
| C | 2.05617100 | 4.48977100 | -1.39183600 |
| C | 2.27015400 | 3.13991500 | -3.38734700 |
| C | 1.91139700 | 4.33820600 | -2.77101900 |
| H | 1.75294700 | 5.42670100 | -0.92167900 |
| H | 2.12697200 | 3.02561900 | -4.46348000 |
| H | 1.49902100 | 5.15566200 | -3.36807800 |
| C | -3.31593300 | 2.27934100 | 0.45371400 |
| C | -3.53251400 | 2.71418400 | 1.77755200 |
| C | -2.55566100 | 3.01778100 | -0.47534400 |
| C | -2.97123800 | 3.94139800 | 2.15675400 |
| C | -2.01081500 | 4.23569200 | -0.04480500 |
| C | -2.22040700 | 4.69599600 | 1.25450200 |
| H | -3.10722100 | 4.30463800 | 3.17722000 |
| H | -1.39465800 | 4.82042600 | -0.73072100 |
| H | -1.77865900 | 5.64337300 | 1.57335300 |
| C | -3.58552600 | -2.48527600 | -0.49786000 |
| C | -3.00311300 | -2.89687300 | -1.71211700 |
| C | -3.78068700 | -3.35666000 | 0.59062000 |
| C | -2.62010800 | -4.24015900 | -1.82262900 |
| C | -3.38056300 | -4.69038300 | 0.43015100 |
| C | -2.80915700 | -5.12871200 | -0.76442300 |
| H | -2.15114400 | -4.59293600 | -2.74348600 |
| H | -3.50341600 | -5.39374700 | 1.25619700 |
| H | -2.49657900 | -6.17119400 | -0.86699500 |
| C | 4.33532700 | -2.94532200 | -1.15707100 |
| H | 4.67146500 | -1.91918200 | -1.36844300 |
| C | 3.00863500 | -3.15552900 | -1.91155200 |
| H | 3.15070600 | -3.02737100 | -2.99659300 |
| H | 2.61552900 | -4.16912300 | -1.73064500 |
| H | 2.24551300 | -2.43895600 | -1.57448800 |
| C | 5.42909100 | -3.89269700 | -1.66745300 |
| H | 5.13075500 | -4.94997200 | -1.58308200 |
| H | 5.63272000 | -3.69719700 | -2.73243400 |
| H | 6.36908300 | -3.76042700 | -1.10858200 |
| C | 3.14356300 | 0.75260100 | -3.31403500 |
| H | 3.81124300 | 0.19453000 | -2.64085000 |
| C | 3.88683000 | 0.91897000 | -4.64679700 |
| H | 3.24966700 | 1.37582300 | -5.42092600 |
| H | 4.78471100 | 1.54679500 | -4.53274100 |
| H | 4.20243500 | -0.06586100 | -5.02681500 |
| C | 1.86488600 | -0.08488600 | -3.48287000 |
| H | 1.38706600 | -0.26524200 | -2.50856900 |
| H | 1.14140100 | 0.43551400 | -4.13026600 |
| H | 2.09157300 | -1.06057500 | -3.93917200 |
| C | 2.74007000 | 3.63560700 | 0.90616400 |
| H | 2.76061900 | 2.62955400 | 1.35029300 |
| C | 4.06610400 | 4.34495000 | 1.23801600 |
| H | 4.93781100 | 3.79658400 | 0.85256400 |
| H | 4.08452700 | 5.35691400 | 0.80015100 |
| H | 4.18662300 | 4.44486100 | 2.32905700 |
| C | 1.55975500 | 4.38111000 | 1.54608300 |
| H | 0.60283100 | 3.91732300 | 1.27381700 |
| H | 1.64925400 | 4.34619100 | 2.64347700 |
| H | 1.53725300 | 5.44410900 | 1.25427200 |
| C | 3.00857300 | -0.76842800 | 3.27111500 |
| H | 2.86183700 | 0.05549200 | 2.56004700 |
| C | 4.12527100 | -0.36321500 | 4.24633200 |
| H | 3.84599200 | 0.54953600 | 4.79764900 |
| H | 4.31565300 | -1.16076600 | 4.98408000 |
| H | 5.06959700 | -0.16435300 | 3.71424000 |
| C | 1.65965000 | -0.95428200 | 3.98268600 |
| H | 1.33588100 | -0.00038700 | 4.42596600 |
| H | 0.88870100 | -1.25952600 | 3.26024000 |
| H | 1.71544500 | -1.70389100 | 4.78881100 |
| C | -2.25583600 | 2.49216700 | -1.87274400 |
| H | -2.91696900 | 1.63307800 | -2.06106600 |
| C | -2.53792000 | 3.53317300 | -2.96709500 |
| H | -3.56987400 | 3.91465400 | -2.90797700 |
| H | -1.85308200 | 4.39352000 | -2.89662800 |
| H | -2.39425300 | 3.08346900 | -3.96280300 |
| C | -0.80764800 | 1.98511800 | -1.94755000 |
| H | -0.62825700 | 1.18219100 | -1.21944300 |
| H | -0.58400200 | 1.59644600 | -2.95110800 |
| H | -0.09401600 | 2.79017600 | -1.72649200 |
| C | -4.25608600 | 1.83774300 | 2.79308700 |
| H | -4.84428300 | 1.09237700 | 2.23647900 |
| C | -5.23672900 | 2.61880800 | 3.67857400 |
| H | -5.80496800 | 1.92401200 | 4.31741000 |
| H | -4.71505200 | 3.32153700 | 4.34794400 |
| H | -5.95530100 | 3.19576300 | 3.07490800 |
| C | -3.22588000 | 1.06511300 | 3.63664200 |
| H | -3.72815300 | 0.37941000 | 4.33790500 |
| H | -2.56167400 | 0.47556400 | 2.98801500 |
| H | -2.59552000 | 1.75881400 | 4.21638800 |
| C | -4.32171900 | -2.85961300 | 1.92580800 |

| | | | |
|---|---|---|---|
| H | -4.80018200 | -1.88350000 | 1.75228300 |
| C | -5.38872600 | -3.78728200 | 2.52423600 |
| H | -4.96868900 | -4.76458400 | 2.81165200 |
| H | -5.81596900 | -3.33677300 | 3.43459600 |
| H | -6.21061500 | -3.96853400 | 1.81324400 |
| C | -3.15930200 | -2.62637100 | 2.90723800 |
| H | -2.61811700 | -3.56605800 | 3.10408600 |
| H | -2.44042600 | -1.91012600 | 2.48532600 |
| H | -3.53047700 | -2.22888300 | 3.86566000 |
| C | -2.72069300 | -1.91153200 | -2.83958600 |
| H | -3.31207200 | -1.00310800 | -2.65005600 |
| C | -3.14515900 | -2.44505500 | -4.21582100 |
| H | -4.20168800 | -2.75763200 | -4.21996200 |
| H | -3.01545800 | -1.66401800 | -4.98229200 |
| H | -2.53594200 | -3.30938600 | -4.52589000 |
| C | -1.24085400 | -1.49303100 | -2.83153100 |
| H | -0.95693500 | -1.04550900 | -1.87053800 |
| H | -0.58479400 | -2.36373100 | -2.99301500 |
| H | -1.04473800 | -0.76237500 | -3.63123800 |
| Cl | 0.28821400 | 1.18203700 | 1.64137400 |

**Cat**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.573147 (Hartree/Particle)
Thermal correction to Energy= 0.606193
Thermal correction to Enthalpy= 0.607137
Thermal correction to Gibbs Free Energy= 0.508016
Sum of electronic and zero-point Energies= -3127.088497
Sum of electronic and thermal Energies= -3127.055451
Sum of electronic and thermal Enthalpies= -3127.054507
Sum of electronic and thermal Free Energies= -3127.153628

| | | | |
|---|---|---|---|
| Ni | -1.38935600 | -0.08923900 | 0.04180800 |
| Cl | 0.69087600 | -0.69401400 | 0.11447500 |
| C | -3.26233600 | 0.10526500 | 0.01082400 |
| C | -5.43119200 | -0.05869900 | -0.66551000 |
| C | -5.44008900 | 0.18713600 | 0.67281100 |
| N | -4.10944500 | 0.28726800 | 1.06394200 |
| N | -4.09567900 | -0.10031000 | -1.04938800 |
| H | -6.25877700 | 0.29961400 | 1.37739400 |
| H | -6.24031100 | -0.20494800 | -1.37493300 |
| C | -3.66352300 | 0.47433100 | 2.41838900 |
| C | -3.36684300 | -0.66421700 | 3.19361300 |
| C | -3.52548200 | 1.79082200 | 2.90691000 |
| C | -2.94839800 | -0.45308500 | 4.51624100 |
| C | -3.10771200 | 1.94642900 | 4.23524900 |
| C | -2.82921300 | 0.83551600 | 5.03434700 |
| H | -2.70650300 | -1.31182000 | 5.14627700 |
| H | -2.98417300 | 2.94851800 | 4.64956100 |
| H | -2.50315600 | 0.97826700 | 6.06773900 |
| C | -3.62850700 | -0.40276400 | -2.37565800 |
| C | -3.29962000 | -1.73723600 | -2.68667600 |
| C | -3.50032200 | 0.65341000 | -3.30256800 |
| C | -2.85805400 | -2.00551500 | -3.99133200 |
| C | -3.05781800 | 0.33131900 | -4.59233700 |
| C | -2.74643800 | -0.98616900 | -4.93544600 |
| H | -2.59219400 | -3.02827500 | -4.26779900 |
| H | -2.94099600 | 1.12040200 | -5.33702700 |
| H | -2.40128300 | -1.21666100 | -5.94655600 |
| C | -3.44646200 | -2.07794000 | 2.63040100 |
| C | -4.43571300 | -2.95288900 | 3.41647200 |
| C | -2.04956300 | -2.72022300 | 2.55912300 |
| H | -3.82227600 | -2.01114100 | 1.59966200 |
| H | -5.43995300 | -2.50037600 | 3.43861600 |
| H | -4.51860500 | -3.94862900 | 2.95180000 |
| H | -4.10837700 | -3.09937100 | 4.45860500 |
| H | -1.35397100 | -2.10491500 | 1.96708600 |
| H | -1.61852500 | -2.85113500 | 3.56510800 |
| H | -2.10974300 | -3.71367200 | 2.08572800 |
| C | -3.71120300 | 2.99259400 | 1.98846100 |
| C | -2.35329400 | 3.36298200 | 1.36155300 |
| C | -4.36022000 | 4.20098900 | 2.67519500 |
| H | -4.37708100 | 2.68827800 | 1.16623600 |
| H | -1.91057600 | 2.49360700 | 0.85194800 |
| H | -2.46788400 | 4.17435700 | 0.62491700 |
| H | -1.64614400 | 3.69674600 | 2.13843500 |
| H | -5.31362600 | 3.92973400 | 3.15556500 |
| H | -3.70416100 | 4.63798500 | 3.44483000 |
| H | -4.56136100 | 4.99165900 | 1.93511900 |
| C | -3.37830200 | -2.85965500 | -1.65910500 |
| C | -1.98835500 | -3.46124200 | -1.38734700 |
| C | -4.39422200 | -3.93640800 | -2.07341400 |
| H | -3.73118800 | -2.42753600 | -0.71233000 |
| H | -1.27185300 | -2.68813600 | -1.06845300 |
| H | -2.05061800 | -4.21672700 | -0.58730700 |
| H | -1.58275900 | -3.95528500 | -2.28526900 |
| H | -5.39552200 | -3.50344800 | -2.22789200 |
| H | -4.09428000 | -4.43478300 | -3.00961000 |
| H | -4.47222400 | -4.71100600 | -1.29344500 |
| C | -3.72603400 | 2.09972500 | -2.87890200 |
| C | -4.37293300 | 2.96810800 | -3.96555000 |
| C | -2.39090500 | 2.70183200 | -2.39979200 |
| H | -4.41018200 | 2.09454300 | -2.01630300 |
| H | -5.30739700 | 2.52033900 | -4.33923100 |
| H | -4.60803100 | 3.96514100 | -3.56061500 |
| H | -3.70085200 | 3.11900700 | -4.82543100 |
| H | -1.94630900 | 2.08356400 | -1.60532900 |
| H | -1.66962400 | 2.75376700 | -3.23172300 |
| H | -2.53812700 | 3.71990900 | -2.00474400 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3128.9249772

PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3127.4013293

**I-1**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.724868 (Hartree/Particle)
Thermal correction to Energy= 0.764760
Thermal correction to Enthalpy= 0.765704
Thermal correction to Gibbs Free Energy= 0.650889
Sum of electronic and zero-point Energies= -2939.029832
Sum of electronic and thermal Energies= -2938.989941
Sum of electronic and thermal Enthalpies= -2938.988996
Sum of electronic and thermal Free Energies= -2939.103812

| | | | |
|---|---|---|---|
| Ni | -1.60628200 | 0.28530200 | -0.62553000 |
| C | -3.42270500 | -0.08482700 | -0.32637900 |
| C | -5.61543400 | -0.67163600 | -0.55132200 |
| C | -5.44929300 | -0.20845500 | 0.71697300 |
| N | -4.10819500 | 0.14003900 | 0.83546700 |
| N | -4.37185800 | -0.58550500 | -1.17086400 |
| H | -6.15065400 | -0.09654500 | 1.53861700 |
| H | -6.49216000 | -1.04984000 | -1.06876700 |
| C | -3.47936400 | 0.69268200 | 2.00330500 |
| C | -2.97926500 | -0.19190300 | 2.98306200 |
| C | -3.33467600 | 2.09177900 | 2.09437900 |
| C | -2.33354500 | 0.36963900 | 4.09268700 |
| C | -2.67967900 | 2.60248600 | 3.22498700 |
| C | -2.18842600 | 1.75289500 | 4.21486000 |
| H | -1.92462600 | -0.28209200 | 4.86697700 |
| H | -2.54265700 | 3.68152500 | 3.32424300 |
| H | -1.67691600 | 2.17050400 | 5.08577000 |
| C | -4.09460600 | -0.97049500 | -2.52673100 |
| C | -3.59160200 | -2.26374800 | -2.77352200 |
| C | -4.31408100 | -0.02673900 | -3.55267700 |
| C | -3.32034300 | -2.60876500 | -4.10597900 |
| C | -4.03073900 | -0.42282000 | -4.86698300 |
| C | -3.54332600 | -1.70193800 | -5.14150900 |
| H | -2.91984600 | -3.59875500 | -4.33464300 |
| H | -4.18077200 | 0.28043900 | -5.68810400 |

| | | | |
|---|---|---|---|
| H | -3.32517700 | -1.99007800 | -6.17305300 |
| O | 0.12086000 | 0.70275500 | -1.04881400 |
| C | 1.16815000 | 0.73227600 | -0.12195600 |
| C | 0.69231000 | 1.37535400 | 1.19891400 |
| H | 0.30905200 | 2.38949600 | 1.00398900 |
| H | -0.13195100 | 0.78256000 | 1.63291100 |
| H | 1.48768200 | 1.43885300 | 1.95963100 |
| C | 2.30062900 | 1.57491200 | -0.76026300 |
| H | 2.52742600 | 1.10419500 | -1.73275800 |
| H | 1.85997300 | 2.55924200 | -0.99748300 |
| C | 1.64427000 | -0.70760000 | 0.16097700 |
| H | 0.78831800 | -1.29547300 | 0.52912800 |
| H | 1.99771700 | -1.17544200 | -0.77212600 |
| H | 2.45187100 | -0.76150300 | 0.91006300 |
| C | 3.59104600 | 1.75894900 | 0.04051900 |
| H | 4.07643800 | 0.79503000 | 0.26502900 |
| H | 4.31916400 | 2.36773700 | -0.52075600 |
| H | 3.41120100 | 2.27016000 | 1.00043300 |
| C | -3.27600400 | -3.23609200 | -1.64353100 |
| C | -1.75378600 | -3.31582800 | -1.43047400 |
| C | -3.89306700 | -4.62468400 | -1.86695700 |
| H | -3.71113900 | -2.83095100 | -0.71793600 |
| H | -1.34525300 | -2.31687700 | -1.21310400 |
| H | -1.51263100 | -3.97685000 | -0.58282900 |
| H | -1.24786600 | -3.70767700 | -2.32791000 |
| H | -4.98229400 | -4.56060900 | -2.01894700 |
| H | -3.45837700 | -5.12991500 | -2.74433800 |
| H | -3.70610100 | -5.26833500 | -0.99243500 |
| C | -4.74804000 | 1.39980800 | -3.23575100 |
| C | -5.76003300 | 1.96777700 | -4.23979100 |
| C | -3.50663600 | 2.30379300 | -3.11581700 |
| H | -5.23967800 | 1.39100700 | -2.25100100 |
| H | -6.63391700 | 1.30644400 | -4.35121900 |
| H | -6.11630400 | 2.95297100 | -3.89934800 |
| H | -5.31440700 | 2.11200900 | -5.23705700 |
| H | -2.80743600 | 1.91180300 | -2.36134600 |
| H | -2.97172600 | 2.36093400 | -4.07792100 |
| H | -3.79397800 | 3.32545600 | -2.81922600 |
| C | -3.04450000 | -1.70284600 | 2.79247400 |
| C | -3.36770100 | -2.46743900 | 4.08315300 |
| C | -1.73316000 | -2.20078900 | 2.15657100 |
| H | -3.85354100 | -1.91699700 | 2.07767300 |
| H | -4.28769300 | -2.08992800 | 4.55695100 |
| H | -3.50930700 | -3.53724700 | 3.86203400 |
| H | -2.55188000 | -2.39470600 | 4.82005100 |
| H | -1.53151800 | -1.67314800 | 1.21204900 |
| H | -0.88015600 | -2.02260700 | 2.83158500 |
| H | -1.78598400 | -3.28063100 | 1.94339400 |
| C | -3.80991100 | 3.03307700 | 0.99376600 |
| C | -2.60854000 | 3.66879300 | 0.27262200 |
| C | -4.78332600 | 4.09731200 | 1.52432100 |
| H | -4.35366500 | 2.43583600 | 0.24757300 |
| H | -1.95404200 | 2.88996200 | -0.14777300 |
| H | -2.94985700 | 4.31330700 | -0.55296800 |
| H | -2.00869700 | 4.28524900 | 0.96182800 |
| H | -5.64984400 | 3.63540300 | 2.02380400 |
| H | -4.29540500 | 4.76994100 | 2.24811500 |
| H | -5.15734000 | 4.71946900 | 0.69532800 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -2941.1224533
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -2939.4632154

**TS-I-II-1**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.845670 (Hartree/Particle)
Thermal correction to Energy= 0.898555
Thermal correction to Enthalpy= 0.899499
Thermal correction to Gibbs Free Energy= 0.758413
Sum of electronic and zero-point Energies= -4131.262484
Sum of electronic and thermal Energies= -4131.209600
Sum of electronic and thermal Enthalpies= -4131.208656
Sum of electronic and thermal Free Energies= -4131.349741

| | | | |
|---|---|---|---|
| Ni | 7.94656600 | -3.26953800 | -0.39845200 |
| C | 8.35797100 | -1.49223500 | 0.28399500 |
| C | 9.06233300 | 0.64422900 | 0.51221900 |
| C | 9.00431300 | 0.10133800 | 1.75449300 |
| N | 8.56542900 | -1.20737600 | 1.59882500 |
| N | 8.67564000 | -0.35252500 | -0.37803900 |
| H | 9.25819100 | 0.51539800 | 2.72344900 |
| H | 9.36801900 | 1.62925900 | 0.17673800 |
| C | 8.48087200 | -2.18179000 | 2.66204600 |
| C | 9.50724200 | -3.15303400 | 2.74727200 |
| C | 7.39752100 | -2.12718600 | 3.56647600 |
| C | 9.39490200 | -4.11919300 | 3.75634400 |
| C | 7.34879200 | -3.11320500 | 4.56440500 |
| C | 8.32651200 | -4.10228100 | 4.65227700 |
| H | 10.15706600 | -4.89330200 | 3.84883900 |
| H | 6.52494300 | -3.11276000 | 5.27857400 |
| H | 8.25829100 | -4.86618300 | 5.43097900 |
| C | 8.66699100 | -0.17873000 | -1.81045100 |
| C | 7.60489800 | 0.55626600 | -2.37437700 |
| C | 9.73885800 | -0.70198800 | -2.57696800 |
| C | 7.61850100 | 0.75451200 | -3.76375500 |
| C | 9.69121000 | -0.47736200 | -3.96041500 |
| C | 8.64691100 | 0.24056700 | -4.54732400 |
| H | 6.81029100 | 1.31795600 | -4.23324300 |
| H | 10.48358500 | -0.86315000 | -4.60031900 |
| H | 8.64148800 | 0.40001700 | -5.62859400 |
| C | 5.27815100 | -5.44701900 | 0.56604200 |
| C | 4.92842700 | -5.80003300 | -0.74555600 |
| C | 5.14443700 | -4.91058900 | -1.80435600 |
| C | 5.71598800 | -3.65385000 | -1.56639700 |
| C | 6.08683000 | -3.34938900 | -0.24887100 |
| C | 5.83466100 | -4.19493700 | 0.84106600 |
| H | 5.10785400 | -6.14669700 | 1.38790100 |
| H | 4.47530800 | -6.77441700 | -0.94094100 |
| H | 4.85689900 | -5.18422000 | -2.82252200 |
| H | 5.84521800 | -2.92111000 | -2.36325800 |
| H | 6.08283100 | -3.88589900 | 1.85638200 |
| O | 5.35482200 | -1.45818200 | 0.07064000 |
| S | 3.93852000 | -1.32644500 | 0.62506200 |
| O | 3.49763500 | -2.50077600 | 1.38838000 |
| O | 3.71562800 | 0.01134800 | 1.19379100 |
| C | 2.79153300 | -1.39054500 | -0.89974900 |
| F | 2.36427600 | -0.17185600 | -1.22994100 |
| F | 1.73123000 | -2.14283600 | -0.61724900 |
| F | 3.41264500 | -1.92299300 | -1.95962900 |
| O | 9.07916800 | -4.64411300 | -0.69317300 |
| C | 9.34587400 | -5.39075000 | -1.85679800 |
| C | 8.56334600 | -6.72051700 | -1.72111900 |
| H | 7.51143800 | -6.44429300 | -1.54574400 |
| H | 8.91118200 | -7.20439700 | -0.79237500 |
| C | 8.88702400 | -4.61118300 | -3.10373000 |
| H | 9.27884500 | -3.58454500 | -3.06368600 |
| H | 9.23005100 | -5.07490100 | -4.04145100 |
| H | 7.78942700 | -4.54895800 | -3.13171900 |
| C | 10.86113300 | -5.64242000 | -1.90988400 |
| H | 11.18000400 | -6.21963200 | -1.02903900 |
| H | 11.15728000 | -6.19214800 | -2.81697000 |
| H | 11.39558100 | -4.68304600 | -1.89724100 |
| C | 8.65811400 | -7.70133200 | -2.89030300 |
| H | 9.69662000 | -8.01658400 | -3.08214300 |
| H | 8.07322800 | -8.61221700 | -2.68328600 |
| H | 8.26436900 | -7.26607000 | -3.82298900 |
| C | 6.32794000 | -1.04100700 | 3.50651900 |
| C | 6.72998200 | 0.18422200 | 4.35196600 |
| C | 4.94638500 | -1.52787000 | 3.96909300 |

| | | | |
|---|---|---|---|
| H | 6.23292200 | -0.72344200 | 2.45675000 |
| H | 7.68449500 | 0.62768800 | 4.04047600 |
| H | 5.95651800 | 0.96468800 | 4.27490000 |
| H | 6.82527500 | -0.09872700 | 5.41318300 |
| H | 4.65923000 | -2.46865100 | 3.48435000 |
| H | 4.91129300 | -1.66250500 | 5.06232100 |
| H | 4.18761300 | -0.78240800 | 3.69311100 |
| C | 10.73825600 | -3.10868300 | 1.84442000 |
| C | 11.36948000 | -4.48096600 | 1.59144100 |
| C | 11.77314300 | -2.12082400 | 2.41543400 |
| H | 10.42130100 | -2.73639300 | 0.86189400 |
| H | 10.61978100 | -5.18123500 | 1.20042900 |
| H | 12.16126700 | -4.38619600 | 0.83226300 |
| H | 11.83403900 | -4.89837400 | 2.49940700 |
| H | 11.35517400 | -1.10998000 | 2.53404300 |
| H | 12.12633600 | -2.45914600 | 3.40334000 |
| H | 12.64536700 | -2.04830200 | 1.74638400 |
| C | 6.49298100 | 1.15588800 | -1.52431200 |
| C | 5.10340200 | 0.93662300 | -2.13225500 |
| C | 6.73605800 | 2.65615400 | -1.27805100 |
| H | 6.48853900 | 0.63816700 | -0.55662600 |
| H | 4.95383900 | -0.11418400 | -2.41078100 |
| H | 4.33539600 | 1.20192700 | -1.39349700 |
| H | 4.93828800 | 1.55873200 | -3.02707100 |
| H | 7.70231400 | 2.84857400 | -0.78858600 |
| H | 6.72791300 | 3.21347100 | -2.22943100 |
| H | 5.94266000 | 3.06907100 | -0.63476200 |
| C | 10.90880200 | -1.46218300 | -1.94267300 |
| C | 11.79789300 | -0.55224600 | -1.07121100 |
| C | 11.80405100 | -2.17475800 | -2.96504100 |
| H | 10.47187100 | -2.23957800 | -1.29278200 |
| H | 12.62737600 | -1.13724000 | -0.64405900 |
| H | 12.23200200 | 0.25715500 | -1.68064800 |
| H | 11.25752500 | -0.09624900 | -0.23383600 |
| H | 11.24106800 | -2.84923400 | -3.62469400 |
| H | 12.34855200 | -1.45297200 | -3.59498600 |
| H | 12.55821600 | -2.77679300 | -2.43680400 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4134.4485155
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4131.9398709

**II-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.846470 (Hartree/Particle)
Thermal correction to Energy= 0.900201
Thermal correction to Enthalpy= 0.901145
Thermal correction to Gibbs Free Energy= 0.758583
Sum of electronic and zero-point Energies= -4131.320610
Sum of electronic and thermal Energies= -4131.266879
Sum of electronic and thermal Enthalpies= -4131.265935
Sum of electronic and thermal Free Energies= -4131.408497

| | | | |
|---|---|---|---|
| C | 1.00985100 | 0.71068200 | 0.79166400 |
| C | 2.19671000 | 2.43275500 | -0.08968800 |
| C | 2.54747400 | 2.31987800 | 1.21670400 |
| N | 1.80815300 | 1.26978000 | 1.74453300 |
| N | 1.25379200 | 1.44472200 | -0.32874300 |
| H | 3.25470000 | 2.87704700 | 1.82339800 |
| H | 2.53958900 | 3.10214500 | -0.87182000 |
| C | 2.04430200 | 0.83456400 | 3.10460800 |
| C | 1.56138000 | 1.64498100 | 4.15311600 |
| C | 2.83720100 | -0.30766200 | 3.31768300 |
| C | 1.93893900 | 1.29535300 | 5.45425700 |
| C | 3.17624000 | -0.61574400 | 4.64290000 |
| C | 2.74471900 | 0.18339400 | 5.69678200 |
| H | 1.58215600 | 1.88399900 | 6.29909900 |
| H | 3.78862600 | -1.49548400 | 4.84873400 |
| H | 3.01700400 | -0.07512800 | 6.72282400 |
| C | 0.74780600 | 1.16701500 | -1.64782000 |
| C | -0.36930900 | 1.89071200 | -2.10933000 |
| C | 1.42426100 | 0.20649200 | -2.42496100 |
| C | -0.82251300 | 1.60861400 | -3.40424900 |
| C | 0.91809100 | -0.04921200 | -3.70831300 |
| C | -0.19234700 | 0.64295700 | -4.19122100 |
| H | -1.68961000 | 2.13967200 | -3.79958700 |
| H | 1.40818700 | -0.79311700 | -4.34009000 |
| H | -0.57018300 | 0.43030500 | -5.19444300 |
| C | -3.85574200 | -0.05462300 | 0.40056600 |
| C | -4.11814100 | -0.42380600 | -0.92212800 |
| C | -3.06865500 | -0.84219400 | -1.74761900 |
| C | -1.76395500 | -0.92593300 | -1.24534000 |
| C | -1.53187100 | -0.58531300 | 0.08485500 |
| C | -2.55258500 | -0.12724900 | 0.91408500 |
| H | -4.66493400 | 0.28745500 | 1.05123300 |
| H | -5.13695800 | -0.37268100 | -1.31397600 |
| H | -3.25830500 | -1.11527000 | -2.78902000 |
| H | -0.94951400 | -1.25968800 | -1.88697000 |
| H | -2.35416800 | 0.14093600 | 1.94887100 |
| Ni | 0.12562000 | -1.05361200 | 0.89676300 |
| O | 0.22720500 | -2.75825600 | 0.44349900 |
| C | -0.41824400 | -4.01047000 | 0.32848300 |
| C | -1.82194900 | -3.92949000 | 0.94012900 |
| H | -2.35072400 | -4.89067600 | 0.85088800 |
| H | -1.74348300 | -3.66197200 | 1.99965400 |
| H | -2.41465800 | -3.16006500 | 0.42617100 |
| C | 0.47556600 | -5.00234900 | 1.11524500 |
| H | 1.49405300 | -4.91380800 | 0.70000000 |
| H | 0.52110300 | -4.62650500 | 2.14828500 |
| C | -0.49796100 | -4.37911200 | -1.16178400 |
| H | -1.00246500 | -5.34614000 | -1.31005900 |
| H | -1.06587100 | -3.61217300 | -1.70748800 |
| H | 0.51048000 | -4.44249800 | -1.59940100 |
| C | 0.03993500 | -6.46838000 | 1.10987000 |
| H | 0.73871600 | -7.07752700 | 1.70587300 |
| H | -0.96186600 | -6.60049900 | 1.54884300 |
| H | 0.01938100 | -6.89486300 | 0.09386400 |
| C | 2.68453900 | -0.50162100 | -1.93883100 |
| C | 3.90918400 | -0.03894800 | -2.74732600 |
| C | 2.53808200 | -2.02997200 | -1.94978700 |
| H | 2.86253400 | -0.20907600 | -0.89435900 |
| H | 4.03323800 | 1.05468000 | -2.69915800 |
| H | 4.82639400 | -0.50585000 | -2.35380800 |
| H | 3.81511000 | -0.32145300 | -3.80857400 |
| H | 1.69738000 | -2.34673800 | -1.31714400 |
| H | 2.37886800 | -2.41668000 | -2.96943000 |
| H | 3.45462800 | -2.49880800 | -1.55604900 |
| C | -1.03694700 | 2.95521400 | -1.24692400 |
| C | -2.56552700 | 2.96572300 | -1.37363500 |
| C | -0.45985300 | 4.34835000 | -1.56205200 |
| H | -0.80195300 | 2.72044900 | -0.19701600 |
| H | -2.98761400 | 1.96888800 | -1.19576800 |
| H | -2.99690900 | 3.65840500 | -0.63388000 |
| H | -2.89188400 | 3.30865000 | -2.36869800 |
| H | 0.62955300 | 4.38873000 | -1.41654500 |
| H | -0.66872900 | 4.62484100 | -2.60862600 |
| H | -0.91642600 | 5.11082700 | -0.91066800 |
| C | 3.34391400 | -1.18587500 | 2.17931000 |
| C | 3.10679500 | -2.67808200 | 2.45200100 |
| C | 4.81507300 | -0.88195900 | 1.85277500 |
| H | 2.76676500 | -0.94387600 | 1.27491800 |
| H | 2.06157300 | -2.86193600 | 2.73615600 |
| H | 3.32034900 | -3.26643300 | 1.54648300 |
| H | 3.75822500 | -3.05391600 | 3.25694700 |
| H | 4.95635500 | 0.17906400 | 1.59156100 |
| H | 5.46176600 | -1.10667000 | 2.71677500 |
| H | 5.15710900 | -1.49294700 | 1.00132400 |
| C | 0.61218500 | 2.80967800 | 3.87995100 |
| C | 0.55251100 | 3.83836300 | 5.01528700 |

| | | | |
|---|---|---|---|
| C | -0.79813400 | 2.28432500 | 3.55018900 |
| H | 0.97886500 | 3.34366900 | 2.98759400 |
| H | 1.55495300 | 4.19373500 | 5.30162800 |
| H | -0.04156100 | 4.70997800 | 4.69888400 |
| H | 0.06753000 | 3.42402900 | 5.91364700 |
| H | -0.79227500 | 1.64997500 | 2.65515100 |
| H | -1.18344100 | 1.66707000 | 4.37475300 |
| H | -1.49113200 | 3.12454000 | 3.38036300 |
| S | -0.57097800 | -1.66584500 | 4.11286400 |
| O | -0.27108200 | -3.09570200 | 3.93995400 |
| O | -0.10010200 | -1.01008300 | 5.33592100 |
| O | -0.34293200 | -0.82936800 | 2.87188000 |
| C | -2.43967900 | -1.57609700 | 4.29558000 |
| F | -2.83647000 | -0.29497200 | 4.34062700 |
| F | -3.07376100 | -2.16584200 | 3.27835100 |
| F | -2.80876700 | -2.17212800 | 5.42798600 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4134.5079469
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4131.9957003

**II'-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.959138 (Hartree/Particle)
Thermal correction to Energy= 1.018331
Thermal correction to Enthalpy= 1.019276
Thermal correction to Gibbs Free Energy= 0.867084
Sum of electronic and zero-point Energies= -4288.314858
Sum of electronic and thermal Energies= -4288.255665
Sum of electronic and thermal Enthalpies= -4288.254721
Sum of electronic and thermal Free Energies= -4288.406913

| | | | |
|---|---|---|---|
| C | 0.88496400 | 0.52095700 | 0.84000500 |
| C | 2.63455300 | 1.71050300 | -0.00737200 |
| C | 2.87209900 | 1.51770100 | 1.31164100 |
| N | 1.78896200 | 0.80094200 | 1.81573000 |
| N | 1.41101800 | 1.10677600 | -0.28100700 |
| H | 3.70147400 | 1.81785600 | 1.94353300 |
| H | 3.21268200 | 2.22104100 | -0.76977500 |
| C | 1.65459200 | 0.62941000 | 3.24837800 |
| C | 1.22523000 | 1.74761200 | 3.99510300 |
| C | 2.07394000 | -0.57386100 | 3.85018100 |
| C | 1.26048200 | 1.64780200 | 5.39130600 |
| C | 2.07291900 | -0.62194100 | 5.25039700 |
| C | 1.68839600 | 0.47907600 | 6.01302700 |
| H | 0.93213800 | 2.49302300 | 5.99895100 |
| H | 2.36732900 | -1.53919300 | 5.75791700 |
| H | 1.70007500 | 0.41388300 | 7.10387000 |
| C | 0.70804800 | 1.31919000 | -1.52769200 |
| C | -0.00797500 | 2.53190700 | -1.68212000 |
| C | 0.79166100 | 0.35347500 | -2.55617200 |
| C | -0.72642700 | 2.71731300 | -2.87209600 |
| C | 0.06030000 | 0.59988100 | -3.72913800 |
| C | -0.70447900 | 1.75563700 | -3.87963800 |
| H | -1.30111600 | 3.63332000 | -3.01697400 |
| H | 0.08514300 | -0.12516900 | -4.54204400 |
| H | -1.27409100 | 1.91529300 | -4.79856800 |
| C | -4.37992900 | -2.89702100 | -0.27091700 |
| C | -4.39699500 | -2.70464100 | -1.65731300 |
| C | -3.36347600 | -1.98954600 | -2.27185700 |
| C | -2.31255900 | -1.47604200 | -1.50153000 |
| C | -2.31385800 | -1.66777400 | -0.11961300 |
| C | -3.33323600 | -2.38068300 | 0.50583100 |
| H | -5.18612900 | -3.45253900 | 0.21633000 |
| H | -5.21413800 | -3.11341000 | -2.25711100 |
| H | -3.36254400 | -1.83874900 | -3.35499300 |
| H | -1.50058400 | -0.93365000 | -1.99029100 |
| H | -3.32527200 | -2.52792400 | 1.58402000 |
| C | -1.79827000 | 1.35685700 | 1.49678000 |
| H | -1.41498500 | 1.16274100 | 2.49696500 |
| H | -1.30349500 | 2.11816700 | 0.90076800 |
| C | -2.95354500 | 0.79514100 | 1.07140100 |
| H | -3.45940300 | 0.10188400 | 1.74677700 |
| C | -3.68813800 | 1.19030200 | -0.17625000 |
| H | -2.97509900 | 1.57533600 | -0.92390000 |
| H | -4.16425300 | 0.30317900 | -0.61824000 |
| C | -4.76579000 | 2.24368500 | 0.12887900 |
| H | -4.32135800 | 3.16703500 | 0.53322800 |
| H | -5.32431000 | 2.50208100 | -0.78462700 |
| H | -5.48800500 | 1.86902500 | 0.87213100 |
| Ni | -0.80589800 | -0.78320100 | 0.73806000 |
| O | 0.27017200 | -2.14911400 | 0.10124300 |
| C | 0.24990000 | -3.56966600 | 0.20269700 |
| C | -0.30767300 | -4.03642900 | 1.55222000 |
| H | -0.25955900 | -5.13245400 | 1.63927700 |
| H | 0.23613900 | -3.58460900 | 2.38735100 |
| H | -1.35403200 | -3.73099700 | 1.65502200 |
| C | 1.75801500 | -3.93494900 | 0.05720300 |
| H | 2.07461600 | -3.61188900 | -0.94769600 |
| H | 2.31091900 | -3.30296200 | 0.76475000 |
| C | -0.54970200 | -4.22643400 | -0.93583400 |
| H | -0.38316700 | -5.31479900 | -0.94331300 |
| H | -1.62671900 | -4.05757400 | -0.82175000 |
| H | -0.23722500 | -3.82193200 | -1.90667800 |
| C | 2.14794600 | -5.39802200 | 0.27265700 |
| H | 3.22859000 | -5.53193900 | 0.10178100 |
| H | 1.93599400 | -5.73251700 | 1.30018600 |
| H | 1.62084600 | -6.07758100 | -0.41575800 |
| C | 1.67016400 | -0.88503200 | -2.42249100 |
| C | 3.15737700 | -0.54273600 | -2.63617800 |
| C | 1.26669300 | -2.01547600 | -3.37607500 |
| H | 1.53404800 | -1.26144100 | -1.39753000 |
| H | 3.52583000 | 0.19985400 | -1.91621700 |
| H | 3.77281800 | -1.44914100 | -2.51768400 |
| H | 3.32768700 | -0.14694800 | -3.65142400 |
| H | 0.19447600 | -2.24727300 | -3.30412200 |
| H | 1.49606100 | -1.77138800 | -4.42637300 |
| H | 1.82503200 | -2.93029600 | -3.12764500 |
| C | 0.06100400 | 3.66582600 | -0.66140400 |
| C | -1.27008300 | 4.40914500 | -0.46318900 |
| C | 1.15893100 | 4.67376200 | -1.05575600 |
| H | 0.35046500 | 3.23535000 | 0.30775600 |
| H | -2.10938600 | 3.72311600 | -0.28615500 |
| H | -1.19482800 | 5.08437000 | 0.40339900 |
| H | -1.52400300 | 5.02828900 | -1.33755600 |
| H | 2.14230800 | 4.19520300 | -1.15969200 |
| H | 0.91452400 | 5.15115900 | -2.01843100 |
| H | 1.24540300 | 5.46420800 | -0.29285100 |
| C | 2.51177700 | -1.76923800 | 3.01197100 |
| C | 2.41907400 | -3.09996500 | 3.77017200 |
| C | 3.93913200 | -1.58921400 | 2.45914500 |
| H | 1.81711500 | -1.82111100 | 2.15732900 |
| H | 1.43366600 | -3.22071200 | 4.24011800 |
| H | 2.58553100 | -3.93767800 | 3.07641500 |
| H | 3.19116800 | -3.17134100 | 4.55381100 |
| H | 4.03433700 | -0.70806400 | 1.81018000 |
| H | 4.66216400 | -1.48556000 | 3.28507500 |
| H | 4.23147600 | -2.46999700 | 1.86472000 |
| C | 0.72729700 | 3.03253500 | 3.34241000 |
| C | 1.78620500 | 4.14786500 | 3.39128700 |
| C | -0.59861800 | 3.51805400 | 3.95399800 |
| H | 0.53254300 | 2.81441800 | 2.28373900 |
| H | 2.72184100 | 3.84671000 | 2.89737600 |
| H | 1.41450700 | 5.05553700 | 2.88755500 |
| H | 2.02436100 | 4.41185600 | 4.43462600 |
| H | -1.32060700 | 2.69549900 | 4.04767800 |
| H | -0.44503100 | 3.94477300 | 4.95801600 |
| H | -1.03761700 | 4.30963800 | 3.32519600 |
| S | -1.42607600 | -1.22136800 | 4.13299100 |

| | | | |
|---|---|---|---|
| O | -0.62929400 | -2.16832700 | 4.92160000 |
| O | -1.46749700 | 0.18531200 | 4.56646000 |
| O | -1.28671500 | -1.40228300 | 2.64683400 |
| C | -3.18137100 | -1.82426400 | 4.38773400 |
| F | -4.05237500 | -1.06721400 | 3.70114700 |
| F | -3.31300700 | -3.08753000 | 3.96343600 |
| F | -3.50831000 | -1.77200400 | 5.67719600 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4291.7523532
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4289.0687522

**TS-II'-III-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.959361 (Hartree/Particle)
Thermal correction to Energy= 1.017424
Thermal correction to Enthalpy= 1.018368
Thermal correction to Gibbs Free Energy= 0.869490
Sum of electronic and zero-point Energies= -4288.306274
Sum of electronic and thermal Energies= -4288.248211
Sum of electronic and thermal Enthalpies= -4288.247267
Sum of electronic and thermal Free Energies= -4288.396145

| | | | |
|---|---|---|---|
| C | 0.87456800 | 0.47671100 | 0.80250700 |
| C | 2.64646200 | 1.61268500 | -0.05099000 |
| C | 2.86979000 | 1.44003000 | 1.27307500 |
| N | 1.76756400 | 0.75603500 | 1.78429900 |
| N | 1.41233500 | 1.02947300 | -0.32648900 |
| H | 3.69899300 | 1.73535700 | 1.90736600 |
| H | 3.23963700 | 2.09660000 | -0.81921300 |
| C | 1.61853500 | 0.62389900 | 3.22061400 |
| C | 1.15370000 | 1.75115900 | 3.93160000 |
| C | 2.06892200 | -0.54901400 | 3.85674600 |
| C | 1.19092500 | 1.69290200 | 5.33075500 |
| C | 2.09364600 | -0.54675200 | 5.25672500 |
| C | 1.67388200 | 0.56387100 | 5.98628000 |
| H | 0.83261600 | 2.54356000 | 5.91327400 |
| H | 2.42155800 | -1.43797200 | 5.79016800 |
| H | 1.69669100 | 0.53561000 | 7.07845600 |
| C | 0.71730100 | 1.26274400 | -1.57567600 |
| C | 0.03326600 | 2.49535500 | -1.72171400 |
| C | 0.78006100 | 0.30412300 | -2.61296600 |
| C | -0.66584500 | 2.71684000 | -2.91678200 |
| C | 0.06851800 | 0.58824400 | -3.79008400 |
| C | -0.65757700 | 1.76881600 | -3.93696700 |
| H | -1.21307500 | 3.65051200 | -3.05535100 |
| H | 0.07909200 | -0.12762700 | -4.61098500 |
| H | -1.20948100 | 1.95686400 | -4.86135900 |
| C | -4.19023300 | -3.12120900 | -0.40323100 |
| C | -4.11752400 | -2.93672400 | -1.78821700 |
| C | -3.23879800 | -1.98221900 | -2.31574100 |
| C | -2.44710100 | -1.21289100 | -1.46024200 |
| C | -2.50633200 | -1.41208600 | -0.07314500 |
| C | -3.38595900 | -2.36067100 | 0.45462000 |
| H | -4.87315900 | -3.86419600 | 0.01715300 |
| H | -4.74653500 | -3.53182000 | -2.45497100 |
| H | -3.17116900 | -1.83119500 | -3.39651100 |
| H | -1.78354500 | -0.45588700 | -1.88704400 |
| H | -3.45723300 | -2.50933100 | 1.53044700 |
| C | -1.68989000 | 1.12596800 | 1.28279000 |
| H | -1.34812700 | 1.17478100 | 2.31520800 |
| H | -1.38240200 | 1.93082400 | 0.61988400 |
| C | -2.89237400 | 0.46392900 | 0.99986200 |
| H | -3.33421000 | -0.08520500 | 1.83163200 |
| C | -3.86085300 | 1.03594300 | -0.00746600 |
| H | -3.30762100 | 1.40735100 | -0.88448600 |
| H | -4.55141700 | 0.25810500 | -0.36150500 |
| C | -4.65646900 | 2.17999800 | 0.64214000 |
| H | -3.99539900 | 2.99592500 | 0.97421100 |
| H | -5.38187000 | 2.59501800 | -0.07492700 |
| H | -5.21514300 | 1.82439400 | 1.52261100 |
| Ni | -0.79738100 | -0.68661600 | 0.75460300 |
| O | 0.25807500 | -2.08490500 | 0.10988600 |
| C | 0.22819100 | -3.50006100 | 0.18709100 |
| C | -0.36463600 | -3.98381000 | 1.51841200 |
| H | -0.35577500 | -5.08307300 | 1.57915400 |
| H | 0.18533100 | -3.57196000 | 2.37016100 |
| H | -1.40014900 | -3.64311500 | 1.61769100 |
| C | 1.72071000 | -3.91881000 | 0.05681900 |
| H | 2.06999000 | -3.56989400 | -0.92959300 |
| H | 2.28205700 | -3.33236300 | 0.79769600 |
| C | -0.58340500 | -4.10723500 | -0.97080400 |
| H | -0.51507700 | -5.20679600 | -0.96684500 |
| H | -1.64171800 | -3.84096000 | -0.89078700 |
| H | -0.20900500 | -3.74293200 | -1.93510700 |
| C | 2.05894900 | -5.40152900 | 0.22186600 |
| H | 3.13713500 | -5.57050900 | 0.06556300 |
| H | 1.81504000 | -5.76786200 | 1.23173100 |
| H | 1.52059200 | -6.03532600 | -0.50113500 |
| C | 1.59679500 | -0.97467700 | -2.47859400 |
| C | 3.10817200 | -0.70377200 | -2.60585000 |
| C | 1.19051000 | -2.05583500 | -3.48680400 |
| H | 1.38657900 | -1.37073600 | -1.47123600 |
| H | 3.48048100 | -0.01578600 | -1.83573900 |
| H | 3.66702400 | -1.64727200 | -2.49768900 |
| H | 3.35178100 | -0.27662500 | -3.59331000 |
| H | 0.10761000 | -2.24764400 | -3.46623800 |
| H | 1.47371700 | -1.78838300 | -4.51847700 |
| H | 1.70273400 | -2.99913300 | -3.24499400 |
| C | 0.10129500 | 3.60857900 | -0.67877900 |
| C | -1.23145800 | 4.34797700 | -0.47401800 |
| C | 1.20519800 | 4.62125900 | -1.04099200 |
| H | 0.38041700 | 3.15858800 | 0.28358400 |
| H | -2.07394200 | 3.65727100 | -0.32635700 |
| H | -1.16578100 | 4.99790400 | 0.41251800 |
| H | -1.47651900 | 4.99131200 | -1.33322400 |
| H | 2.18779900 | 4.14057800 | -1.14434700 |
| H | 0.97289800 | 5.12079000 | -1.99543200 |
| H | 1.28660800 | 5.39418300 | -0.25984000 |
| C | 2.49217000 | -1.77060400 | 3.05125100 |
| C | 2.31926600 | -3.08123300 | 3.83049100 |
| C | 3.94041000 | -1.64928400 | 2.54095700 |
| H | 1.82122000 | -1.81359600 | 2.17758800 |
| H | 1.31811400 | -3.14206300 | 4.27944300 |
| H | 2.45927400 | -3.93920900 | 3.15570300 |
| H | 3.06722800 | -3.17640500 | 4.63484000 |
| H | 4.08483100 | -0.77704200 | 1.88803300 |
| H | 4.64293600 | -1.56243600 | 3.38636300 |
| H | 4.21753800 | -2.54518100 | 1.96205600 |
| C | 0.63706000 | 3.00573800 | 3.23615900 |
| C | 1.68835600 | 4.12931600 | 3.23354900 |
| C | -0.69093900 | 3.50377200 | 3.83156500 |
| H | 0.43901500 | 2.74540700 | 2.18798400 |
| H | 2.62299800 | 3.81369000 | 2.74677800 |
| H | 1.30760800 | 5.01254800 | 2.69438700 |
| H | 1.93004900 | 4.43733700 | 4.26382000 |
| H | -1.41229700 | 2.68262800 | 3.94383700 |
| H | -0.54146200 | 3.95656800 | 4.82479400 |
| H | -1.12698100 | 4.27937900 | 3.18103400 |
| S | -1.47175500 | -1.09673700 | 4.14194200 |
| O | -0.63469400 | -1.83611200 | 5.09286300 |
| O | -1.78066300 | 0.31516500 | 4.43448400 |
| O | -1.13152700 | -1.36038300 | 2.70250000 |
| C | -3.13182400 | -1.95662700 | 4.31083700 |
| F | -4.07583000 | -1.34454200 | 3.57093200 |
| F | -3.05258400 | -3.22670200 | 3.89828900 |
| F | -3.53105600 | -1.94358400 | 5.58030200 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)

HF = -4291.7442046
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4289.0640622

**III-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.960566 (Hartree/Particle)
Thermal correction to Energy= 1.018850
Thermal correction to Enthalpy= 1.019795
Thermal correction to Gibbs Free Energy= 0.868977
Sum of electronic and zero-point Energies= -4288.355388
Sum of electronic and thermal Energies= -4288.297103
Sum of electronic and thermal Enthalpies= -4288.296159
Sum of electronic and thermal Free Energies= -4288.446977

| | | | |
|---|---|---|---|
| Ni | -0.83000400 | -0.37270200 | 0.05569000 |
| N | 1.10614500 | 1.54699500 | 1.45419100 |
| N | -0.57451500 | 1.22265100 | 2.75068900 |
| C | 3.08525700 | 0.92156400 | 0.13961900 |
| C | 3.97961000 | 1.26642100 | -0.88325900 |
| C | 3.71523500 | 2.33191100 | -1.74208500 |
| C | 2.53396200 | 3.06094900 | -1.61837600 |
| C | 1.61722000 | 2.78002700 | -0.59597400 |
| C | 1.93741700 | 1.72636800 | 0.28967300 |
| C | 1.41082400 | 2.17572000 | 2.65731700 |
| C | 0.35243500 | 1.96547700 | 3.47681900 |
| C | -0.11753300 | 0.95006400 | 1.50026300 |
| C | -1.90593900 | 1.03397600 | 3.28256400 |
| C | -2.25351400 | -0.19004400 | 3.88769800 |
| C | -3.49729800 | -0.24926200 | 4.53139900 |
| C | -4.34335000 | 0.85765300 | 4.57267900 |
| C | -3.98441800 | 2.04346300 | 3.93796600 |
| C | -2.75983500 | 2.15733300 | 3.26945400 |
| H | 4.88658800 | 0.67810200 | -1.02717400 |
| H | 4.42052800 | 2.57391200 | -2.54050400 |
| H | 2.32257200 | 3.86109700 | -2.32833800 |
| H | 2.33292300 | 2.72885700 | 2.80218500 |
| H | 0.15384400 | 2.28776800 | 4.49419700 |
| H | -3.81633200 | -1.17770400 | 5.00415400 |
| H | -5.30828300 | 0.78327000 | 5.08037400 |
| H | -4.67961900 | 2.88485400 | 3.93638000 |
| C | -1.29104400 | -1.03595400 | -1.75176500 |
| H | -2.32858000 | -1.36302500 | -1.69586300 |
| H | -0.62554500 | -1.81889400 | -2.11264800 |
| C | -2.33995500 | 0.97885200 | -2.89045000 |
| H | -2.12373100 | 2.00893400 | -3.21402900 |
| H | -3.05384000 | 1.06750000 | -2.06154200 |
| C | 0.21000800 | 0.42262600 | -3.16748700 |
| C | 0.27129400 | 1.17032400 | -4.35279600 |
| C | 1.36636800 | -0.26389100 | -2.75691700 |
| C | 1.44299900 | 1.20794200 | -5.11848800 |
| H | -0.59795400 | 1.72922400 | -4.69989100 |
| C | 2.53229100 | -0.23220200 | -3.52123900 |
| H | 1.36124500 | -0.81972000 | -1.81672400 |
| C | 2.57586100 | 0.50046800 | -4.71156100 |
| H | 1.46267500 | 1.79211300 | -6.04224900 |
| H | 3.41650000 | -0.77192200 | -3.17466900 |
| H | 3.48888000 | 0.52645900 | -5.31164800 |
| C | -2.98107700 | 0.18445900 | -4.03005600 |
| H | -2.28500900 | 0.02267100 | -4.86768100 |
| H | -3.32520600 | -0.80168700 | -3.68340200 |
| H | -3.86142400 | 0.71918400 | -4.41940000 |
| C | -1.05265200 | 0.35533500 | -2.30464000 |
| H | -0.82267300 | 1.05098900 | -1.43240600 |
| O | 0.23554200 | -1.74465000 | 0.58394300 |
| C | 0.22273900 | -3.15956400 | 0.46119600 |
| C | 0.98826100 | -3.61140300 | -0.79297100 |
| H | 0.49577900 | -3.26855000 | -1.71194100 |
| H | 2.01066700 | -3.20947100 | -0.78095200 |
| H | 1.04916800 | -4.70891100 | -0.84607500 |
| C | 0.96419600 | -3.64688000 | 1.73610500 |
| H | 0.45201300 | -3.18979500 | 2.59428100 |
| H | 1.97057100 | -3.19738900 | 1.71050500 |
| C | -1.22279300 | -3.66972300 | 0.42938100 |
| H | -1.77612400 | -3.31044300 | 1.30622400 |
| H | -1.74347900 | -3.28617200 | -0.45858500 |
| H | -1.26599000 | -4.76894600 | 0.39787200 |
| C | 1.07627100 | -5.15652500 | 1.95210200 |
| H | 1.63349700 | -5.36984000 | 2.87869800 |
| H | 0.08739500 | -5.63167600 | 2.05018400 |
| H | 1.60885700 | -5.65829000 | 1.12842600 |
| C | 0.34037700 | 3.60443400 | -0.44192600 |
| C | -0.23437300 | 4.07747600 | -1.78459200 |
| C | 0.55199600 | 4.80345800 | 0.50118100 |
| H | -0.41989800 | 2.95527600 | 0.01769500 |
| H | -0.28444400 | 3.25758900 | -2.51475100 |
| H | -1.25064200 | 4.47422200 | -1.63686200 |
| H | 0.37132000 | 4.88318400 | -2.22928500 |
| H | 0.89140700 | 4.48799100 | 1.49752200 |
| H | 1.30539400 | 5.49288800 | 0.08623500 |
| H | -0.38952300 | 5.36135400 | 0.62870200 |
| C | 3.32704500 | -0.29500200 | 1.02890400 |
| C | 4.13941900 | 0.04915500 | 2.29012000 |
| C | 4.01190900 | -1.43822300 | 0.26510700 |
| H | 2.33513400 | -0.66427500 | 1.33414000 |
| H | 3.63357400 | 0.79121700 | 2.92253500 |
| H | 4.29656400 | -0.85494400 | 2.90042000 |
| H | 5.12937900 | 0.45200300 | 2.01849800 |
| H | 3.50687000 | -1.64319500 | -0.68996800 |
| H | 5.06945900 | -1.21619200 | 0.04959100 |
| H | 3.98936900 | -2.36036300 | 0.86566000 |
| C | -1.31166300 | -1.38920200 | 3.84707800 |
| C | -2.02917000 | -2.72647400 | 4.07003600 |
| C | -0.15735000 | -1.24024300 | 4.85682700 |
| H | -0.87575200 | -1.41414900 | 2.83494800 |
| H | -2.88898700 | -2.82898400 | 3.39514600 |
| H | -1.33576100 | -3.55989700 | 3.87987800 |
| H | -2.38016400 | -2.83051000 | 5.10998200 |
| H | 0.43804700 | -0.33306500 | 4.68399600 |
| H | -0.54795200 | -1.19962500 | 5.88722000 |
| H | 0.52540800 | -2.10283600 | 4.78788600 |
| C | -2.41688200 | 3.42922300 | 2.49952400 |
| C | -2.67875000 | 4.70970900 | 3.30480600 |
| C | -3.15310300 | 3.44972600 | 1.14767300 |
| H | -1.34176300 | 3.41838900 | 2.27458400 |
| H | -2.15954300 | 4.68788100 | 4.27631400 |
| H | -2.32023400 | 5.58871700 | 2.74501400 |
| H | -3.75256200 | 4.86177000 | 3.49793500 |
| H | -2.92920400 | 2.54467800 | 0.56780300 |
| H | -4.24415200 | 3.47760100 | 1.29526900 |
| H | -2.85745200 | 4.33723200 | 0.56353000 |
| S | -4.03068500 | -0.42081100 | 0.81585200 |
| O | -3.75724700 | -1.70086900 | 1.48109500 |
| O | -4.90560000 | 0.55570800 | 1.46489800 |
| O | -2.78920300 | 0.22490000 | 0.21503800 |
| C | -5.03139900 | -0.91444600 | -0.69916500 |
| F | -4.43177700 | -1.89613300 | -1.39208500 |
| F | -6.22568600 | -1.35247300 | -0.30956200 |
| F | -5.20376600 | 0.12661300 | -1.52036300 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4291.7886391
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4289.1116985

**TS-III-IV-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.955944 (Hartree/Particle)
Thermal correction to Energy= 1.014051

Thermal correction to Enthalpy= 1.014995
Thermal correction to Gibbs Free Energy= 0.865547
Sum of electronic and zero-point Energies= -4288.338967
Sum of electronic and thermal Energies= -4288.280861
Sum of electronic and thermal Enthalpies= -4288.279916
Sum of electronic and thermal Free Energies= -4288.429365

| | | | |
|---|---|---|---|
| Ni | -0.84034900 | -0.15457800 | 0.38617700 |
| N | 1.27126200 | 1.61466600 | 1.44325500 |
| N | -0.29426300 | 1.42011800 | 2.91296100 |
| C | 3.06136100 | 0.86534800 | -0.06844100 |
| C | 3.89179900 | 1.18059400 | -1.15289100 |
| C | 3.65247400 | 2.30472000 | -1.94231500 |
| C | 2.56097700 | 3.13100800 | -1.68216000 |
| C | 1.71280100 | 2.88096300 | -0.59491200 |
| C | 2.00170400 | 1.75387900 | 0.20606600 |
| C | 1.71270100 | 2.27813600 | 2.58367200 |
| C | 0.73059400 | 2.15511400 | 3.50572100 |
| C | 0.03881100 | 1.07344300 | 1.64282400 |
| C | -1.54803100 | 1.29768700 | 3.63078100 |
| C | -1.78721600 | 0.15474800 | 4.41736000 |
| C | -2.91854000 | 0.18166900 | 5.24549800 |
| C | -3.75462500 | 1.29433300 | 5.28942200 |
| C | -3.50023600 | 2.40161500 | 4.48348900 |
| C | -2.39117100 | 2.42983900 | 3.63091600 |
| H | 4.73092700 | 0.52788100 | -1.39593000 |
| H | 4.30977500 | 2.52440700 | -2.78711900 |
| H | 2.36974900 | 3.98833000 | -2.32923600 |
| H | 2.67186900 | 2.78388200 | 2.61585600 |
| H | 0.64302500 | 2.52767400 | 4.52112800 |
| H | -3.15700200 | -0.68621700 | 5.85936600 |
| H | -4.63186300 | 1.28782800 | 5.94108600 |
| H | -4.18984900 | 3.24616100 | 4.50297100 |
| C | -1.67071000 | -1.03798800 | -1.36410100 |
| H | -2.64165000 | -1.35422800 | -0.99215300 |
| H | -0.98374500 | -1.82876300 | -1.65158100 |
| C | -2.74845500 | 1.14362000 | -1.97868200 |
| H | -2.44612600 | 2.19000400 | -2.13010700 |
| H | -3.26612600 | 1.09878500 | -1.01393600 |
| C | -0.34469600 | 0.50696000 | -2.78540200 |
| C | -0.44140700 | 1.39210900 | -3.87322500 |
| C | 0.86438600 | -0.19345400 | -2.60196800 |
| C | 0.61839400 | 1.53938100 | -4.77381700 |
| H | -1.35515500 | 1.96109800 | -4.04207000 |
| C | 1.91666700 | -0.04882600 | -3.50155200 |
| H | 0.98798200 | -0.84318500 | -1.73311900 |
| C | 1.79715200 | 0.81278200 | -4.59797100 |
| H | 0.51480900 | 2.22447100 | -5.61880600 |
| H | 2.84488300 | -0.59845500 | -3.33444700 |
| H | 2.62555600 | 0.92666200 | -5.30136100 |
| C | -3.72058600 | 0.69075800 | -3.07874500 |
| H | -4.09751900 | -0.32024500 | -2.86470700 |
| H | -4.58723100 | 1.36859800 | -3.11670200 |
| H | -3.25374300 | 0.67587200 | -4.07532700 |
| C | -1.52123300 | 0.24500500 | -1.89551300 |
| H | -0.94230100 | 1.12300400 | -0.35176100 |
| O | 0.16919800 | -1.60224000 | 0.95442600 |
| C | 0.09124900 | -3.01303500 | 0.95991900 |
| C | 0.63237200 | -3.59717100 | -0.35931500 |
| H | -0.01796100 | -3.35158200 | -1.20966500 |
| H | 1.63537900 | -3.19882000 | -0.56506400 |
| H | 0.69856000 | -4.69520800 | -0.31387500 |
| C | 1.00120600 | -3.46899200 | 2.13366700 |
| H | 0.69461000 | -2.88772700 | 3.01412100 |
| H | 2.02479700 | -3.13335200 | 1.89550200 |
| C | -1.36297300 | -3.45471100 | 1.17836100 |
| H | -1.46076500 | -4.55097100 | 1.20934100 |
| H | -1.76267500 | -3.03293800 | 2.10908100 |
| H | -1.99871600 | -3.08520000 | 0.36286200 |
| C | 1.01303300 | -4.95687000 | 2.48754700 |
| H | 1.72340600 | -5.15345700 | 3.30715900 |
| H | 0.02333100 | -5.30415000 | 2.82415800 |
| H | 1.31566400 | -5.58748600 | 1.63581800 |
| C | 0.55746200 | 3.82612500 | -0.27691000 |
| C | -0.19767800 | 4.28902500 | -1.53046200 |
| C | 1.03326200 | 5.03942100 | 0.54259000 |
| H | -0.16626700 | 3.27396900 | 0.33735500 |
| H | -0.47658800 | 3.43763100 | -2.16551700 |
| H | -1.11687800 | 4.82078100 | -1.23940300 |
| H | 0.40219600 | 4.98218900 | -2.14144300 |
| H | 1.52413400 | 4.73569600 | 1.47795400 |
| H | 1.75039100 | 5.64258700 | -0.03811100 |
| H | 0.17794300 | 5.68302600 | 0.80517000 |
| C | 3.28267100 | -0.39039300 | 0.76863000 |
| C | 4.17729500 | -0.12499900 | 1.99292000 |
| C | 3.86214600 | -1.54585600 | -0.05998600 |
| H | 2.29110500 | -0.71554100 | 1.12290900 |
| H | 3.74747500 | 0.62933900 | 2.66630700 |
| H | 4.30783700 | -1.05130700 | 2.57558300 |
| H | 5.17580600 | 0.22525200 | 1.68194600 |
| H | 3.28956800 | -1.70667600 | -0.98591800 |
| H | 4.91433500 | -1.37142700 | -0.33764300 |
| H | 3.83042900 | -2.47843300 | 0.52333700 |
| C | -0.85889600 | -1.05429000 | 4.36873000 |
| C | -1.53837400 | -2.35363900 | 4.82197000 |
| C | 0.42266600 | -0.83073700 | 5.19486900 |
| H | -0.56558900 | -1.18170300 | 3.31369100 |
| H | -2.49165800 | -2.50400700 | 4.29978000 |
| H | -0.88257200 | -3.21154000 | 4.60848800 |
| H | -1.72583500 | -2.35437800 | 5.90857400 |
| H | 1.01097300 | 0.02741600 | 4.84256700 |
| H | 0.17446600 | -0.66166400 | 6.25587200 |
| H | 1.07155300 | -1.71982900 | 5.13757700 |
| C | -2.15159000 | 3.61151100 | 2.69536400 |
| C | -2.56980000 | 4.96149200 | 3.29316400 |
| C | -2.84521000 | 3.36795900 | 1.34224100 |
| H | -1.06998100 | 3.68022400 | 2.50026100 |
| H | -2.12702800 | 5.12028100 | 4.28918800 |
| H | -2.23858200 | 5.78090400 | 2.63529800 |
| H | -3.66380000 | 5.04650400 | 3.39015200 |
| H | -2.46547700 | 2.45795000 | 0.86308400 |
| H | -3.92678900 | 3.22020600 | 1.48336500 |
| H | -2.68357700 | 4.22358100 | 0.66641300 |
| S | -4.03504800 | -0.36811000 | 1.77481700 |
| O | -3.78496100 | -1.54224900 | 2.62174000 |
| O | -4.84914400 | 0.72605000 | 2.31479500 |
| O | -2.82900800 | 0.12131200 | 1.01216500 |
| C | -5.13575500 | -1.04995400 | 0.41346000 |
| F | -4.57057400 | -2.10360800 | -0.20100200 |
| F | -6.29691800 | -1.44509100 | 0.92905900 |
| F | -5.37923100 | -0.11701900 | -0.51772800 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4291.7687392
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4289.0910775

**IV-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.955112 (Hartree/Particle)
Thermal correction to Energy= 1.014823
Thermal correction to Enthalpy= 1.015767
Thermal correction to Gibbs Free Energy= 0.859240
Sum of electronic and zero-point Energies= -4288.343229
Sum of electronic and thermal Energies= -4288.283518
Sum of electronic and thermal Enthalpies= -4288.282574
Sum of electronic and thermal Free Energies= -4288.439101

| | | | |
|---|---|---|---|
| Ni | 0.94094400 | -0.03926500 | -0.24543600 |
| N | 1.78610800 | 2.13822400 | 1.58028900 |
| N | -0.26573400 | 1.56344500 | 1.89554800 |

| | | | |
|---|---|---|---|
| C | 4.05803600 | 1.27952500 | 1.25856400 |
| C | 5.35561300 | 1.49965100 | 0.77620500 |
| C | 5.67673900 | 2.67206600 | 0.09960300 |
| C | 4.71009900 | 3.65554500 | -0.11726000 |
| C | 3.40039300 | 3.49528400 | 0.34682100 |
| C | 3.11209000 | 2.29484100 | 1.03267300 |
| C | 1.37420000 | 2.75454200 | 2.75288800 |
| C | 0.07775500 | 2.39318100 | 2.95137200 |
| C | 0.78893800 | 1.38435800 | 1.05617500 |
| C | -1.56544400 | 0.96784100 | 1.72566000 |
| C | -1.77443700 | -0.33755100 | 2.21274400 |
| C | -3.05387400 | -0.88516300 | 2.04097300 |
| C | -4.06734600 | -0.15759300 | 1.41765100 |
| C | -3.82685300 | 1.13332400 | 0.94527300 |
| C | -2.56649600 | 1.72914100 | 1.08524700 |
| H | 6.11819700 | 0.73231900 | 0.92008100 |
| H | 6.69009100 | 2.81791900 | -0.28223700 |
| H | 4.98068100 | 4.55230400 | -0.67383100 |
| H | 2.04173000 | 3.38936700 | 3.32770700 |
| H | -0.62427300 | 2.64054000 | 3.74087100 |
| H | -3.25933300 | -1.89441500 | 2.40295800 |
| H | -5.05585000 | -0.60515900 | 1.28923200 |
| H | -4.62959600 | 1.68075300 | 0.44925900 |
| C | -2.92670600 | -0.81720600 | -1.79494900 |
| H | -3.40669800 | -1.74496300 | -1.47175100 |
| H | -2.23029100 | -0.36051400 | -1.08919100 |
| C | -4.16844800 | -0.93224800 | -3.95224200 |
| H | -4.97558200 | -0.22388700 | -4.21025200 |
| H | -4.65829400 | -1.77681900 | -3.44147200 |
| C | -2.51436300 | 0.97427700 | -3.44896800 |
| C | -3.21389900 | 1.96411200 | -4.16797900 |
| C | -1.15784000 | 1.21160300 | -3.15599300 |
| C | -2.58949000 | 3.15682900 | -4.54228200 |
| H | -4.26637000 | 1.81465400 | -4.41825400 |
| C | -0.52857000 | 2.39899500 | -3.53566900 |
| H | -0.57221600 | 0.45558000 | -2.63821500 |
| C | -1.24474500 | 3.38106000 | -4.22568300 |
| H | -3.15863800 | 3.91657400 | -5.08476500 |
| H | 0.52625000 | 2.53159500 | -3.29743600 |
| H | -0.75549100 | 4.31196600 | -4.52362900 |
| C | -3.49852600 | -1.42266900 | -5.24371700 |
| H | -3.03535400 | -0.58880100 | -5.79436600 |
| H | -2.70631700 | -2.15496000 | -5.01874500 |
| H | -4.23112100 | -1.90446000 | -5.91078300 |
| C | -3.19206600 | -0.27507300 | -2.99660400 |
| H | -0.39103200 | 0.36574800 | -0.50765100 |
| O | 1.02391800 | -1.77933200 | -0.54223400 |
| C | 1.06386700 | -2.74807300 | -1.57007100 |
| C | 0.34810900 | -2.20195100 | -2.81097300 |
| H | -0.69648900 | -1.96889200 | -2.56166600 |
| H | 0.83401400 | -1.27985900 | -3.14921100 |
| H | 0.35291700 | -2.92648300 | -3.63891300 |
| C | 2.56384000 | -3.02791300 | -1.83479100 |
| H | 2.98656400 | -3.41975400 | -0.89409900 |
| H | 3.04373000 | -2.05362600 | -2.00365000 |
| C | 0.33971700 | -4.00114700 | -1.05526100 |
| H | 0.34507700 | -4.80747900 | -1.80486000 |
| H | 0.82341500 | -4.37174800 | -0.13825300 |
| H | -0.70757300 | -3.75720500 | -0.81853200 |
| C | 2.89578800 | -3.97226100 | -2.99006700 |
| H | 3.98325100 | -4.14164400 | -3.04615000 |
| H | 2.41554500 | -4.95799500 | -2.87637800 |
| H | 2.58350500 | -3.55265300 | -3.95854400 |
| C | 2.31637800 | 4.54597000 | 0.10767000 |
| C | 1.36622100 | 4.13523000 | -1.03380900 |
| C | 2.87307900 | 5.95272600 | -0.14221600 |
| H | 1.71254200 | 4.60626700 | 1.02812300 |
| H | 0.95825900 | 3.12599100 | -0.89354300 |
| H | 0.52498200 | 4.84388200 | -1.10473100 |
| H | 1.90677600 | 4.12020200 | -1.98984100 |
| H | 3.57539500 | 6.26329500 | 0.64747400 |
| H | 3.39671900 | 6.01543300 | -1.10937100 |
| H | 2.04772600 | 6.68123700 | -0.17259600 |
| C | 3.72275000 | -0.00277000 | 2.01092500 |
| C | 4.32791000 | 0.01656100 | 3.42451500 |
| C | 4.13853100 | -1.25728300 | 1.22739500 |
| H | 2.62955200 | -0.05551700 | 2.12882500 |
| H | 3.97536400 | 0.88657800 | 4.00141100 |
| H | 4.05316400 | -0.89660600 | 3.97728700 |
| H | 5.42808000 | 0.06669800 | 3.37759100 |
| H | 3.74610400 | -1.23055800 | 0.20294000 |
| H | 5.23453500 | -1.35125600 | 1.16661000 |
| H | 3.75186400 | -2.16002500 | 1.72663500 |
| C | -0.68517500 | -1.11169500 | 2.94577100 |
| C | -0.50700000 | -2.53753300 | 2.40645700 |
| C | -0.95519900 | -1.10002900 | 4.46107000 |
| H | 0.27064000 | -0.59166300 | 2.78129800 |
| H | -0.26075600 | -2.51785300 | 1.33587000 |
| H | 0.32148000 | -3.03641300 | 2.93487500 |
| H | -1.40969900 | -3.15043500 | 2.55834200 |
| H | -1.02484300 | -0.07152700 | 4.84973700 |
| H | -1.90296800 | -1.61236500 | 4.69440100 |
| H | -0.14643500 | -1.61702100 | 5.00202100 |
| C | -2.30708900 | 3.15488300 | 0.60920500 |
| C | -2.76397300 | 4.16897600 | 1.67499900 |
| C | -2.95171200 | 3.46839200 | -0.74646600 |
| H | -1.22043100 | 3.27137500 | 0.47894900 |
| H | -2.26950600 | 4.00279200 | 2.64364200 |
| H | -2.53695100 | 5.19705200 | 1.35015300 |
| H | -3.85181600 | 4.09459400 | 1.83681000 |
| H | -2.66075800 | 2.73673500 | -1.50982500 |
| H | -4.05165600 | 3.48503700 | -0.68537300 |
| H | -2.62915300 | 4.46249200 | -1.09269600 |
| S | 3.19499600 | 1.06852300 | -2.46376000 |
| O | 1.82428100 | 0.89459800 | -1.83978100 |
| O | 3.51412800 | 2.47349100 | -2.75103400 |
| O | 4.23493200 | 0.22287700 | -1.86122300 |
| C | 2.96235800 | 0.35495300 | -4.19532500 |
| F | 3.93630700 | 0.80469200 | -4.98550200 |
| F | 1.78753600 | 0.72441100 | -4.71197500 |
| F | 3.01513100 | -0.98097400 | -4.18638000 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4291.7669937
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4289.091339

**V-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.916502 (Hartree/Particle)
Thermal correction to Energy= 0.967522
Thermal correction to Enthalpy= 0.968466
Thermal correction to Gibbs Free Energy= 0.829240
Sum of electronic and zero-point Energies= -3326.877119
Sum of electronic and thermal Energies= -3326.826099
Sum of electronic and thermal Enthalpies= -3326.825155
Sum of electronic and thermal Free Energies= -3326.964381

| | | | |
|---|---|---|---|
| Ni | -0.78785400 | 0.40426100 | -1.76398900 |
| C | -2.62361300 | 0.07913000 | -1.46252400 |
| C | -4.84823100 | -0.40567600 | -1.64533400 |
| C | -4.63569200 | 0.05745000 | -0.38503900 |
| N | -3.27730600 | 0.33994600 | -0.28962400 |
| N | -3.61274000 | -0.37944900 | -2.28659900 |
| H | -5.31541000 | 0.20837300 | 0.44846800 |
| H | -5.75067000 | -0.74546000 | -2.14483500 |
| C | -2.63094400 | 0.87543300 | 0.87761400 |
| C | -2.28727500 | -0.01018200 | 1.92254700 |
| C | -2.35441200 | 2.25536100 | 0.92490500 |
| C | -1.66967200 | 0.53545700 | 3.05486400 |

| | | | |
|---|---|---|---|
| C | -1.72978700 | 2.74977500 | 2.08003100 |
| C | -1.39783800 | 1.90313500 | 3.13507600 |
| H | -1.38232300 | -0.11513700 | 3.88195000 |
| H | -1.49633800 | 3.81459800 | 2.14847400 |
| H | -0.90969000 | 2.30794900 | 4.02520500 |
| C | -3.38156000 | -0.75580500 | -3.65157000 |
| C | -2.86149900 | -2.03747200 | -3.92025500 |
| C | -3.65459300 | 0.18964000 | -4.66463400 |
| C | -2.59410600 | -2.35787100 | -5.26026500 |
| C | -3.39354600 | -0.19006800 | -5.98805700 |
| C | -2.86254000 | -1.44811400 | -6.28204700 |
| H | -2.17100700 | -3.33426200 | -5.50621400 |
| H | -3.58269700 | 0.51280400 | -6.80081900 |
| H | -2.64854600 | -1.71733700 | -7.31931800 |
| O | 0.80063500 | 1.17396300 | -1.34815900 |
| C | 1.85674700 | 0.67562100 | -0.57374800 |
| C | 1.54447300 | 0.94266600 | 0.91060400 |
| H | 1.43986800 | 2.02537800 | 1.08524400 |
| H | 0.58156300 | 0.47388400 | 1.16490600 |
| H | 2.31577500 | 0.54881900 | 1.59309200 |
| C | 3.12979600 | 1.43386800 | -1.02627200 |
| H | 3.22144300 | 1.26823800 | -2.11310200 |
| H | 2.91562100 | 2.50969700 | -0.90061200 |
| C | 2.02326800 | -0.83973000 | -0.80192000 |
| H | 1.09266900 | -1.35479900 | -0.51986000 |
| H | 2.21406800 | -1.03714300 | -1.86663700 |
| H | 2.84693000 | -1.27555700 | -0.21241800 |
| C | 4.44813400 | 1.07998400 | -0.33569600 |
| H | 4.72693700 | 0.02628100 | -0.50067000 |
| H | 5.27432000 | 1.69927400 | -0.72322800 |
| H | 4.40095700 | 1.24321200 | 0.75357800 |
| C | -2.56548600 | -3.03733600 | -2.80771800 |
| C | -1.05156400 | -3.16775200 | -2.57624300 |
| C | -3.21813500 | -4.40405100 | -3.06628600 |
| H | -2.99757200 | -2.64067000 | -1.87729900 |
| H | -0.61340800 | -2.18669000 | -2.33895400 |
| H | -0.84372300 | -3.84533100 | -1.73349300 |
| H | -0.54516000 | -3.56962100 | -3.46888800 |
| H | -4.30388900 | -4.30738900 | -3.22492600 |
| H | -2.78981800 | -4.90052600 | -3.95180900 |
| H | -3.05543700 | -5.07131900 | -2.20476800 |
| C | -4.11496600 | 1.60220900 | -4.31758700 |
| C | -5.08526600 | 2.19978700 | -5.34457400 |
| C | -2.89472300 | 2.52045400 | -4.10839400 |
| H | -4.65110000 | 1.55380800 | -3.35782000 |
| H | -5.93955300 | 1.53049600 | -5.53277000 |
| H | -5.47681600 | 3.16121600 | -4.97660500 |
| H | -4.59128700 | 2.40026200 | -6.30882500 |
| H | -2.19912100 | 2.10600900 | -3.36269300 |
| H | -2.34285700 | 2.64670800 | -5.05382600 |
| H | -3.21367600 | 3.51663700 | -3.76223800 |
| C | -2.49004300 | -1.51405300 | 1.76985800 |
| C | -2.74261800 | -2.24560800 | 3.09353200 |
| C | -1.29132800 | -2.12272500 | 1.01771700 |
| H | -3.38023000 | -1.66997800 | 1.14077600 |
| H | -3.56850600 | -1.78748000 | 3.66048700 |
| H | -3.00279500 | -3.29781600 | 2.89757700 |
| H | -1.84895400 | -2.24929400 | 3.73809800 |
| H | -1.11566200 | -1.59997400 | 0.06639200 |
| H | -0.37198600 | -2.03371600 | 1.61867300 |
| H | -1.46311900 | -3.19018800 | 0.80351600 |
| C | -2.69070900 | 3.19552000 | -0.22579000 |
| C | -1.42238900 | 3.85065400 | -0.79798200 |
| C | -3.73977800 | 4.23945500 | 0.18946900 |
| H | -3.12986600 | 2.59534600 | -1.03438700 |
| H | -0.68405000 | 3.08690900 | -1.08653300 |
| H | -1.67446200 | 4.45263100 | -1.68617500 |
| H | -0.95125900 | 4.52288000 | -0.06189600 |
| H | -4.65967600 | 3.75870400 | 0.55959200 |
| H | -3.35948500 | 4.89813800 | 0.98752600 |
| H | -4.00808000 | 4.87672100 | -0.66908300 |
| C | 3.11733200 | -1.81609200 | -4.48174500 |
| C | 4.29498600 | -1.74186500 | -3.83420700 |
| H | 4.91309800 | -2.63146800 | -3.68318500 |
| H | 4.66465100 | -0.80562000 | -3.40857100 |
| C | 2.59509100 | -3.14564300 | -4.99218200 |
| H | 1.64818000 | -3.38488100 | -4.47595700 |
| H | 3.30104800 | -3.93979900 | -4.70189100 |
| C | 2.27554600 | -0.60554200 | -4.69827600 |
| C | 0.87078400 | -0.68933100 | -4.70527400 |
| C | 2.85563600 | 0.66624900 | -4.87678700 |
| C | 0.07808900 | 0.45209100 | -4.84007300 |
| H | 0.37787500 | -1.65181200 | -4.57450500 |
| C | 2.06513200 | 1.80797000 | -5.01846900 |
| H | 3.94306800 | 0.75853000 | -4.91527900 |
| C | 0.67128300 | 1.70796200 | -4.98790300 |
| H | -1.00641000 | 0.35300200 | -4.81356900 |
| H | 2.54245800 | 2.78275100 | -5.14788400 |
| H | 0.05169500 | 2.60295000 | -5.07657200 |
| C | 2.36541900 | -3.18584600 | -6.50883400 |
| H | 1.62624600 | -2.43293400 | -6.82355400 |
| H | 3.30205500 | -2.98245000 | -7.05266500 |
| H | 1.99637300 | -4.17501700 | -6.82413900 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3329.4968332
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3327.4258565

**(*E*)-TS-V-VI-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.912483 (Hartree/Particle)
Thermal correction to Energy= 0.962127
Thermal correction to Enthalpy= 0.963071
Thermal correction to Gibbs Free Energy= 0.829975
Sum of electronic and zero-point Energies= -3326.830567
Sum of electronic and thermal Energies= -3326.780924
Sum of electronic and thermal Enthalpies= -3326.779979
Sum of electronic and thermal Free Energies= -3326.913076

| | | | |
|---|---|---|---|
| Ni | -0.16247500 | -0.06522900 | -0.68285500 |
| N | 0.36927100 | -0.41863500 | 2.20302900 |
| N | -1.54037400 | -1.27043500 | 1.70105700 |
| C | 2.73778200 | -0.83224200 | 1.83157700 |
| C | 4.03977400 | -0.33395100 | 1.67996000 |
| C | 4.28467500 | 1.03619400 | 1.70989600 |
| C | 3.23308400 | 1.93983700 | 1.87885500 |
| C | 1.91141000 | 1.49992000 | 2.04457100 |
| C | 1.70164800 | 0.10146900 | 2.03817900 |
| C | -0.14553800 | -0.95356900 | 3.38186100 |
| C | -1.35565000 | -1.48422900 | 3.06624500 |
| C | -0.48024200 | -0.61540900 | 1.16301700 |
| C | -2.62786900 | -1.80446600 | 0.92184200 |
| C | -2.60411400 | -3.18254400 | 0.62122000 |
| C | -3.64835500 | -3.68880800 | -0.16686700 |
| C | -4.66063900 | -2.85240000 | -0.63361600 |
| C | -4.65347200 | -1.49124100 | -0.32360700 |
| C | -3.63767400 | -0.92972700 | 0.46322700 |
| H | 4.86753500 | -1.02778200 | 1.52179600 |
| H | 5.30416700 | 1.40992400 | 1.58515700 |
| H | 3.45335300 | 3.00669500 | 1.87401100 |
| H | 0.39132000 | -0.90119600 | 4.32384300 |
| H | -2.09710900 | -1.99327100 | 3.67458800 |
| H | -3.66270700 | -4.74781200 | -0.42992100 |
| H | -5.46304300 | -3.26318000 | -1.25183600 |
| H | -5.45308200 | -0.85706600 | -0.70661300 |
| C | 1.29738900 | -1.84584400 | -2.82047000 |
| C | 0.10147600 | -1.02317400 | -2.46591400 |
| C | 1.23607800 | -3.16674700 | -3.09772400 |
| H | 0.68648400 | -1.23131700 | -0.64693400 |

| | | | |
|---|---|---|---|
| H | 0.29474700 | -3.71803900 | -3.08024600 |
| H | 2.13863400 | -3.73899500 | -3.32574100 |
| C | 2.61402000 | -1.13598400 | -2.90875000 |
| C | 3.46065300 | -1.36240700 | -4.01196400 |
| C | 3.05286800 | -0.22977100 | -1.92331600 |
| C | 4.69547000 | -0.71811400 | -4.12393000 |
| H | 3.13087600 | -2.04218900 | -4.80100500 |
| C | 4.28878200 | 0.41297800 | -2.03152200 |
| H | 2.43880300 | -0.04410900 | -1.04178200 |
| C | 5.11682000 | 0.17447000 | -3.13246600 |
| H | 5.32774400 | -0.90849300 | -4.99541800 |
| H | 4.60259800 | 1.09754300 | -1.23977900 |
| H | 6.08135000 | 0.68157200 | -3.21909800 |
| O | -1.08725300 | 1.55960100 | -0.79596900 |
| C | -0.81279100 | 2.63520800 | -1.65479100 |
| C | -1.54999100 | 2.37010900 | -2.99456200 |
| H | -1.22024200 | 1.38109800 | -3.35229900 |
| H | -2.61982600 | 2.25841900 | -2.74992900 |
| C | 0.70676200 | 2.77439200 | -1.88379800 |
| H | 0.97789700 | 3.69328600 | -2.42761600 |
| H | 1.21785400 | 2.78278400 | -0.90979900 |
| H | 1.09972500 | 1.91628000 | -2.45090900 |
| C | -1.35734900 | 3.91492600 | -0.99448100 |
| H | -1.17826900 | 4.81607800 | -1.60286600 |
| H | -2.44094100 | 3.81343600 | -0.82719400 |
| H | -0.87589800 | 4.05990200 | -0.01782700 |
| C | -1.37375000 | 3.39918300 | -4.11282700 |
| H | -1.94927600 | 3.10920200 | -5.00739800 |
| H | -1.72217900 | 4.40027200 | -3.81107200 |
| H | -0.31946500 | 3.49326400 | -4.41985800 |
| C | -3.61667100 | 0.55392100 | 0.81627200 |
| C | -4.03877500 | 0.78451600 | 2.27923200 |
| C | -4.45909400 | 1.41854000 | -0.12579600 |
| H | -2.58210100 | 0.90197600 | 0.67960300 |
| H | -3.40164300 | 0.23518300 | 2.98754100 |
| H | -3.96945100 | 1.85513400 | 2.53188900 |
| H | -5.08136200 | 0.46350500 | 2.44297700 |
| H | -4.17407000 | 1.25584700 | -1.17541900 |
| H | -5.54055000 | 1.22971700 | -0.01900300 |
| H | -4.28704900 | 2.48172200 | 0.10141400 |
| C | -1.45154800 | -4.08534700 | 1.05455500 |
| C | -0.39362800 | -4.17202100 | -0.05891800 |
| C | -1.90883200 | -5.48219200 | 1.49745700 |
| H | -0.96228700 | -3.62410900 | 1.92450300 |
| H | -0.02881400 | -3.17582100 | -0.34550600 |
| H | 0.47063200 | -4.76980800 | 0.27122900 |
| H | -0.81256000 | -4.64881400 | -0.95932900 |
| H | -2.68884100 | -5.42600800 | 2.27320300 |
| H | -2.30871600 | -6.07100000 | 0.65657700 |
| H | -1.05540700 | -6.04415500 | 1.90890800 |
| C | 2.47990500 | -2.33511600 | 1.78409800 |
| C | 2.94773300 | -3.00844900 | 3.08605200 |
| C | 3.10870800 | -3.00187000 | 0.55126500 |
| H | 1.39549400 | -2.49130400 | 1.70362500 |
| H | 2.45454400 | -2.56783200 | 3.96674100 |
| H | 2.71720100 | -4.08603000 | 3.06910100 |
| H | 4.03636700 | -2.89605300 | 3.21864200 |
| H | 2.73310000 | -2.55628600 | -0.38049200 |
| H | 4.20689900 | -2.91761100 | 0.55092300 |
| H | 2.86009900 | -4.07458700 | 0.53670000 |
| C | 0.74777800 | 2.48226300 | 2.18744700 |
| C | 1.13125800 | 3.92865500 | 1.84910500 |
| C | 0.12018400 | 2.45566700 | 3.59509300 |
| H | -0.01403800 | 2.16205300 | 1.45274000 |
| H | 1.56991900 | 4.02217100 | 0.84536000 |
| H | 0.23543200 | 4.56658200 | 1.88151900 |
| H | 1.84810600 | 4.34037400 | 2.57843900 |
| H | -0.27991500 | 1.47143700 | 3.86686100 |
| H | 0.86356600 | 2.74518300 | 4.35657400 |
| H | -0.71452800 | 3.17288300 | 3.64806700 |
| C | -1.26409600 | -1.63736600 | -2.73885800 |
| H | -1.33053100 | -2.01950900 | -3.77484800 |
| H | -1.48424600 | -2.47513700 | -2.06203000 |
| H | -2.05975500 | -0.89163700 | -2.59635600 |
| H | 0.19886400 | -0.04855300 | -2.97555800 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3329.4421338
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3327.3712832

**(*E*)-VI-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.913248 (Hartree/Particle)
Thermal correction to Energy= 0.963421
Thermal correction to Enthalpy= 0.964365
Thermal correction to Gibbs Free Energy= 0.829355
Sum of electronic and zero-point Energies= -3326.829916
Sum of electronic and thermal Energies= -3326.779743
Sum of electronic and thermal Enthalpies= -3326.778798
Sum of electronic and thermal Free Energies= -3326.913808

| | | | |
|---|---|---|---|
| Ni | -0.24204900 | -0.01264100 | -0.70957500 |
| N | 0.34412100 | -0.34883700 | 2.17768500 |
| N | -1.57257500 | -1.20050300 | 1.69855800 |
| C | 2.70597600 | -0.73320400 | 1.73064200 |
| C | 3.99747000 | -0.21723500 | 1.55099800 |
| C | 4.23087700 | 1.15431900 | 1.60925200 |
| C | 3.17774000 | 2.04300300 | 1.83749700 |
| C | 1.86710500 | 1.58382300 | 2.03263000 |
| C | 1.66884200 | 0.18479100 | 1.99374700 |
| C | -0.14734400 | -0.90392500 | 3.35709200 |
| C | -1.36163000 | -1.43453700 | 3.05606000 |
| C | -0.52430000 | -0.53500800 | 1.15123900 |
| C | -2.67092800 | -1.72141700 | 0.92528400 |
| C | -2.63421700 | -3.08492800 | 0.56799500 |
| C | -3.68387900 | -3.57121900 | -0.22553200 |
| C | -4.71369200 | -2.72943200 | -0.64180900 |
| C | -4.72101400 | -1.38308600 | -0.27214400 |
| C | -3.70071100 | -0.84312800 | 0.52317300 |
| H | 4.82625900 | -0.89795200 | 1.34836600 |
| H | 5.24238300 | 1.54086200 | 1.46095800 |
| H | 3.38663200 | 3.11221900 | 1.85523300 |
| H | 0.40767700 | -0.86677000 | 4.28919300 |
| H | -2.08831200 | -1.95825700 | 3.66972300 |
| H | -3.68759500 | -4.61820300 | -0.53377000 |
| H | -5.51887000 | -3.12413500 | -1.26684300 |
| H | -5.53444000 | -0.74319600 | -0.61461700 |
| C | 1.16517500 | -1.68636200 | -2.92604400 |
| C | -0.02154200 | -0.86581500 | -2.54894500 |
| C | 1.09532100 | -3.00492100 | -3.21734800 |
| H | 0.67555000 | -1.12414700 | -0.59911400 |
| H | 0.15138400 | -3.55133100 | -3.19602300 |
| H | 1.99226300 | -3.58077900 | -3.45809300 |
| C | 2.48574800 | -0.98415600 | -3.02424500 |
| C | 3.33609400 | -1.23261800 | -4.12032100 |
| C | 2.92675600 | -0.06277900 | -2.05407300 |
| C | 4.57573000 | -0.59856900 | -4.23709100 |
| H | 3.00584900 | -1.92166700 | -4.90104200 |
| C | 4.16722800 | 0.57027700 | -2.16650700 |
| H | 2.30689400 | 0.14210800 | -1.18145400 |
| C | 4.99951500 | 0.30721800 | -3.25857000 |
| H | 5.21026000 | -0.80728000 | -5.10277500 |
| H | 4.48143500 | 1.26644300 | -1.38490200 |
| H | 5.96820400 | 0.80573500 | -3.34896000 |
| O | -1.28001000 | 1.53094700 | -0.86513600 |
| C | -0.97681100 | 2.68255000 | -1.60901200 |
| C | -1.66734700 | 2.54358900 | -2.99227300 |
| H | -1.31866900 | 1.59556800 | -3.43337500 |
| H | -2.74463700 | 2.40676600 | -2.79689100 |

| | | | |
|---|---|---|---|
| C | 0.54896300 | 2.84297000 | -1.77350400 |
| H | 0.83423700 | 3.81763500 | -2.20032500 |
| H | 1.02959000 | 2.74058500 | -0.78915800 |
| H | 0.96217900 | 2.05586600 | -2.42231200 |
| C | -1.54663300 | 3.89478100 | -0.84914500 |
| H | -1.32887800 | 4.85152200 | -1.35047600 |
| H | -2.63750900 | 3.79101900 | -0.74794700 |
| H | -1.11516100 | 3.93055600 | 0.16057600 |
| C | -1.45871400 | 3.67985300 | -3.99530400 |
| H | -2.00337100 | 3.48051700 | -4.93284500 |
| H | -1.82075000 | 4.64512300 | -3.60580300 |
| H | -0.39522900 | 3.80450400 | -4.25602600 |
| C | -3.70136500 | 0.61893800 | 0.95647400 |
| C | -4.16334100 | 0.75653500 | 2.41903300 |
| C | -4.52736500 | 1.52695900 | 0.04163700 |
| H | -2.66572400 | 0.97746100 | 0.86870500 |
| H | -3.54223200 | 0.16430900 | 3.10704600 |
| H | -4.10744100 | 1.80918700 | 2.74110600 |
| H | -5.20780400 | 0.42091100 | 2.53393800 |
| H | -4.19246400 | 1.43858400 | -1.00154100 |
| H | -5.60715500 | 1.30911300 | 0.09397900 |
| H | -4.39137100 | 2.57594400 | 0.34612800 |
| C | -1.46713800 | -3.99093100 | 0.95098700 |
| C | -0.44635400 | -4.06170500 | -0.19726200 |
| C | -1.91186400 | -5.39304300 | 1.39082600 |
| H | -0.95084200 | -3.53978800 | 1.81053100 |
| H | -0.09049800 | -3.06102700 | -0.47963700 |
| H | 0.42750900 | -4.66538600 | 0.09535000 |
| H | -0.89505100 | -4.52462500 | -1.09051800 |
| H | -2.66332200 | -5.34591800 | 2.19489800 |
| H | -2.34386500 | -5.96847300 | 0.55657100 |
| H | -1.04579100 | -5.96289900 | 1.76324400 |
| C | 2.45779700 | -2.23635300 | 1.65470200 |
| C | 2.93097000 | -2.93000400 | 2.94408100 |
| C | 3.08887900 | -2.87714400 | 0.40970300 |
| H | 1.37404200 | -2.39686100 | 1.57170500 |
| H | 2.43369100 | -2.51077400 | 3.83282700 |
| H | 2.71018600 | -4.00913100 | 2.90675200 |
| H | 4.01852000 | -2.80966200 | 3.07865200 |
| H | 2.72481600 | -2.40157300 | -0.51177000 |
| H | 4.18805600 | -2.80647700 | 0.42012600 |
| H | 2.82799000 | -3.94605400 | 0.36506700 |
| C | 0.69948900 | 2.54678100 | 2.25058000 |
| C | 1.03378300 | 4.00084800 | 1.89346800 |
| C | 0.16659700 | 2.50057400 | 3.69611000 |
| H | -0.10375800 | 2.21314700 | 1.56914600 |
| H | 1.41560400 | 4.10256400 | 0.86777900 |
| H | 0.12814800 | 4.62033300 | 1.97586700 |
| H | 1.78051800 | 4.42593700 | 2.58375100 |
| H | -0.18565300 | 1.50361900 | 3.98768600 |
| H | 0.95181100 | 2.80723300 | 4.40689800 |
| H | -0.68187500 | 3.19443400 | 3.80840900 |
| C | -1.39425800 | -1.46906700 | -2.81065800 |
| H | -1.48449900 | -1.82770600 | -3.85366600 |
| H | -1.60586100 | -2.32196000 | -2.14932200 |
| H | -2.18040900 | -0.72092000 | -2.63295700 |
| H | 0.06922900 | 0.11929600 | -3.03773400 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3329.44441
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3327.3707625

**(*E*)-VII-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.913809 (Hartree/Particle)
Thermal correction to Energy= 0.963754
Thermal correction to Enthalpy= 0.964698
Thermal correction to Gibbs Free Energy= 0.831788
Sum of electronic and zero-point Energies= -3326.832564
Sum of electronic and thermal Energies= -3326.782618
Sum of electronic and thermal Enthalpies= -3326.781674
Sum of electronic and thermal Free Energies= -3326.914585

| | | | |
|---|---|---|---|
| Ni | 0.26581100 | 0.17141400 | -0.77121800 |
| N | 0.44277800 | -0.11954800 | 2.22014900 |
| N | -1.27437300 | -1.19504500 | 1.50474100 |
| C | 2.88005100 | -0.24352300 | 2.20270700 |
| C | 4.11928100 | 0.39571700 | 2.34849200 |
| C | 4.19219000 | 1.77094800 | 2.55819000 |
| C | 3.02837700 | 2.53817300 | 2.60982600 |
| C | 1.75988300 | 1.95322200 | 2.47372300 |
| C | 1.71762200 | 0.55350100 | 2.28717000 |
| C | -0.17042600 | -0.67712500 | 3.33955600 |
| C | -1.25756400 | -1.35111300 | 2.89050800 |
| C | -0.22803000 | -0.43906900 | 1.08027600 |
| C | -2.20445000 | -1.91827900 | 0.67204800 |
| C | -1.94417000 | -3.28972800 | 0.45377700 |
| C | -2.89037000 | -4.02161700 | -0.27761500 |
| C | -4.05027600 | -3.41165500 | -0.75243500 |
| C | -4.27210900 | -2.05232400 | -0.53535700 |
| C | -3.35026200 | -1.26416700 | 0.17044600 |
| H | 5.03887900 | -0.18915300 | 2.29391800 |
| H | 5.16602500 | 2.25436500 | 2.67113500 |
| H | 3.11505100 | 3.61459000 | 2.75501300 |
| H | 0.22403400 | -0.54220500 | 4.34133700 |
| H | -2.01241400 | -1.93040500 | 3.41323800 |
| H | -2.72108800 | -5.08066800 | -0.47672200 |
| H | -4.78337200 | -3.99835800 | -1.31189700 |
| H | -5.17559600 | -1.59542000 | -0.93749900 |
| C | 0.42263600 | -1.01410200 | -3.19891400 |
| C | 1.02732800 | -2.22909100 | -3.15022000 |
| C | 1.01854900 | 0.22154700 | -2.63213300 |
| H | 1.56946700 | -0.47435400 | -0.57823300 |
| H | 2.11524800 | 0.23561500 | -2.66396800 |
| H | 0.62669600 | 1.13008900 | -3.09967500 |
| C | -0.93806700 | -0.90237300 | -3.81014500 |
| C | -1.14591100 | -0.07897100 | -4.93185000 |
| C | -2.03849100 | -1.58881000 | -3.27185900 |
| C | -2.41348200 | 0.05270700 | -5.50182700 |
| H | -0.29963200 | 0.46852400 | -5.35475900 |
| C | -3.31059300 | -1.45559700 | -3.83981300 |
| H | -1.90077900 | -2.20968900 | -2.38385500 |
| C | -3.50373300 | -0.63517300 | -4.95501300 |
| H | -2.55318400 | 0.69716200 | -6.37384600 |
| H | -4.15391100 | -1.98913800 | -3.39675900 |
| H | -4.49891000 | -0.52779300 | -5.39434900 |
| O | -0.74080400 | 1.73230700 | -0.55388300 |
| C | -0.99019900 | 2.88694600 | -1.31940000 |
| C | -1.78805000 | 2.49311300 | -2.58540800 |
| H | -1.25870700 | 1.65879200 | -3.05738600 |
| H | -2.74641600 | 2.07259400 | -2.24573400 |
| C | 0.33947600 | 3.58180900 | -1.67137000 |
| H | 0.18348600 | 4.56888200 | -2.13478800 |
| H | 0.92581500 | 3.72009700 | -0.75109600 |
| H | 0.93737600 | 2.96675400 | -2.35776500 |
| C | -1.83998800 | 3.83374400 | -0.44898000 |
| H | -2.12228000 | 4.75262500 | -0.98762300 |
| H | -2.75944700 | 3.32003600 | -0.12955600 |
| H | -1.28348000 | 4.12414300 | 0.45115800 |
| C | -2.04566500 | 3.57917400 | -3.62967600 |
| H | -2.64343400 | 3.17441500 | -4.46281600 |
| H | -2.59856800 | 4.43774000 | -3.21382500 |
| H | -1.10764300 | 3.96565200 | -4.06026200 |
| C | -3.56483300 | 0.23408900 | 0.36581500 |
| C | -3.99187600 | 0.57774400 | 1.80529000 |
| C | -4.57453800 | 0.82392100 | -0.62702900 |
| H | -2.59469600 | 0.72260200 | 0.16772400 |
| H | -3.25702400 | 0.24727100 | 2.55201800 |
| H | -4.10446300 | 1.66859700 | 1.91442700 |

| | | | |
|---|---|---|---|
| H | -4.96053600 | 0.10977500 | 2.04943800 |
| H | -4.32754000 | 0.55758300 | -1.66586600 |
| H | -5.60345100 | 0.48523200 | -0.42021400 |
| H | -4.57320200 | 1.92144000 | -0.55044900 |
| C | -0.64655200 | -3.93996700 | 0.92495900 |
| C | 0.43789300 | -3.76500100 | -0.15052600 |
| C | -0.80087000 | -5.41318200 | 1.32367200 |
| H | -0.30236400 | -3.40365800 | 1.82187000 |
| H | 0.58337300 | -2.70569600 | -0.39889400 |
| H | 1.40156500 | -4.17332500 | 0.19240600 |
| H | 0.15456300 | -4.28359700 | -1.08002200 |
| H | -1.61636400 | -5.55442200 | 2.05036400 |
| H | -1.00501100 | -6.05699100 | 0.45324000 |
| H | 0.13324600 | -5.77606200 | 1.78079900 |
| C | 2.81167200 | -1.74997300 | 1.97733900 |
| C | 2.85932000 | -2.51883700 | 3.31006200 |
| C | 3.90219800 | -2.25703300 | 1.02250100 |
| H | 1.84743900 | -1.96849400 | 1.49999900 |
| H | 2.04631300 | -2.21579400 | 3.98576400 |
| H | 2.76473700 | -3.60284400 | 3.13297300 |
| H | 3.81522700 | -2.34011400 | 3.82959400 |
| H | 3.93886400 | -1.65571700 | 0.10259600 |
| H | 4.90095100 | -2.23285000 | 1.48696600 |
| H | 3.69912100 | -3.30166600 | 0.73956800 |
| C | 0.48752300 | 2.79778200 | 2.51167600 |
| C | 0.74827600 | 4.28269200 | 2.22389000 |
| C | -0.25558000 | 2.67816900 | 3.85653200 |
| H | -0.16287800 | 2.41117500 | 1.70743200 |
| H | 1.29092100 | 4.43230200 | 1.27917400 |
| H | -0.20760300 | 4.82265300 | 2.15287600 |
| H | 1.32588900 | 4.76089700 | 3.03157900 |
| H | -0.56137800 | 1.64953400 | 4.08333900 |
| H | 0.37884300 | 3.03619700 | 4.68470100 |
| H | -1.16898700 | 3.29454700 | 3.83915400 |
| C | 2.38666600 | -2.46298900 | -2.56578400 |
| H | 2.48059100 | -1.95573100 | -1.58882800 |
| H | 2.59503400 | -3.53331900 | -2.42170200 |
| H | 3.18804100 | -2.04793900 | -3.20454900 |
| H | 0.49327600 | -3.08793700 | -3.57037200 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3329.4498983
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3327.3733344

**(*E*)-TS-VII-B-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.912461 (Hartree/Particle)
Thermal correction to Energy= 0.962379
Thermal correction to Enthalpy= 0.963323
Thermal correction to Gibbs Free Energy= 0.828954
Sum of electronic and zero-point Energies= -3326.831599
Sum of electronic and thermal Energies= -3326.781681
Sum of electronic and thermal Enthalpies= -3326.780737
Sum of electronic and thermal Free Energies= -3326.915106

| | | | |
|---|---|---|---|
| Ni | 0.05483100 | 0.22923100 | -0.76834100 |
| N | 0.43617200 | -0.15741300 | 2.19362800 |
| N | -1.22566900 | -1.30429000 | 1.45299500 |
| C | 2.85158000 | 0.13353100 | 1.94336400 |
| C | 3.97559900 | 0.96678100 | 2.03444300 |
| C | 3.85020900 | 2.29823600 | 2.42813700 |
| C | 2.59676500 | 2.82857200 | 2.73154500 |
| C | 1.43726700 | 2.04328000 | 2.65063500 |
| C | 1.59598000 | 0.69475000 | 2.26022700 |
| C | -0.09538900 | -0.83843300 | 3.28611600 |
| C | -1.15037700 | -1.55417400 | 2.81995700 |
| C | -0.24588800 | -0.44986200 | 1.05087200 |
| C | -2.17641700 | -1.92459200 | 0.56383500 |
| C | -1.95046400 | -3.26507300 | 0.18424500 |
| C | -2.86023500 | -3.84339700 | -0.71202200 |
| C | -3.94614000 | -3.11501800 | -1.19557600 |
| C | -4.15608000 | -1.79990000 | -0.78241400 |
| C | -3.28055700 | -1.17010400 | 0.11290800 |
| H | 4.96390000 | 0.57027100 | 1.79705100 |
| H | 4.73822800 | 2.93198400 | 2.49442200 |
| H | 2.52094900 | 3.87528000 | 3.02747500 |
| H | 0.32941300 | -0.75672600 | 4.28086500 |
| H | -1.84608100 | -2.21795200 | 3.32410600 |
| H | -2.71317200 | -4.87161600 | -1.04539600 |
| H | -4.63358300 | -3.57407200 | -1.91021700 |
| H | -5.01028700 | -1.25104600 | -1.17726000 |
| C | 0.26967300 | -1.50471800 | -3.23329200 |
| C | 1.02914500 | -2.62668300 | -3.31059000 |
| C | 0.81389800 | -0.27494800 | -2.58637100 |
| H | 1.18264400 | -0.68096600 | -0.83307100 |
| H | 1.90587100 | -0.22458800 | -2.66922700 |
| H | 0.39667800 | 0.63981200 | -3.02943800 |
| C | -1.11758400 | -1.47942600 | -3.79229700 |
| C | -1.52179200 | -2.39362800 | -4.79097400 |
| C | -2.06929000 | -0.53140200 | -3.36326500 |
| C | -2.81538300 | -2.38215200 | -5.31320500 |
| H | -0.80491400 | -3.11436900 | -5.18863900 |
| C | -3.36275400 | -0.51582400 | -3.89440300 |
| H | -1.81748700 | 0.20559500 | -2.59866500 |
| C | -3.74989600 | -1.44018800 | -4.86624100 |
| H | -3.09034500 | -3.10386300 | -6.08747700 |
| H | -4.07632900 | 0.22906800 | -3.53290700 |
| H | -4.76189200 | -1.42377800 | -5.27950200 |
| C | 2.43174100 | -2.74550900 | -2.79057400 |
| H | 3.14924600 | -2.15303100 | -3.38816300 |
| H | 2.51264900 | -2.37261700 | -1.75642300 |
| H | 2.77874400 | -3.78926300 | -2.79815500 |
| H | 0.59750000 | -3.52886600 | -3.75184900 |
| O | -1.17704200 | 1.59963400 | -1.04142900 |
| C | -0.85910200 | 2.93936400 | -1.30281200 |
| C | -1.11540000 | 3.19717900 | -2.81151900 |
| H | -0.47509800 | 2.49989400 | -3.37762800 |
| H | -2.15312400 | 2.88328800 | -3.01572700 |
| C | 0.61597400 | 3.22179600 | -0.94872500 |
| H | 0.88464800 | 4.28741100 | -1.02880000 |
| H | 0.81102800 | 2.89399200 | 0.08274800 |
| H | 1.28461900 | 2.64850000 | -1.61159600 |
| C | -1.78808300 | 3.81887000 | -0.44439700 |
| H | -1.52909000 | 4.88898200 | -0.48713800 |
| H | -2.83017000 | 3.69603200 | -0.77564700 |
| H | -1.72834500 | 3.48836500 | 0.60163800 |
| C | -0.89175600 | 4.62265300 | -3.31988200 |
| H | -1.09573500 | 4.69045600 | -4.40108100 |
| H | -1.55308700 | 5.34588500 | -2.81610700 |
| H | 0.14674900 | 4.95596300 | -3.16142700 |
| C | -3.52242100 | 0.25253500 | 0.60761700 |
| C | -4.14142300 | 0.24130500 | 2.01779900 |
| C | -4.37136500 | 1.09678100 | -0.34624700 |
| H | -2.54374900 | 0.75089200 | 0.64699500 |
| H | -3.51499400 | -0.30119400 | 2.74094200 |
| H | -4.26594500 | 1.27135500 | 2.39039000 |
| H | -5.13475100 | -0.23808700 | 2.00575400 |
| H | -3.91021200 | 1.13222100 | -1.34210600 |
| H | -5.40512000 | 0.72366900 | -0.43420900 |
| H | -4.42741200 | 2.12927500 | 0.02994500 |
| C | -0.72970500 | -4.03310100 | 0.68273500 |
| C | 0.47526000 | -3.75957400 | -0.23004600 |
| C | -0.97087200 | -5.53928400 | 0.84393800 |
| H | -0.47392700 | -3.64583200 | 1.68014800 |
| H | 0.61200000 | -2.68287300 | -0.39663400 |
| H | 1.40138300 | -4.17012100 | 0.20418200 |
| H | 0.32146600 | -4.22011300 | -1.21729700 |
| H | -1.85624500 | -5.74611800 | 1.46575800 |
| H | -1.11344500 | -6.03847400 | -0.12782500 |

| | | | |
|---|---|---|---|
| H | -0.09722400 | -6.00947100 | 1.32272700 |
| C | 2.99540800 | -1.33625700 | 1.56623600 |
| C | 3.25558600 | -2.19401000 | 2.81839000 |
| C | 4.07031600 | -1.58366900 | 0.50037100 |
| H | 2.04074400 | -1.66287800 | 1.13409600 |
| H | 2.45382900 | -2.07788400 | 3.56323800 |
| H | 3.31501300 | -3.26120000 | 2.54907000 |
| H | 4.20661800 | -1.90788900 | 3.29710500 |
| H | 3.91969800 | -0.93404100 | -0.37495600 |
| H | 5.08677600 | -1.40827700 | 0.88745500 |
| H | 4.02798900 | -2.63004400 | 0.16101500 |
| C | 0.06938000 | 2.63307600 | 2.98900700 |
| C | -0.03177800 | 4.13776400 | 2.69461700 |
| C | -0.30400300 | 2.38456300 | 4.46385700 |
| H | -0.67101400 | 2.11626100 | 2.35573400 |
| H | 0.31016400 | 4.38498000 | 1.68100000 |
| H | -1.07781400 | 4.46637900 | 2.78964200 |
| H | 0.56004800 | 4.72982700 | 3.41094800 |
| H | -0.33540400 | 1.31728100 | 4.71630200 |
| H | 0.42771400 | 2.86965700 | 5.13050700 |
| H | -1.29724100 | 2.80871400 | 4.68256300 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3329.4478185
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3327.3732364

**(*E*)-B-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.915876 (Hartree/Particle)
Thermal correction to Energy= 0.967255
Thermal correction to Enthalpy= 0.968199
Thermal correction to Gibbs Free Energy= 0.828308
Sum of electronic and zero-point Energies= -3326.877548
Sum of electronic and thermal Energies= -3326.826169
Sum of electronic and thermal Enthalpies= -3326.825225
Sum of electronic and thermal Free Energies= -3326.965116

| | | | |
|---|---|---|---|
| Ni | 0.45064800 | 1.54961600 | 0.82101700 |
| N | 0.72931700 | -0.01923000 | 3.30842000 |
| N | -0.86832700 | -0.73288900 | 2.06304000 |
| C | 3.13112100 | 0.45370800 | 3.36173600 |
| C | 4.18126700 | 1.25452100 | 3.83566700 |
| C | 3.93570000 | 2.32280200 | 4.69726700 |
| C | 2.63141800 | 2.62370600 | 5.09514300 |
| C | 1.54631100 | 1.85902000 | 4.64622700 |
| C | 1.82736800 | 0.77348400 | 3.78870500 |
| C | 0.11967900 | -1.05713400 | 4.00547400 |
| C | -0.89715500 | -1.50397800 | 3.21825900 |
| C | 0.13018300 | 0.19444000 | 2.10180000 |
| C | -1.75287400 | -0.86285400 | 0.93759800 |
| C | -1.40033900 | -1.76607600 | -0.08657000 |
| C | -2.24016000 | -1.83558400 | -1.20573800 |
| C | -3.38547300 | -1.04133000 | -1.28797800 |
| C | -3.71153300 | -0.16052200 | -0.25765100 |
| C | -2.89873000 | -0.04719100 | 0.88015100 |
| H | 5.20482500 | 1.04300700 | 3.51875100 |
| H | 4.76738900 | 2.93463300 | 5.05591500 |
| H | 2.45628600 | 3.47540900 | 5.75472800 |
| H | 0.46073900 | -1.37205600 | 4.98727100 |
| H | -1.62826700 | -2.29301100 | 3.36793700 |
| H | -1.99226200 | -2.50068900 | -2.03303300 |
| H | -4.01883400 | -1.10577400 | -2.17584800 |
| H | -4.60337600 | 0.46444400 | -0.34385600 |
| C | 1.00477800 | -1.80098300 | -4.57607800 |
| C | 2.05598600 | -2.60059700 | -4.86302700 |
| C | 1.14858700 | -0.32847000 | -4.26721800 |
| H | 0.51877800 | -0.03576500 | -3.41533800 |
| H | 2.18116200 | -0.04650500 | -4.02780300 |
| H | 0.83166000 | 0.29326200 | -5.12207200 |
| C | -0.38512400 | -2.34471300 | -4.57144000 |
| C | -1.48909800 | -1.50651600 | -4.82704100 |
| C | -0.65524000 | -3.70001100 | -4.28481600 |
| C | -2.79632400 | -2.00155900 | -4.82027700 |
| H | -1.33315400 | -0.44882000 | -5.03726600 |
| C | -1.95981900 | -4.19597800 | -4.27456600 |
| H | 0.16798300 | -4.37200800 | -4.03495400 |
| C | -3.04158000 | -3.34919700 | -4.54417500 |
| H | -3.62827500 | -1.32292800 | -5.02607900 |
| H | -2.13421100 | -5.24822500 | -4.03514700 |
| H | -4.06391200 | -3.73461300 | -4.52627600 |
| C | 3.51162700 | -2.24340300 | -4.89779400 |
| H | 4.09441500 | -2.93295400 | -4.26157400 |
| H | 3.91682800 | -2.35466800 | -5.91980500 |
| H | 3.72178400 | -1.21751200 | -4.56601800 |
| H | 1.84467700 | -3.64280800 | -5.12728900 |
| O | 0.04439600 | 2.99732000 | -0.18946000 |
| C | -0.17115900 | 3.03734400 | -1.57414200 |
| C | -1.23401100 | 1.97010700 | -1.94638000 |
| H | -0.80526300 | 0.98192500 | -1.70053800 |
| H | -2.07191000 | 2.10344100 | -1.24520400 |
| C | 1.15735600 | 2.75806200 | -2.30154600 |
| H | 1.06179600 | 2.75963800 | -3.39995800 |
| H | 1.90242300 | 3.51799500 | -2.01650200 |
| H | 1.53815200 | 1.77549000 | -1.97919000 |
| C | -0.67358900 | 4.44999900 | -1.92305500 |
| H | -0.78565400 | 4.60962600 | -3.00781000 |
| H | -1.64720700 | 4.63283700 | -1.43968300 |
| H | 0.04138700 | 5.19203400 | -1.53437100 |
| C | -1.77020900 | 1.96721200 | -3.37772000 |
| H | -2.47088000 | 1.12956500 | -3.52444900 |
| H | -2.31369700 | 2.89639700 | -3.61214400 |
| H | -0.96568100 | 1.85874400 | -4.12244800 |
| C | -3.24017000 | 0.95334500 | 1.97859000 |
| C | -4.62047100 | 0.66967000 | 2.59286900 |
| C | -3.12973400 | 2.40089600 | 1.46950600 |
| H | -2.49742800 | 0.84034100 | 2.78185700 |
| H | -4.68307700 | -0.35931800 | 2.98193800 |
| H | -4.81984800 | 1.36398400 | 3.42516900 |
| H | -5.42669400 | 0.79919500 | 1.85253500 |
| H | -2.12453800 | 2.60840700 | 1.07288500 |
| H | -3.85979900 | 2.59599000 | 0.66657400 |
| H | -3.33430100 | 3.10898900 | 2.28895800 |
| C | -0.10583400 | -2.56750600 | -0.02005600 |
| C | 0.99516600 | -1.84591600 | -0.81698900 |
| C | -0.27276000 | -4.02202000 | -0.48014100 |
| H | 0.21914500 | -2.59562500 | 1.03076000 |
| H | 1.09725100 | -0.80311000 | -0.47861700 |
| H | 1.96673600 | -2.35029300 | -0.68888500 |
| H | 0.75503200 | -1.83977200 | -1.88976300 |
| H | -1.06198600 | -4.53660700 | 0.09091100 |
| H | -0.53109700 | -4.08362600 | -1.54778100 |
| H | 0.66993600 | -4.57447000 | -0.33738700 |
| C | 3.40340800 | -0.66751100 | 2.36579500 |
| C | 4.50284700 | -1.62800400 | 2.84320700 |
| C | 3.73027500 | -0.07788000 | 0.98208900 |
| H | 2.48106400 | -1.25700600 | 2.25723200 |
| H | 4.26618500 | -2.04765900 | 3.83375600 |
| H | 4.61138100 | -2.46392100 | 2.13366700 |
| H | 5.48210900 | -1.12782400 | 2.91305900 |
| H | 2.90378900 | 0.55598200 | 0.62172300 |
| H | 4.64116400 | 0.54134400 | 1.02030300 |
| H | 3.88770700 | -0.87941400 | 0.24333300 |
| C | 0.11144900 | 2.24547100 | 4.98919200 |
| C | -0.40667500 | 3.28112500 | 3.97281000 |
| C | -0.05996100 | 2.74345000 | 6.43049800 |
| H | -0.51413700 | 1.34621000 | 4.88355900 |
| H | -0.31453700 | 2.90639000 | 2.94213700 |
| H | -1.46747200 | 3.51371100 | 4.15950400 |
| H | 0.17036600 | 4.21765500 | 4.04435800 |

| | | | |
|---|---|---|---|
| H | 0.34493500 | 2.02324900 | 7.15914700 |
| H | 0.44116900 | 3.71084300 | 6.59467600 |
| H | -1.12859600 | 2.89224000 | 6.65228800 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3329.497375
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3327.4275785

**(*Z*)-TS-V-VI-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.912259 (Hartree/Particle)
Thermal correction to Energy= 0.962113
Thermal correction to Enthalpy= 0.963057
Thermal correction to Gibbs Free Energy= 0.828626
Sum of electronic and zero-point Energies= -3326.821684
Sum of electronic and thermal Energies= -3326.771830
Sum of electronic and thermal Enthalpies= -3326.770886
Sum of electronic and thermal Free Energies= -3326.905317

| | | | |
|---|---|---|---|
| Ni | 0.27182500 | 0.18448900 | -0.62210500 |
| N | 0.38075100 | -0.36001300 | 2.26337700 |
| N | -1.58982400 | -0.92437900 | 1.61745800 |
| C | 2.68403400 | -1.15022600 | 2.39297400 |
| C | 4.05561500 | -0.86003200 | 2.35669600 |
| C | 4.50808400 | 0.44200400 | 2.15102500 |
| C | 3.59818600 | 1.48904900 | 1.99245700 |
| C | 2.21578800 | 1.26120800 | 2.04161100 |
| C | 1.79022500 | -0.07001600 | 2.23825100 |
| C | -0.31539400 | -0.72671500 | 3.40824600 |
| C | -1.55423500 | -1.09992600 | 2.99880600 |
| C | -0.38987100 | -0.47522800 | 1.14507300 |
| C | -2.70687700 | -1.33588200 | 0.80583500 |
| C | -2.60077200 | -2.55761300 | 0.10883000 |
| C | -3.68649200 | -2.94669700 | -0.69023100 |
| C | -4.84056500 | -2.17022100 | -0.76180400 |
| C | -4.93389100 | -0.98403000 | -0.03319500 |
| C | -3.87121700 | -0.53442100 | 0.76278600 |
| H | 4.77835600 | -1.67036900 | 2.46810000 |
| H | 5.58126800 | 0.64419700 | 2.10797700 |
| H | 3.97198800 | 2.50079800 | 1.83144200 |
| H | 0.14076200 | -0.70762700 | 4.39343800 |
| H | -2.39842800 | -1.49497600 | 3.55259400 |
| H | -3.62638900 | -3.87711900 | -1.25891400 |
| H | -5.67701500 | -2.49145400 | -1.38764000 |
| H | -5.84598800 | -0.38977700 | -0.09922600 |
| C | 1.98510200 | -1.30971300 | -2.82597100 |
| C | 1.39817300 | -0.03613200 | -2.29746600 |
| C | 1.26296000 | -2.10105200 | -3.64893700 |
| H | 1.23288800 | -0.90468300 | -0.57812400 |
| H | 0.24947000 | -1.81954200 | -3.94828800 |
| H | 1.63668300 | -3.06230300 | -4.00941000 |
| C | 3.38365200 | -1.69033000 | -2.46430500 |
| C | 4.22007400 | -2.31564000 | -3.41181000 |
| C | 3.92310400 | -1.42945400 | -1.18984300 |
| C | 5.52913200 | -2.68520200 | -3.09544800 |
| H | 3.84221500 | -2.49230500 | -4.42124200 |
| C | 5.23346700 | -1.79557200 | -0.87291100 |
| H | 3.30555700 | -0.94987800 | -0.43051600 |
| C | 6.04406300 | -2.42746800 | -1.82066200 |
| H | 6.15420200 | -3.16475900 | -3.85359500 |
| H | 5.62033900 | -1.58134000 | 0.12530700 |
| H | 7.07085600 | -2.70781300 | -1.57154900 |
| O | -0.42942700 | 1.87204100 | -0.86334200 |
| C | -1.41756600 | 2.37290500 | -1.71858900 |
| C | -2.39760400 | 1.22684400 | -2.07793600 |
| H | -1.79852900 | 0.43445100 | -2.55989400 |
| H | -2.73336400 | 0.79495600 | -1.12435300 |
| C | -0.76274700 | 2.93934300 | -2.99512700 |
| H | -1.50013300 | 3.42659900 | -3.65351300 |
| H | -0.00153400 | 3.68571400 | -2.72044000 |
| H | -0.26718000 | 2.13969500 | -3.56605700 |
| C | -2.12553100 | 3.51632300 | -0.96824800 |
| H | -2.94907500 | 3.96725400 | -1.54497300 |
| H | -2.52284600 | 3.14209700 | -0.01402700 |
| H | -1.39152500 | 4.30458500 | -0.73881900 |
| C | -3.60372300 | 1.55205200 | -2.95856300 |
| H | -4.22842000 | 0.65547900 | -3.10341300 |
| H | -4.24682000 | 2.32748300 | -2.51179700 |
| H | -3.30227600 | 1.90924000 | -3.95642300 |
| C | -3.99560600 | 0.76783400 | 1.54959800 |
| C | -4.61031500 | 0.52836900 | 2.94323000 |
| C | -4.82563600 | 1.83625600 | 0.81936300 |
| H | -2.97604200 | 1.16538600 | 1.68357600 |
| H | -4.02404200 | -0.17087200 | 3.55279700 |
| H | -4.68134400 | 1.47765300 | 3.49827600 |
| H | -5.62776600 | 0.11571000 | 2.84492800 |
| H | -4.51404300 | 1.95877300 | -0.22498800 |
| H | -5.89893600 | 1.58780400 | 0.82784800 |
| H | -4.71384700 | 2.80779800 | 1.32477300 |
| C | -1.37055900 | -3.45321400 | 0.19430800 |
| C | -0.60836900 | -3.45405300 | -1.13780000 |
| C | -1.72811400 | -4.87679500 | 0.65073000 |
| H | -0.69242000 | -3.03666400 | 0.95213200 |
| H | -0.27214900 | -2.43985900 | -1.38821500 |
| H | 0.28507700 | -4.09467800 | -1.07821800 |
| H | -1.23785300 | -3.82633600 | -1.96223800 |
| H | -2.27684500 | -4.86715900 | 1.60603400 |
| H | -2.35056800 | -5.40153900 | -0.09184600 |
| H | -0.80959100 | -5.46985600 | 0.78904000 |
| C | 2.20730300 | -2.59459200 | 2.53196900 |
| C | 2.90183300 | -3.33631000 | 3.68384400 |
| C | 2.35811500 | -3.35353700 | 1.20259400 |
| H | 1.13444400 | -2.58073400 | 2.76713600 |
| H | 2.79442200 | -2.79259300 | 4.63591600 |
| H | 2.46137600 | -4.33836300 | 3.80923800 |
| H | 3.97805600 | -3.47494500 | 3.49322200 |
| H | 3.41524500 | -3.43462500 | 0.90643600 |
| H | 1.94510200 | -4.37148100 | 1.29315400 |
| H | 1.82554700 | -2.83749700 | 0.39160800 |
| C | 1.21214300 | 2.40402900 | 1.93706900 |
| C | 1.71050200 | 3.58024700 | 1.09214400 |
| C | 0.78548200 | 2.86571600 | 3.34271500 |
| H | 0.32189100 | 2.02623800 | 1.41745100 |
| H | 2.04655600 | 3.23653900 | 0.10362600 |
| H | 0.88735900 | 4.29318400 | 0.93271100 |
| H | 2.53461200 | 4.12820000 | 1.57856200 |
| H | 0.35709800 | 2.03779900 | 3.92911900 |
| H | 1.64658800 | 3.26651200 | 3.90329700 |
| H | 0.02370700 | 3.65924800 | 3.27268200 |
| H | 0.52856100 | 0.20317700 | -2.92922200 |
| C | 2.34855300 | 1.16217600 | -2.24516900 |
| H | 2.91594100 | 1.25439100 | -3.19004200 |
| H | 1.77523300 | 2.08263700 | -2.08392700 |
| H | 3.08498600 | 1.08573700 | -1.43243800 |

**(*Z*)-VI-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.912939 (Hartree/Particle)
Thermal correction to Energy= 0.963160
Thermal correction to Enthalpy= 0.964105
Thermal correction to Gibbs Free Energy= 0.830606
Sum of electronic and zero-point Energies= -3326.822647
Sum of electronic and thermal Energies= -3326.772426
Sum of electronic and thermal Enthalpies= -3326.771482
Sum of electronic and thermal Free Energies= -3326.904980

| | | | |
|---|---|---|---|
| Ni | 0.05137600 | 0.04006300 | -0.97971000 |
| N | 0.34659300 | -0.15006000 | 2.05756400 |
| N | -1.46402500 | -1.12277300 | 1.42318300 |
| C | 2.76453400 | -0.38325700 | 1.72047400 |

| | | | |
|---|---|---|---|
| C | 4.04167800 | 0.18619500 | 1.80043200 |
| C | 4.21811700 | 1.50995000 | 2.20650600 |
| C | 3.11618900 | 2.29915600 | 2.52323000 |
| C | 1.81151300 | 1.78454300 | 2.45254700 |
| C | 1.66395600 | 0.43747000 | 2.06548600 |
| C | -0.29948500 | -0.58008700 | 3.21399400 |
| C | -1.44196200 | -1.19222400 | 2.81338200 |
| C | -0.36497800 | -0.47693300 | 0.94435700 |
| C | -2.43623500 | -1.83114500 | 0.62342900 |
| C | -2.19898700 | -3.20034400 | 0.37232600 |
| C | -3.17047000 | -3.90549000 | -0.35280000 |
| C | -4.32127700 | -3.26823900 | -0.81141500 |
| C | -4.51647400 | -1.90793400 | -0.57066400 |
| C | -3.57851200 | -1.15088600 | 0.14741500 |
| H | 4.91759000 | -0.40905400 | 1.54163200 |
| H | 5.22516500 | 1.93059900 | 2.26579900 |
| H | 3.27053700 | 3.33602500 | 2.82554600 |
| H | 0.12216900 | -0.43211100 | 4.20222500 |
| H | -2.23253600 | -1.67215700 | 3.38094900 |
| H | -3.02130600 | -4.96538700 | -0.56504300 |
| H | -5.06921600 | -3.83296500 | -1.37411700 |
| H | -5.41392500 | -1.42651300 | -0.95900300 |
| C | -0.34921000 | -1.33374600 | -3.05982500 |
| C | 0.40390700 | -0.05378900 | -2.98665800 |
| C | -1.69710900 | -1.33467100 | -2.85322000 |
| H | 1.53592300 | 0.04683600 | -0.91749200 |
| H | -2.23881900 | -0.39335300 | -2.73640800 |
| H | -2.26658200 | -2.26105200 | -2.75741500 |
| C | 0.37199300 | -2.63398600 | -3.19377200 |
| C | -0.13571300 | -3.64583100 | -4.02849000 |
| C | 1.55451500 | -2.89407000 | -2.47581400 |
| C | 0.51498600 | -4.87765000 | -4.14205100 |
| H | -1.04584600 | -3.45553200 | -4.60218600 |
| C | 2.21009300 | -4.12075800 | -2.59618000 |
| H | 1.93682500 | -2.12998300 | -1.79813800 |
| C | 1.69414800 | -5.11877700 | -3.42968200 |
| H | 0.10289100 | -5.64939800 | -4.79753100 |
| H | 3.12549100 | -4.30300300 | -2.02851000 |
| H | 2.20810400 | -6.07878800 | -3.52303600 |
| O | -1.15104500 | 1.54530700 | -0.88715600 |
| C | -1.15903400 | 2.83621600 | -1.42194100 |
| C | -1.99270400 | 2.84506600 | -2.73337200 |
| H | -1.51489600 | 2.14720700 | -3.44022800 |
| H | -2.96976800 | 2.39970600 | -2.48503600 |
| C | 0.28441800 | 3.31215000 | -1.68266200 |
| H | 0.33652700 | 4.37101900 | -1.98283300 |
| H | 0.87590000 | 3.17646300 | -0.76446800 |
| H | 0.75528900 | 2.70282600 | -2.46741600 |
| C | -1.82253100 | 3.75991900 | -0.37764100 |
| H | -1.79512900 | 4.82470600 | -0.66095000 |
| H | -2.87311900 | 3.46521000 | -0.22888900 |
| H | -1.30259300 | 3.64274500 | 0.58193700 |
| C | -2.19999900 | 4.19307700 | -3.42826500 |
| H | -2.79115600 | 4.07249300 | -4.35118900 |
| H | -2.73915300 | 4.90892600 | -2.78719100 |
| H | -1.24248600 | 4.65903200 | -3.71278500 |
| C | -3.76819500 | 0.34410600 | 0.37890000 |
| C | -4.23539600 | 0.65424600 | 1.81273100 |
| C | -4.72923600 | 0.98846900 | -0.62732000 |
| H | -2.78429300 | 0.81440600 | 0.20597300 |
| H | -3.53084800 | 0.28870900 | 2.57216800 |
| H | -4.33220200 | 1.74347800 | 1.95139300 |
| H | -5.21959600 | 0.19810000 | 2.01480600 |
| H | -4.44938400 | 0.75119300 | -1.66479400 |
| H | -5.77431500 | 0.67186900 | -0.47173100 |
| H | -4.70082500 | 2.08298200 | -0.51738200 |
| C | -0.94842100 | -3.91483500 | 0.87466800 |
| C | -0.36729300 | -4.89269600 | -0.15716800 |
| C | -1.21785900 | -4.63967400 | 2.20613900 |
| H | -0.18099700 | -3.15035200 | 1.06164200 |
| H | -0.25657300 | -4.42399200 | -1.14372500 |
| H | 0.62793500 | -5.23464200 | 0.16793500 |
| H | -0.99801400 | -5.78891000 | -0.27087800 |
| H | -1.57919800 | -3.95210300 | 2.98414500 |
| H | -1.97824800 | -5.42641500 | 2.07085700 |
| H | -0.29626600 | -5.11632900 | 2.57769500 |
| C | 2.57462800 | -1.83387600 | 1.28370800 |
| C | 2.34704400 | -2.76772400 | 2.48703700 |
| C | 3.71734300 | -2.36531700 | 0.41199600 |
| H | 1.66893200 | -1.85660000 | 0.65965000 |
| H | 1.48089900 | -2.46338900 | 3.09079000 |
| H | 2.16555700 | -3.79849200 | 2.14182600 |
| H | 3.23285300 | -2.77883700 | 3.14322500 |
| H | 3.91597600 | -1.70293200 | -0.44447700 |
| H | 4.65351000 | -2.48073300 | 0.98128600 |
| H | 3.45058200 | -3.35915000 | 0.02371700 |
| C | 0.61830200 | 2.66704000 | 2.80580500 |
| C | 0.77046100 | 4.10396000 | 2.28252200 |
| C | 0.37464800 | 2.69374500 | 4.32687600 |
| H | -0.26921300 | 2.23060200 | 2.32095300 |
| H | 1.01282700 | 4.12233900 | 1.21089400 |
| H | -0.16880600 | 4.65896400 | 2.42876600 |
| H | 1.55843900 | 4.65307300 | 2.82198800 |
| H | 0.19450100 | 1.69130900 | 4.73898800 |
| H | 1.24785300 | 3.11814900 | 4.84926100 |
| H | -0.50139600 | 3.31794700 | 4.56611300 |
| H | -0.25652900 | 0.77616900 | -3.25526200 |
| C | 1.74512700 | 0.09428600 | -3.68018700 |
| H | 1.63442500 | -0.02166400 | -4.77510500 |
| H | 2.15642600 | 1.09747300 | -3.49333800 |
| H | 2.49618300 | -0.63452600 | -3.34915600 |

**(*Z*)-VII-1**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.912855 (Hartree/Particle)

Thermal correction to Energy= 0.963344

Thermal correction to Enthalpy= 0.964288

Thermal correction to Gibbs Free Energy= 0.829112

Sum of electronic and zero-point Energies= -3326.830999

Sum of electronic and thermal Energies= -3326.780511

Sum of electronic and thermal Enthalpies= -3326.779567

Sum of electronic and thermal Free Energies= -3326.914743

| | | | |
|---|---|---|---|
| Ni | 0.19979900 | 0.14787300 | -0.68716500 |
| N | 0.38765100 | -0.14782200 | 2.28637000 |
| N | -1.33869300 | -1.21615200 | 1.58919300 |
| C | 2.81878100 | -0.26825100 | 2.18427600 |
| C | 4.06159400 | 0.37625600 | 2.26632300 |
| C | 4.13838700 | 1.75509700 | 2.44721000 |
| C | 2.97476500 | 2.52136200 | 2.53528900 |
| C | 1.70425300 | 1.93046900 | 2.46639700 |
| C | 1.66082500 | 0.52705100 | 2.30976800 |
| C | -0.17992500 | -0.75233800 | 3.40507000 |
| C | -1.27548300 | -1.42279100 | 2.96708300 |
| C | -0.31348000 | -0.43829400 | 1.15922200 |
| C | -2.27913800 | -1.90501100 | 0.74238600 |
| C | -2.01478500 | -3.26049800 | 0.45191000 |
| C | -2.96172300 | -3.95671800 | -0.31342600 |
| C | -4.12351600 | -3.32575000 | -0.75327600 |
| C | -4.34513000 | -1.97734600 | -0.47101800 |
| C | -3.42096400 | -1.22353300 | 0.26771500 |
| H | 4.97954500 | -0.20909200 | 2.18350700 |
| H | 5.11444800 | 2.24327900 | 2.50879800 |
| H | 3.06469400 | 3.60075900 | 2.65509600 |
| H | 0.24825600 | -0.64922100 | 4.39710800 |
| H | -2.00812500 | -2.02755100 | 3.49273200 |
| H | -2.78743900 | -5.00265600 | -0.57074400 |
| H | -4.85717500 | -3.88418500 | -1.34011300 |
| H | -5.24968000 | -1.50198800 | -0.84908600 |
| C | 0.58057700 | -1.05682100 | -3.18471300 |
| C | 1.27952500 | -2.21214800 | -3.25299200 |

| | | | |
|---|---|---|---|
| C | 1.07974400 | 0.16360300 | -2.48399400 |
| H | 1.46150800 | -0.54285900 | -0.47036900 |
| H | 2.17734800 | 0.18737000 | -2.43711900 |
| H | 0.72639600 | 1.07560300 | -2.97911500 |
| C | -0.77511500 | -0.93022200 | -3.81274200 |
| C | -0.91437500 | -0.29862500 | -5.06011100 |
| C | -1.93145900 | -1.37232700 | -3.15087600 |
| C | -2.17503700 | -0.11184000 | -5.63345000 |
| H | -0.01990100 | 0.05783900 | -5.57789300 |
| C | -3.19445400 | -1.18599100 | -3.72302600 |
| H | -1.84415500 | -1.85307800 | -2.17342700 |
| C | -3.32141300 | -0.55427400 | -4.96381900 |
| H | -2.26354900 | 0.38381500 | -6.60391500 |
| H | -4.08076900 | -1.53506900 | -3.19033100 |
| H | -4.30960000 | -0.40562500 | -5.40693300 |
| O | -0.77769300 | 1.72982600 | -0.53246600 |
| C | -1.01503000 | 2.85019100 | -1.34967200 |
| C | -1.78137800 | 2.39578800 | -2.61572800 |
| H | -1.21960000 | 1.56542700 | -3.05988800 |
| H | -2.72999900 | 1.95393600 | -2.27339500 |
| C | 0.31670200 | 3.54339100 | -1.69961100 |
| H | 0.16099900 | 4.50874100 | -2.20679700 |
| H | 0.87965600 | 3.72701000 | -0.77246200 |
| H | 0.93768500 | 2.90899500 | -2.34617400 |
| C | -1.88381500 | 3.82682900 | -0.53239200 |
| H | -2.14085200 | 4.73482900 | -1.10129700 |
| H | -2.81700300 | 3.33058100 | -0.22663200 |
| H | -1.34876700 | 4.13282400 | 0.37646700 |
| C | -2.06081000 | 3.44734800 | -3.68967600 |
| H | -2.63122200 | 3.00342000 | -4.52176700 |
| H | -2.64899700 | 4.29518300 | -3.30164100 |
| H | -1.13007600 | 3.85639600 | -4.11542700 |
| C | -3.61428000 | 0.27118300 | 0.51080300 |
| C | -4.00775200 | 0.58176200 | 1.96707500 |
| C | -4.63199400 | 0.90301700 | -0.44702000 |
| H | -2.64101500 | 0.75010000 | 0.30287600 |
| H | -3.26499100 | 0.21787900 | 2.69007000 |
| H | -4.09967800 | 1.67074300 | 2.10870500 |
| H | -4.97953800 | 0.12329200 | 2.21656700 |
| H | -4.39909500 | 0.67333900 | -1.49769000 |
| H | -5.66105300 | 0.56526000 | -0.23972500 |
| H | -4.61978500 | 1.99713100 | -0.33302700 |
| C | -0.70746800 | -3.92769500 | 0.86826300 |
| C | 0.32403300 | -3.79473400 | -0.26534100 |
| C | -0.87702000 | -5.39120200 | 1.29805000 |
| H | -0.30764400 | -3.38702500 | 1.73831000 |
| H | 0.50641200 | -2.74365800 | -0.53052400 |
| H | 1.28662800 | -4.24295100 | 0.02796700 |
| H | -0.03209100 | -4.30823900 | -1.17165200 |
| H | -1.65075500 | -5.49770800 | 2.07471200 |
| H | -1.15270400 | -6.04082100 | 0.45203600 |
| H | 0.07225400 | -5.77512000 | 1.70407100 |
| C | 2.75162000 | -1.77888400 | 1.98394600 |
| C | 3.09365700 | -2.52025100 | 3.28774100 |
| C | 3.63488600 | -2.25326400 | 0.82004000 |
| H | 1.71921400 | -2.04032900 | 1.71609300 |
| H | 2.41886300 | -2.22340600 | 4.10586500 |
| H | 3.00341300 | -3.61015400 | 3.14984400 |
| H | 4.12614100 | -2.30160500 | 3.60643400 |
| H | 3.37079600 | -1.72702400 | -0.11009200 |
| H | 4.70579400 | -2.08921300 | 1.01885300 |
| H | 3.49317900 | -3.33270900 | 0.65310400 |
| C | 0.42675500 | 2.76531000 | 2.53562700 |
| C | 0.66401700 | 4.25236500 | 2.24225800 |
| C | -0.28393300 | 2.63351900 | 3.89659200 |
| H | -0.23677600 | 2.37578200 | 1.74343100 |
| H | 1.17531800 | 4.40748400 | 1.28112600 |
| H | -0.29992100 | 4.78132600 | 2.20012100 |
| H | 1.26149400 | 4.73617200 | 3.03219100 |
| H | -0.56414800 | 1.59911200 | 4.13133600 |
| H | 0.36234000 | 3.00432700 | 4.70984100 |
| H | -1.20900000 | 3.23250300 | 3.89963400 |
| H | 2.25853900 | -2.23253800 | -2.75605700 |
| C | 0.87227500 | -3.47462200 | -3.95281800 |
| H | 1.56764300 | -3.71408300 | -4.77825300 |
| H | 0.90101300 | -4.34144100 | -3.26892600 |
| H | -0.14127400 | -3.40832300 | -4.37469200 |

**(*Z*)-TS-VII-B-1**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.911828 (Hartree/Particle)
Thermal correction to Energy= 0.961931
Thermal correction to Enthalpy= 0.962876
Thermal correction to Gibbs Free Energy= 0.827657
Sum of electronic and zero-point Energies= -3326.830734
Sum of electronic and thermal Energies= -3326.780631
Sum of electronic and thermal Enthalpies= -3326.779687
Sum of electronic and thermal Free Energies= -3326.914906

| | | | |
|---|---|---|---|
| Ni | -0.22389500 | -0.10175200 | -0.76063100 |
| N | 0.36342200 | -0.10439500 | 2.24222600 |
| N | -1.31142400 | -1.31150800 | 1.64335900 |
| C | 2.72325600 | 0.29502200 | 1.68866900 |
| C | 3.81894100 | 1.16844200 | 1.71214000 |
| C | 3.70532800 | 2.45723400 | 2.23732200 |
| C | 2.48519700 | 2.91048800 | 2.73250900 |
| C | 1.35055200 | 2.08485900 | 2.72230100 |
| C | 1.50154100 | 0.77780000 | 2.21483800 |
| C | -0.12260500 | -0.71920700 | 3.39716300 |
| C | -1.18211600 | -1.47966400 | 3.01766500 |
| C | -0.36216900 | -0.47234400 | 1.15299400 |
| C | -2.21543400 | -2.04668200 | 0.79947800 |
| C | -1.84253700 | -3.35126300 | 0.42041900 |
| C | -2.74973900 | -4.08109900 | -0.36218600 |
| C | -3.96020600 | -3.51789000 | -0.76194300 |
| C | -4.27526800 | -2.20128000 | -0.41811500 |
| C | -3.40379000 | -1.42517100 | 0.35794400 |
| H | 4.78055700 | 0.84183100 | 1.31554700 |
| H | 4.57656200 | 3.11705700 | 2.24890100 |
| H | 2.40822300 | 3.92707700 | 3.12219600 |
| H | 0.33524200 | -0.56568800 | 4.36851200 |
| H | -1.84517300 | -2.12363400 | 3.58721400 |
| H | -2.49769300 | -5.09763300 | -0.67182600 |
| H | -4.65553400 | -4.09926300 | -1.37256200 |
| H | -5.20929100 | -1.76779300 | -0.77632600 |
| C | 0.51131300 | -1.54054500 | -3.28846200 |
| C | 1.15617800 | -2.68064100 | -3.61634200 |
| C | 1.04042600 | -0.57128500 | -2.28712600 |
| H | 0.37792700 | -1.41341900 | -0.74435700 |
| H | 2.06109000 | -0.82579000 | -1.97146300 |
| H | 1.02600200 | 0.45533500 | -2.68900500 |
| C | -0.81371700 | -1.18452700 | -3.89039100 |
| C | -2.00348900 | -1.43095200 | -3.18627400 |
| C | -0.89045700 | -0.55683900 | -5.14345300 |
| C | -3.23957600 | -1.06626900 | -3.72540300 |
| H | -1.95864800 | -1.90726800 | -2.20448400 |
| C | -2.12677400 | -0.18301100 | -5.68188000 |
| H | 0.03105300 | -0.35711000 | -5.69685600 |
| C | -3.30576100 | -0.43697100 | -4.97359100 |
| H | -4.15282200 | -1.27125200 | -3.16236600 |
| H | -2.16840500 | 0.30857400 | -6.65767600 |
| H | -4.27259700 | -0.14522500 | -5.39219900 |
| O | -1.25849300 | 1.32326900 | -1.25604600 |
| C | -0.96648300 | 2.68183600 | -1.40617600 |
| C | -1.08986400 | 2.99834900 | -2.91874900 |
| H | -0.37893600 | 2.33528600 | -3.44077400 |
| H | -2.09289200 | 2.66029300 | -3.23050800 |
| C | 0.45601800 | 2.98516900 | -0.89535300 |
| H | 0.69713100 | 4.06048400 | -0.90069200 |
| H | 0.55673200 | 2.61138800 | 0.13344200 |
| H | 1.20318300 | 2.45962500 | -1.51036900 |

| | | | |
|---|---|---|---|
| C | -1.99980400 | 3.48021700 | -0.58831600 |
| H | -1.80086400 | 4.56413300 | -0.58571400 |
| H | -3.00937600 | 3.30785200 | -0.99189300 |
| H | -1.98808200 | 3.12344500 | 0.45294700 |
| C | -0.86587300 | 4.44830200 | -3.34917300 |
| H | -0.97561100 | 4.55523600 | -4.44092100 |
| H | -1.59149100 | 5.13211000 | -2.87943900 |
| H | 0.14370000 | 4.80433400 | -3.08612200 |
| C | -3.69622800 | 0.03552800 | 0.68818900 |
| C | -4.24713000 | 0.19335900 | 2.11641000 |
| C | -4.62016700 | 0.71019100 | -0.33105400 |
| H | -2.73615000 | 0.56899900 | 0.61461500 |
| H | -3.56180200 | -0.21873800 | 2.87158600 |
| H | -4.40255300 | 1.25898500 | 2.35117700 |
| H | -5.21620500 | -0.32271500 | 2.22088100 |
| H | -4.22472500 | 0.60004700 | -1.35105300 |
| H | -5.64615400 | 0.30752100 | -0.29867300 |
| H | -4.68394400 | 1.78653900 | -0.11147400 |
| C | -0.49653000 | -3.95430500 | 0.80644100 |
| C | 0.29135900 | -4.41625700 | -0.43019200 |
| C | -0.66402000 | -5.08834100 | 1.83064100 |
| H | 0.10527800 | -3.16739400 | 1.28224500 |
| H | 0.39733500 | -3.59997600 | -1.16093100 |
| H | 1.30087900 | -4.74577100 | -0.13461700 |
| H | -0.19849000 | -5.26343100 | -0.93682000 |
| H | -1.17669600 | -4.73474900 | 2.73933500 |
| H | -1.25698900 | -5.91740600 | 1.41075700 |
| H | 0.31810100 | -5.49088600 | 2.12708500 |
| C | 2.84219500 | -1.11964200 | 1.12531800 |
| C | 2.91968700 | -2.17412500 | 2.24491500 |
| C | 4.00717900 | -1.29764300 | 0.14471300 |
| H | 1.92362700 | -1.30357800 | 0.55176100 |
| H | 2.05943100 | -2.11954300 | 2.92708300 |
| H | 2.93782400 | -3.18783200 | 1.81252200 |
| H | 3.83629900 | -2.04131900 | 2.84310800 |
| H | 4.00281400 | -0.52258800 | -0.63659200 |
| H | 4.98561800 | -1.26722800 | 0.65154500 |
| H | 3.92543600 | -2.27743400 | -0.35110100 |
| C | 0.01695300 | 2.60440000 | 3.25146500 |
| C | -0.29799800 | 4.03128100 | 2.77201400 |
| C | -0.03072800 | 2.54268500 | 4.78961400 |
| H | -0.77519900 | 1.94786200 | 2.85875400 |
| H | -0.19809800 | 4.12496100 | 1.68273600 |
| H | -1.33152400 | 4.29850500 | 3.04318600 |
| H | 0.36485300 | 4.77519600 | 3.24202200 |
| H | 0.13846200 | 1.52503900 | 5.16999600 |
| H | 0.74438700 | 3.19448100 | 5.22509200 |
| H | -1.01035600 | 2.88447200 | 5.16082700 |
| C | 0.67750800 | -3.74807300 | -4.55642400 |
| H | 0.56414800 | -4.71386500 | -4.03010000 |
| H | -0.29165800 | -3.49615800 | -5.01120800 |
| H | 1.40174400 | -3.92375200 | -5.37206400 |
| H | 2.12209600 | -2.86979900 | -3.12935000 |

**(*Z*)-B-1**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.915729 (Hartree/Particle)

Thermal correction to Energy= 0.967119

Thermal correction to Enthalpy= 0.968063

Thermal correction to Gibbs Free Energy= 0.827701

Sum of electronic and zero-point Energies= -3326.875878

Sum of electronic and thermal Energies= -3326.824489

Sum of electronic and thermal Enthalpies= -3326.823545

Sum of electronic and thermal Free Energies= -3326.963906

| | | | |
|---|---|---|---|
| Ni | 0.43918400 | 1.52473600 | 0.82502500 |
| N | 0.69339800 | -0.00936600 | 3.33809600 |
| N | -0.92716600 | -0.70279300 | 2.11144100 |
| C | 3.10780200 | 0.39515200 | 3.37574200 |
| C | 4.18208300 | 1.17511000 | 3.82991400 |
| C | 3.97010900 | 2.26709600 | 4.67050900 |
| C | 2.67644100 | 2.61270000 | 5.06654100 |
| C | 1.56830800 | 1.87039400 | 4.63658400 |
| C | 1.81515700 | 0.76077300 | 3.79984300 |
| C | 0.06103200 | -1.02012100 | 4.05452700 |
| C | -0.96987500 | -1.45454800 | 3.27865500 |
| C | 0.09472100 | 0.19949300 | 2.13029600 |
| C | -1.81302500 | -0.83401100 | 0.98756800 |
| C | -1.46590300 | -1.74494400 | -0.03058700 |
| C | -2.30217300 | -1.81183700 | -1.15260000 |
| C | -3.44241500 | -1.01175000 | -1.24131800 |
| C | -3.76503700 | -0.12437800 | -0.21505000 |
| C | -2.95237200 | -0.00964200 | 0.92258000 |
| H | 5.19800300 | 0.92804800 | 3.51417300 |
| H | 4.82011100 | 2.86221200 | 5.01404700 |
| H | 2.52792900 | 3.48205900 | 5.70943300 |
| H | 0.39823100 | -1.32737800 | 5.04007900 |
| H | -1.71942800 | -2.22288100 | 3.44392800 |
| H | -2.05350700 | -2.48025500 | -1.97684900 |
| H | -4.07408200 | -1.07577100 | -2.13068100 |
| H | -4.65178500 | 0.50705700 | -0.30641300 |
| C | 1.02513300 | -1.79019800 | -4.65969200 |
| C | 2.09957600 | -2.48715100 | -5.09134800 |
| C | 1.18374200 | -0.34679100 | -4.23203300 |
| H | 0.65188900 | -0.13558200 | -3.29317200 |
| H | 2.24176200 | -0.08059100 | -4.09567000 |
| H | 0.76861900 | 0.34256400 | -4.98683500 |
| C | -0.35643900 | -2.34604500 | -4.60117400 |
| C | -1.46968300 | -1.54579300 | -4.92922700 |
| C | -0.60729400 | -3.66416600 | -4.16787700 |
| C | -2.77061600 | -2.05055500 | -4.86313100 |
| H | -1.32009600 | -0.51256900 | -5.24437900 |
| C | -1.90760400 | -4.17125800 | -4.10086600 |
| H | 0.22588500 | -4.29060200 | -3.84711300 |
| C | -2.99751700 | -3.36855800 | -4.45355100 |
| H | -3.61262800 | -1.40611700 | -5.12881000 |
| H | -2.07048700 | -5.19451800 | -3.75268800 |
| H | -4.01531000 | -3.76189800 | -4.39458000 |
| O | 0.05193900 | 2.97000900 | -0.19701200 |
| C | -0.18863400 | 2.98976300 | -1.57839700 |
| C | -1.21986200 | 1.88358700 | -1.92386000 |
| H | -0.75231400 | 0.91338400 | -1.67817400 |
| H | -2.04914800 | 1.99409600 | -1.20884200 |
| C | 1.13759100 | 2.74808300 | -2.32267300 |
| H | 1.02488700 | 2.72752900 | -3.41911700 |
| H | 1.85910200 | 3.53866800 | -2.06153500 |
| H | 1.55764900 | 1.78527100 | -1.99006700 |
| C | -0.74472700 | 4.38065000 | -1.93330100 |
| H | -0.87702300 | 4.52451000 | -3.01803400 |
| H | -1.71781700 | 4.53500700 | -1.43895500 |
| H | -0.05105900 | 5.15142300 | -1.56233600 |
| C | -1.78025800 | 1.84766700 | -3.34515500 |
| H | -2.44209200 | 0.97658200 | -3.47589900 |
| H | -2.37006100 | 2.74966900 | -3.57427300 |
| H | -0.98443200 | 1.77154100 | -4.10269000 |
| C | -3.28035400 | 1.00705900 | 2.01015700 |
| C | -4.67147500 | 0.76205800 | 2.61614800 |
| C | -3.13157100 | 2.44702500 | 1.48833000 |
| H | -2.54639100 | 0.88325600 | 2.82001000 |
| H | -4.76238200 | -0.26219700 | 3.01207200 |
| H | -4.85951400 | 1.46708900 | 3.44203000 |
| H | -5.46920600 | 0.90635000 | 1.86941500 |
| H | -2.11992200 | 2.62716600 | 1.09464300 |
| H | -3.85254200 | 2.65165100 | 0.67950000 |
| H | -3.32318100 | 3.16768900 | 2.29997800 |
| C | -0.18092300 | -2.56075600 | 0.03962300 |
| C | 0.90335900 | -1.90002200 | -0.82852400 |
| C | -0.38693600 | -4.03503800 | -0.33542600 |
| H | 0.17787400 | -2.53864400 | 1.07925300 |
| H | 1.03526600 | -0.84507500 | -0.54082700 |
| H | 1.86970100 | -2.41659100 | -0.71078600 |

| | | | |
|---|---|---|---|
| H | 0.62462000 | -1.93829600 | -1.89142900 |
| H | -1.15589200 | -4.50657700 | 0.29709600 |
| H | -0.69516900 | -4.14803000 | -1.38552900 |
| H | 0.55380700 | -4.59421000 | -0.20602100 |
| C | 3.34400200 | -0.75370200 | 2.40244900 |
| C | 4.42127400 | -1.73249700 | 2.89309100 |
| C | 3.67669700 | -0.20269900 | 1.00427800 |
| H | 2.40587300 | -1.32124200 | 2.31269400 |
| H | 4.18149500 | -2.12370100 | 3.89447900 |
| H | 4.50188900 | -2.58645900 | 2.20155000 |
| H | 5.41417300 | -1.25757700 | 2.94443300 |
| H | 2.86620900 | 0.44714400 | 0.63632400 |
| H | 4.60544400 | 0.39038200 | 1.02300700 |
| H | 3.80545700 | -1.02385100 | 0.28172000 |
| C | 0.14659400 | 2.30481600 | 4.97696100 |
| C | -0.34220400 | 3.34037900 | 3.94614500 |
| C | -0.00522500 | 2.82936000 | 6.41108600 |
| H | -0.50628900 | 1.42353200 | 4.88614000 |
| H | -0.26393200 | 2.94686400 | 2.92139600 |
| H | -1.39498100 | 3.60822100 | 4.13123100 |
| H | 0.26344000 | 4.25976700 | 4.00209800 |
| H | 0.37740800 | 2.10703600 | 7.14961600 |
| H | 0.52830900 | 3.78180500 | 6.55961600 |
| H | -1.06784500 | 3.01670000 | 6.63258600 |
| C | 2.16108300 | -3.86766700 | -5.68050200 |
| H | 2.54349700 | -4.60692000 | -4.95270900 |
| H | 1.18380200 | -4.22568500 | -6.03478000 |
| H | 2.86178600 | -3.88347200 | -6.53207300 |
| H | 3.06439800 | -1.96635400 | -5.04563300 |

**NaO*t*-Am**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.151483 (Hartree/Particle)
Thermal correction to Energy= 0.160867
Thermal correction to Enthalpy= 0.161811
Thermal correction to Gibbs Free Energy= 0.116984
Sum of electronic and zero-point Energies= -434.338340
Sum of electronic and thermal Energies= -434.328956
Sum of electronic and thermal Enthalpies= -434.328012
Sum of electronic and thermal Free Energies= -434.372838

| | | | |
|---|---|---|---|
| C | -2.82835000 | 0.59097800 | 0.08185800 |
| C | -1.28597500 | 0.67981000 | -0.03407800 |
| H | -3.26141700 | 1.60509500 | 0.04897900 |
| H | -3.22245300 | 0.02815000 | -0.78054400 |
| H | -3.17663500 | 0.09348300 | 1.00340700 |
| C | -0.70247400 | -0.75332900 | 0.04194300 |
| C | -0.72008200 | 1.54134400 | 1.13581300 |
| H | 0.39821500 | -0.70819000 | -0.01689400 |
| H | -0.98012200 | -1.29985200 | 0.95981700 |
| H | -1.06242700 | -1.33345900 | -0.82375000 |
| H | 0.36930500 | 1.61643400 | 0.96527300 |
| H | -1.11993400 | 2.56127600 | 0.98943200 |
| C | -0.98625700 | 1.08576600 | 2.57323400 |
| H | -0.53334200 | 1.77968900 | 3.30163400 |
| H | -2.06488700 | 1.03939600 | 2.79600300 |
| H | -0.56583100 | 0.08620400 | 2.77173000 |
| O | -0.93678900 | 1.26499000 | -1.22712500 |
| Na | -0.44266500 | 2.11563600 | -2.97137500 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -434.7813505
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -434.4028672

**NaCl**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.000735 (Hartree/Particle)
Thermal correction to Energy= 0.003488
Thermal correction to Enthalpy= 0.004432
Thermal correction to Gibbs Free Energy= -0.021746
Sum of electronic and zero-point Energies= -622.413620
Sum of electronic and thermal Energies= -622.410867
Sum of electronic and thermal Enthalpies= -622.409923
Sum of electronic and thermal Free Energies= -622.436101

| | | | |
|---|---|---|---|
| Na | -1.61062200 | 0.60067700 | 0.00000000 |
| Cl | -4.02811000 | 0.60067700 | 0.00000000 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -622.6048618
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -622.3566268

**PhOTf**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.119381 (Hartree/Particle)
Thermal correction to Energy= 0.131657
Thermal correction to Enthalpy= 0.132601
Thermal correction to Gibbs Free Energy= 0.078251
Sum of electronic and zero-point Energies= -1192.241396
Sum of electronic and thermal Energies= -1192.229121
Sum of electronic and thermal Enthalpies= -1192.228176
Sum of electronic and thermal Free Energies= -1192.282527

| | | | |
|---|---|---|---|
| C | -1.32807100 | 0.51491600 | -0.63656900 |
| C | -0.02534600 | 0.00911700 | -0.61323400 |
| C | 0.97114700 | 0.76462900 | 0.00411100 |
| C | 0.70646700 | 1.99841500 | 0.59756600 |
| C | -0.60229200 | 2.48761200 | 0.57307500 |
| C | -1.61816200 | 1.74954000 | -0.04496500 |
| H | -2.12001000 | -0.06327400 | -1.11815300 |
| H | 0.22468500 | -0.94967200 | -1.06769000 |
| H | 1.51851700 | 2.55280100 | 1.07081400 |
| H | -0.82666500 | 3.45061900 | 1.03748700 |
| H | -2.63934700 | 2.13700700 | -0.06426900 |
| O | 2.28125700 | 0.26410500 | 0.09865100 |
| S | 3.23143900 | 0.13870800 | -1.23181800 |
| O | 4.33371500 | -0.71433900 | -0.84292800 |
| O | 2.42918600 | -0.06876100 | -2.42494000 |
| C | 3.88576000 | 1.90519100 | -1.30715400 |
| F | 2.88705300 | 2.72893000 | -1.60063300 |
| F | 4.81401500 | 1.97056500 | -2.24855800 |
| F | 4.40690900 | 2.23585900 | -0.13496700 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1193.3450038
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1192.5031262

**AlkeneSM**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.107810 (Hartree/Particle)
Thermal correction to Energy= 0.113056
Thermal correction to Enthalpy= 0.114000
Thermal correction to Gibbs Free Energy= 0.080321
Sum of electronic and zero-point Energies= -157.006093
Sum of electronic and thermal Energies= -157.000847
Sum of electronic and thermal Enthalpies= -156.999903
Sum of electronic and thermal Free Energies= -157.033581

| | | | |
|---|---|---|---|
| C | -2.38466600 | 2.64472300 | -0.07039300 |
| H | -2.36799500 | 3.31380100 | 0.80628800 |
| H | -2.07159600 | 3.23392600 | -0.94719400 |
| H | -3.42855900 | 2.32786900 | -0.22695200 |
| C | -1.46717700 | 1.43142700 | 0.13983200 |
| H | -0.42546800 | 1.78845900 | 0.24595900 |
| H | -1.48604500 | 0.78333300 | -0.75328300 |
| C | -1.83322700 | 0.62890500 | 1.35797300 |
| H | -1.80035200 | 1.17471600 | 2.31147600 |
| C | -2.20290500 | -0.65569900 | 1.36220600 |

| | | | |
|---|---|---|---|
| H | -2.25523700 | -1.23768000 | 0.43503400 |
| H | -2.46428700 | -1.17579700 | 2.28858800 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -157.2524276
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -157.0798653

**HO*t*-Am**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.163747 (Hartree/Particle)
Thermal correction to Energy= 0.171587
Thermal correction to Enthalpy= 0.172532
Thermal correction to Gibbs Free Energy= 0.132865
Sum of electronic and zero-point Energies= -272.640113
Sum of electronic and thermal Energies= -272.632272
Sum of electronic and thermal Enthalpies= -272.631328
Sum of electronic and thermal Free Energies= -272.670994

| | | | |
|---|---|---|---|
| C | -2.72484900 | 0.81560400 | -0.02869900 |
| C | -1.19063300 | 0.81371200 | 0.02333900 |
| H | -3.10539000 | 1.84782000 | 0.01308500 |
| H | -3.07422000 | 0.35816300 | -0.96961200 |
| H | -3.16608900 | 0.24278300 | 0.80104600 |
| C | -0.64661600 | -0.61953800 | -0.05958500 |
| C | -0.65870100 | 1.55763200 | 1.26226200 |
| H | 0.45414800 | -0.60976400 | -0.04274100 |
| H | -1.00653900 | -1.24624500 | 0.77050600 |
| H | -0.97146500 | -1.09636600 | -0.99964600 |
| H | 0.43955500 | 1.59829900 | 1.16577700 |
| H | -1.00964300 | 2.60076300 | 1.18529100 |
| C | -1.04178900 | 0.97778800 | 2.62316200 |
| H | -0.61116800 | 1.58538200 | 3.43449700 |
| H | -2.13317100 | 0.96058600 | 2.77218500 |
| H | -0.66996900 | -0.05102800 | 2.75354500 |
| O | -0.67999500 | 1.57687600 | -1.07727000 |
| H | -0.98222400 | 1.15907400 | -1.89530800 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -273.0547447
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -272.7778593

**NaOTf**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.028421 (Hartree/Particle)
Thermal correction to Energy= 0.037456
Thermal correction to Enthalpy= 0.038400
Thermal correction to Gibbs Free Energy= -0.006908
Sum of electronic and zero-point Energies= -1123.209022
Sum of electronic and thermal Energies= -1123.199988
Sum of electronic and thermal Enthalpies= -1123.199043
Sum of electronic and thermal Free Energies= -1123.244351

| | | | |
|---|---|---|---|
| O | -0.19721800 | 0.97397600 | -1.15884100 |
| Na | -2.16604000 | 1.71265900 | -2.13048600 |
| S | -0.90902300 | 0.43746600 | 0.04547300 |
| O | -2.39089300 | 0.52892800 | -0.15704200 |
| O | -0.39298200 | -0.80062200 | 0.62620800 |
| C | -0.59050800 | 1.76245600 | 1.32709700 |
| F | -1.21247100 | 1.47876500 | 2.46997400 |
| F | 0.71366800 | 1.88822300 | 1.56593600 |
| F | -1.05367100 | 2.93968500 | 0.87304900 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1124.0689004
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1123.3689881

**OTf**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.027156 (Hartree/Particle)
Thermal correction to Energy= 0.034367
Thermal correction to Enthalpy= 0.035311
Thermal correction to Gibbs Free Energy= -0.005506
Sum of electronic and zero-point Energies= -960.977963
Sum of electronic and thermal Energies= -960.970753
Sum of electronic and thermal Enthalpies= -960.969809
Sum of electronic and thermal Free Energies= -961.010625

| | | | |
|---|---|---|---|
| O | 2.54310100 | 1.69826400 | -0.00021700 |
| S | 4.01934600 | 1.80517500 | -0.00012800 |
| O | 4.68905800 | 1.38428700 | 1.25082900 |
| O | 4.68884900 | 1.38918800 | -1.25283300 |
| C | 4.28896100 | 3.66546800 | 0.00349400 |
| F | 3.74026200 | 4.24042600 | 1.08780200 |
| F | 3.74051300 | 4.24464700 | -1.07869700 |
| F | 5.59751100 | 3.97424200 | 0.00424600 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -961.8053058
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -961.2091066

**O*t*-Am**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.148001 (Hartree/Particle)
Thermal correction to Energy= 0.155661
Thermal correction to Enthalpy= 0.156605
Thermal correction to Gibbs Free Energy= 0.117212
Sum of electronic and zero-point Energies= -272.078281
Sum of electronic and thermal Energies= -272.070621
Sum of electronic and thermal Enthalpies= -272.069677
Sum of electronic and thermal Free Energies= -272.109070

| | | | |
|---|---|---|---|
| C | -2.71967300 | 0.82099900 | -0.01999700 |
| C | -1.14844900 | 0.87690800 | -0.05506700 |
| H | -3.10790700 | 1.85429800 | 0.02362700 |
| H | -3.06225700 | 0.38613200 | -0.97499000 |
| H | -3.16570700 | 0.23919700 | 0.81147700 |
| C | -0.64044500 | -0.61146000 | -0.05615900 |
| C | -0.65276400 | 1.56309000 | 1.27857700 |
| H | 0.46413000 | -0.60663300 | -0.04087500 |
| H | -1.00291800 | -1.24852600 | 0.77554100 |
| H | -0.94921800 | -1.07369900 | -1.00997500 |
| H | 0.44878400 | 1.60704800 | 1.18839900 |
| H | -0.99446200 | 2.61250800 | 1.20450200 |
| C | -1.04547800 | 0.97645900 | 2.63875900 |
| H | -0.62581700 | 1.55886200 | 3.48034700 |
| H | -2.14059700 | 0.95748000 | 2.77426400 |
| H | -0.68726300 | -0.06105000 | 2.75491300 |
| O | -0.70422300 | 1.54862100 | -1.11359400 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -272.489235
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -272.2128793

**UnsubAlk**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.189893 (Hartree/Particle)
Thermal correction to Energy= 0.199170
Thermal correction to Enthalpy= 0.200114
Thermal correction to Gibbs Free Energy= 0.155175
Sum of electronic and zero-point Energies= -387.827702
Sum of electronic and thermal Energies= -387.818425
Sum of electronic and thermal Enthalpies= -387.817481
Sum of electronic and thermal Free Energies= -387.862420

| | | | |
|---|---|---|---|
| C | -0.89964600 | -1.06601900 | -2.63077100 |

| | | | |
|---|---|---|---|
| C | 0.31809400 | -1.20279800 | -2.07523000 |
| H | 0.68489700 | -2.18149800 | -1.75266800 |
| H | 0.97833200 | -0.34772800 | -1.90780700 |
| C | -1.81195200 | -2.26403400 | -2.81472300 |
| H | -2.75031200 | -2.10361500 | -2.25427000 |
| H | -1.33682000 | -3.14652900 | -2.35763400 |
| C | -1.39243400 | 0.26333700 | -3.09653500 |
| C | -2.75160500 | 0.61794800 | -2.98699100 |
| C | -0.51208400 | 1.20744500 | -3.66198800 |
| C | -3.20660500 | 1.87295700 | -3.40000100 |
| H | -3.46536000 | -0.08894200 | -2.55918500 |
| C | -0.96528600 | 2.46126900 | -4.07732300 |
| H | 0.53935400 | 0.94395300 | -3.79658500 |
| C | -2.31574300 | 2.80250100 | -3.94560700 |
| H | -4.26505700 | 2.12517500 | -3.29439100 |
| H | -0.26085200 | 3.17234600 | -4.51701200 |
| H | -2.67241100 | 3.78199100 | -4.27410400 |
| C | -2.14854600 | -2.55810600 | -4.28309000 |
| H | -2.66312700 | -1.70656700 | -4.75515800 |
| H | -1.23277800 | -2.75846600 | -4.86236700 |
| H | -2.80494800 | -3.43883200 | -4.36706500 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -388.3589946
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -387.9482009

**EProd**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.189014 (Hartree/Particle)
Thermal correction to Energy= 0.198729
Thermal correction to Enthalpy= 0.199674
Thermal correction to Gibbs Free Energy= 0.153890
Sum of electronic and zero-point Energies= -387.831042
Sum of electronic and thermal Energies= -387.821327
Sum of electronic and thermal Enthalpies= -387.820383
Sum of electronic and thermal Free Energies= -387.866167

| | | | |
|---|---|---|---|
| C | -1.55294200 | -0.92021000 | 0.09780500 |
| H | -1.84060500 | -1.96058000 | -0.13628100 |
| H | -0.60572300 | -0.98559400 | 0.66316200 |
| H | -2.31406000 | -0.50271800 | 0.77137800 |
| C | -1.36426000 | -0.13005900 | -1.16277900 |
| H | -0.65164100 | -0.57365700 | -1.86764600 |
| C | -1.93305500 | 1.04529700 | -1.51040100 |
| C | -2.87546300 | 1.81041200 | -0.60815400 |
| H | -3.74181900 | 2.18905000 | -1.17402900 |
| H | -3.25072900 | 1.19895600 | 0.22244500 |
| H | -2.37805800 | 2.69025200 | -0.16424500 |
| C | -1.62212300 | 1.67419200 | -2.82804500 |
| C | -1.60980900 | 3.07617700 | -2.97719800 |
| C | -1.34753800 | 0.89675000 | -3.97272900 |
| C | -1.30552600 | 3.67322200 | -4.20393900 |
| H | -1.82440400 | 3.71715000 | -2.12007900 |
| C | -1.04530600 | 1.49129900 | -5.19909100 |
| H | -1.39586200 | -0.19236800 | -3.90604600 |
| C | -1.01874000 | 2.88506200 | -5.32216800 |
| H | -1.29333100 | 4.76353400 | -4.28448200 |
| H | -0.84275700 | 0.86079800 | -6.06907100 |
| H | -0.78693600 | 3.35128900 | -6.28312400 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -388.3636323
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -387.9510108

**ZProd**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.188865 (Hartree/Particle)
Thermal correction to Energy= 0.198536
Thermal correction to Enthalpy= 0.199480
Thermal correction to Gibbs Free Energy= 0.153805
Sum of electronic and zero-point Energies= -387.830642
Sum of electronic and thermal Energies= -387.820970
Sum of electronic and thermal Enthalpies= -387.820026
Sum of electronic and thermal Free Energies= -387.865702

| | | | |
|---|---|---|---|
| C | -1.29870200 | -0.09331000 | -1.19973500 |
| C | -1.93196600 | 1.02325200 | -1.61264700 |
| C | -3.02895900 | 1.65335900 | -0.78387700 |
| H | -3.96980000 | 1.71434400 | -1.35797000 |
| H | -3.22010900 | 1.08420400 | 0.13822900 |
| H | -2.77400900 | 2.68751600 | -0.49544400 |
| C | -1.61879800 | 1.70821500 | -2.90252600 |
| C | -1.32107400 | 3.08398200 | -2.93828300 |
| C | -1.64688300 | 1.00625600 | -4.12230500 |
| C | -1.04147300 | 3.72913200 | -4.14578200 |
| H | -1.29249400 | 3.65459500 | -2.00677700 |
| C | -1.37204700 | 1.65053600 | -5.33208300 |
| H | -1.89912000 | -0.05668000 | -4.11741100 |
| C | -1.06597300 | 3.01504000 | -5.34880000 |
| H | -0.80205200 | 4.79588300 | -4.14717300 |
| H | -1.40276100 | 1.08421000 | -6.26676700 |
| H | -0.85123500 | 3.52032700 | -6.29392800 |
| C | -0.15943900 | -0.81271400 | -1.86260200 |
| H | -0.47625500 | -1.80036900 | -2.24408700 |
| H | 0.26778200 | -0.24980900 | -2.70435400 |
| H | 0.64624200 | -1.00825300 | -1.13385400 |
| H | -1.63201400 | -0.52877900 | -0.24880800 |

**(*E*)-tetrasub**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.269955 (Hartree/Particle)
Thermal correction to Energy= 0.284260
Thermal correction to Enthalpy= 0.285205
Thermal correction to Gibbs Free Energy= 0.227801
Sum of electronic and zero-point Energies= -618.649183
Sum of electronic and thermal Energies= -618.634877
Sum of electronic and thermal Enthalpies= -618.633933
Sum of electronic and thermal Free Energies= -618.691337

| | | | |
|---|---|---|---|
| C | -2.59794000 | 0.20667100 | -1.06952200 |
| C | -1.72315700 | -0.16962100 | -0.03369200 |
| C | -1.59515800 | 0.69008500 | 1.07233000 |
| C | -2.30730600 | 1.89127900 | 1.13739400 |
| C | -3.16487100 | 2.25685100 | 0.09471600 |
| C | -3.30621600 | 1.40989800 | -1.01017800 |
| H | -2.71327100 | -0.44449700 | -1.94009900 |
| H | -0.92703100 | 0.40541100 | 1.88910200 |
| H | -2.19308200 | 2.54312800 | 2.00761900 |
| H | -3.72189900 | 3.19603800 | 0.14313800 |
| H | -3.97150200 | 1.68843100 | -1.83181600 |
| C | -0.98094700 | -1.46740300 | -0.08310200 |
| C | 0.37424800 | -1.51818600 | -0.08249400 |
| C | -1.86996600 | -2.69086300 | -0.12233900 |
| H | -1.31283000 | -3.61820500 | -0.30724900 |
| H | -2.42133100 | -2.80298500 | 0.82772700 |
| H | -2.63475400 | -2.58542600 | -0.90969900 |
| C | 1.26277100 | -0.29494600 | -0.13902200 |
| H | 0.70613600 | 0.62834700 | -0.34458200 |
| H | 1.80791000 | -0.16449600 | 0.81234300 |
| H | 2.03262400 | -0.41439800 | -0.91934900 |
| C | 1.11686900 | -2.81490500 | -0.01391300 |
| C | 1.99046000 | -3.20687500 | -1.04493100 |
| C | 0.99061700 | -3.65748600 | 1.10540600 |
| C | 2.69917700 | -4.40884100 | -0.96792100 |
| H | 2.10441400 | -2.56917400 | -1.92560500 |
| C | 1.70323100 | -4.85733600 | 1.18810000 |
| H | 0.32341000 | -3.36049800 | 1.91852500 |
| C | 2.55954800 | -5.23870200 | 0.15008300 |
| H | 3.36348300 | -4.69983200 | -1.78603000 |

| | | | |
|---|---|---|---|
| H | 1.59031700 | -5.49569600 | 2.06843500 |
| H | 3.11697400 | -6.17684200 | 0.21225300 |

**(*Z*)-tetrasub**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.269879 (Hartree/Particle)
Thermal correction to Energy= 0.284197
Thermal correction to Enthalpy= 0.285142
Thermal correction to Gibbs Free Energy= 0.227948
Sum of electronic and zero-point Energies= -618.648697
Sum of electronic and thermal Energies= -618.634379
Sum of electronic and thermal Enthalpies= -618.633435
Sum of electronic and thermal Free Energies= -618.690628

| | | | |
|---|---|---|---|
| C | -1.74450300 | -3.79475800 | -0.79943300 |
| C | -1.79507800 | -2.81638300 | 0.21162200 |
| C | -2.67467800 | -3.02548800 | 1.29108500 |
| C | -3.45347500 | -4.18316600 | 1.37230500 |
| C | -3.38278700 | -5.15099600 | 0.36473600 |
| C | -2.52805900 | -4.94795300 | -0.72450700 |
| H | -1.07891600 | -3.64363400 | -1.65145400 |
| H | -2.73572600 | -2.27917900 | 2.08775400 |
| H | -4.11824000 | -4.33001800 | 2.22777400 |
| H | -3.99419800 | -6.05499300 | 0.42507900 |
| H | -2.47304200 | -5.69211600 | -1.52352000 |
| C | -0.96847400 | -1.57783000 | 0.13265500 |
| C | 0.36826600 | -1.58522500 | -0.11319700 |
| C | -1.69902100 | -0.25945900 | 0.30470400 |
| H | -1.27991800 | 0.33912600 | 1.13162800 |
| H | -1.61266100 | 0.36218500 | -0.60332000 |
| H | -2.76967100 | -0.40699000 | 0.49947700 |
| C | 1.11568500 | -0.27499400 | -0.27469700 |
| H | 0.70206900 | 0.33737700 | -1.09422900 |
| H | 1.04050100 | 0.33863300 | 0.63980000 |
| H | 2.18365300 | -0.43491400 | -0.47439500 |
| C | 1.17938900 | -2.83341800 | -0.20155500 |
| C | 2.05396200 | -3.04665200 | -1.28426400 |
| C | 1.11882700 | -3.81725500 | 0.80359600 |
| C | 2.81796000 | -4.21347600 | -1.37448500 |
| H | 2.12255600 | -2.29610100 | -2.07633600 |
| C | 1.88768600 | -4.97970900 | 0.71969800 |
| H | 0.45692700 | -3.66307600 | 1.65795700 |
| C | 2.73734900 | -5.18662100 | -0.37276900 |
| H | 3.47895400 | -4.36332300 | -2.23235300 |
| H | 1.82514700 | -5.72811300 | 1.51418600 |
| H | 3.33722400 | -6.09782100 | -0.44015000 |

**(*E*)-trisub**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.189025 (Hartree/Particle)
Thermal correction to Energy= 0.198723
Thermal correction to Enthalpy= 0.199667
Thermal correction to Gibbs Free Energy= 0.153953
Sum of electronic and zero-point Energies= -387.831023
Sum of electronic and thermal Energies= -387.821324
Sum of electronic and thermal Enthalpies= -387.820380
Sum of electronic and thermal Free Energies= -387.866095

| | | | |
|---|---|---|---|
| C | -1.53755500 | -3.69154900 | -1.00102800 |
| C | -1.73776000 | -2.74927200 | 0.02950000 |
| C | -2.67234100 | -3.07403200 | 1.03406600 |
| C | -3.34968800 | -4.29677300 | 1.02742900 |
| C | -3.12353600 | -5.22491800 | 0.00696600 |
| C | -2.21471800 | -4.91232600 | -1.01028900 |
| H | -0.85724400 | -3.45298600 | -1.82150900 |
| H | -2.86533100 | -2.37097500 | 1.84653300 |
| H | -4.05986000 | -4.52406100 | 1.82704700 |
| H | -3.65735100 | -6.17858700 | -0.00210200 |
| H | -2.04123700 | -5.61932500 | -1.82606500 |
| C | -1.00525000 | -1.44889500 | 0.05465100 |
| C | 0.25511000 | -1.36513900 | -0.42506200 |
| C | -1.73979200 | -0.27718600 | 0.66725300 |
| H | -1.78599500 | -0.36483900 | 1.76667300 |
| H | -1.26043100 | 0.68370300 | 0.44036500 |
| H | -2.78103500 | -0.23432900 | 0.30930400 |
| C | 1.14787300 | -0.16203300 | -0.49397000 |
| H | 0.65859400 | 0.76990500 | -0.17876000 |
| H | 2.04091800 | -0.30221500 | 0.14157700 |
| H | 1.52487400 | -0.01682900 | -1.52189200 |
| H | 0.71584700 | -2.28774800 | -0.79632600 |

**(*Z*)-trisub**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.188831 (Hartree/Particle)
Thermal correction to Energy= 0.198525
Thermal correction to Enthalpy= 0.199469
Thermal correction to Gibbs Free Energy= 0.153686
Sum of electronic and zero-point Energies= -387.830677
Sum of electronic and thermal Energies= -387.820983
Sum of electronic and thermal Enthalpies= -387.820038
Sum of electronic and thermal Free Energies= -387.865821

| | | | |
|---|---|---|---|
| C | -1.73724600 | -3.66620000 | -1.06081100 |
| C | -1.74673800 | -2.82370200 | 0.06678000 |
| C | -2.57134800 | -3.17960900 | 1.15117100 |
| C | -3.34128700 | -4.34513200 | 1.11796300 |
| C | -3.31430600 | -5.17607800 | -0.00747400 |
| C | -2.51049000 | -4.83013800 | -1.09832500 |
| H | -1.12196900 | -3.39441700 | -1.92166800 |
| H | -2.59968200 | -2.54379800 | 2.03955500 |
| H | -3.96573100 | -4.60650800 | 1.97647400 |
| H | -3.91964000 | -6.08575700 | -0.03529700 |
| H | -2.48834600 | -5.46694000 | -1.98674800 |
| C | -0.93487100 | -1.57032400 | 0.09777000 |
| C | 0.39156200 | -1.54675400 | -0.14359800 |
| C | -1.69691900 | -0.30100900 | 0.40676400 |
| H | -1.04095500 | 0.58222600 | 0.38637400 |
| H | -2.51383600 | -0.14638800 | -0.31927700 |
| H | -2.17108200 | -0.34661100 | 1.40210400 |
| C | 1.30723500 | -2.70691300 | -0.40877700 |
| H | 0.82627900 | -3.67898100 | -0.23039500 |
| H | 1.67341400 | -2.69894600 | -1.45150900 |
| H | 2.20335000 | -2.64254000 | 0.23250900 |
| H | 0.88099000 | -0.56436300 | -0.12453600 |

**Ni(0)**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.571144 (Hartree/Particle)
Thermal correction to Energy= 0.602008
Thermal correction to Enthalpy= 0.602952
Thermal correction to Gibbs Free Energy= 0.510765
Sum of electronic and zero-point Energies= -2666.885043
Sum of electronic and thermal Energies= -2666.854180
Sum of electronic and thermal Enthalpies= -2666.853236
Sum of electronic and thermal Free Energies= -2666.945423

| | | | |
|---|---|---|---|
| Ni | 6.31522300 | -2.02419500 | 0.26118200 |
| C | 7.87181100 | -1.23684200 | 0.31979900 |
| C | 9.68420300 | 0.06554000 | -0.21685200 |
| C | 9.94352000 | -0.50490200 | 0.98713400 |
| N | 8.83991800 | -1.29542300 | 1.30226000 |
| N | 8.42803400 | -0.38888700 | -0.61765100 |
| H | 10.80566400 | -0.43162500 | 1.64364500 |
| H | 10.27088100 | 0.74667300 | -0.82645600 |
| C | 8.74643800 | -2.15082000 | 2.44563300 |
| C | 9.20752600 | -3.47946300 | 2.32893600 |
| C | 8.21137600 | -1.63363000 | 3.64402600 |
| C | 9.10171000 | -4.30521500 | 3.45718200 |
| C | 8.12931900 | -2.49842700 | 4.74466500 |
| C | 8.56853400 | -3.82044200 | 4.65252300 |
| H | 9.43617900 | -5.34330400 | 3.40020300 |
| H | 7.71095000 | -2.13774800 | 5.68641400 |
| H | 8.49417600 | -4.47944600 | 5.52162100 |
| C | 7.79915500 | -0.03207000 | -1.85524700 |

| | | | |
|---|---|---|---|
| C | 7.82044800 | -0.95369300 | -2.92816000 |
| C | 7.20382000 | 1.24302300 | -1.96069300 |
| C | 7.27417500 | -0.53338200 | -4.14883600 |
| C | 6.67512000 | 1.61554100 | -3.20534000 |
| C | 6.72279900 | 0.74179500 | -4.29157400 |
| H | 7.27170700 | -1.21100400 | -5.00358500 |
| H | 6.20990100 | 2.59508500 | -3.32691400 |
| H | 6.31017500 | 1.04981000 | -5.25596200 |
| C | 7.04072000 | 2.12466000 | -0.72627400 |
| C | 5.78175200 | 1.68641400 | 0.04878000 |
| C | 7.01002600 | 3.62722900 | -1.02979000 |
| H | 7.90474300 | 1.94505000 | -0.06838900 |
| H | 5.81407600 | 0.60836000 | 0.27790200 |
| H | 5.69338400 | 2.24159800 | 0.99717800 |
| H | 4.87613600 | 1.88033300 | -0.55027900 |
| H | 7.88298300 | 3.94104000 | -1.62422800 |
| H | 6.10146700 | 3.91737100 | -1.58196400 |
| H | 7.01189600 | 4.20064400 | -0.08926200 |
| C | 7.66924300 | -0.21027900 | 3.71143000 |
| C | 7.98185500 | 0.49795800 | 5.03645600 |
| C | 6.15886200 | -0.20904700 | 3.41303600 |
| H | 8.15567400 | 0.36578300 | 2.90926500 |
| H | 9.05933400 | 0.47257100 | 5.26521900 |
| H | 7.66697600 | 1.55246200 | 4.98425900 |
| H | 7.44521300 | 0.04177200 | 5.88405900 |
| H | 5.96584800 | -0.66846800 | 2.42848600 |
| H | 5.60935900 | -0.78258600 | 4.17825900 |
| H | 5.76328000 | 0.81986400 | 3.40018700 |
| C | 9.73911500 | -4.02165100 | 1.00599400 |
| C | 8.64273500 | -4.82035100 | 0.27934200 |
| C | 11.02612600 | -4.84278000 | 1.16687400 |
| H | 9.98004800 | -3.16032100 | 0.36586000 |
| H | 7.75828500 | -4.18016600 | 0.12201500 |
| H | 9.00049400 | -5.16732700 | -0.70427400 |
| H | 8.33856400 | -5.70185500 | 0.86812600 |
| H | 11.80332800 | -4.27392800 | 1.70185200 |
| H | 10.85095100 | -5.77935000 | 1.72040800 |
| H | 11.42423800 | -5.11917800 | 0.17726400 |
| C | 8.36750700 | -2.36541100 | -2.72944300 |
| C | 9.90522600 | -2.40610100 | -2.72578400 |
| C | 7.80812100 | -3.38667500 | -3.72581200 |
| H | 8.00898900 | -2.67378400 | -1.73303000 |
| H | 10.33527100 | -1.73343600 | -1.97081200 |
| H | 10.25952800 | -3.42629100 | -2.50402800 |
| H | 10.30576100 | -2.11375500 | -3.71106700 |
| H | 6.70706200 | -3.36888300 | -3.74857000 |
| H | 8.17435400 | -3.21387800 | -4.75139000 |
| H | 8.12453900 | -4.40062100 | -3.43362800 |

**Ni(II)**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.574909 (Hartree/Particle)
Thermal correction to Energy= 0.609810
Thermal correction to Enthalpy= 0.610755
Thermal correction to Gibbs Free Energy= 0.507529
Sum of electronic and zero-point Energies= -3587.203846
Sum of electronic and thermal Energies= -3587.168944
Sum of electronic and thermal Enthalpies= -3587.168000
Sum of electronic and thermal Free Energies= -3587.271225

| | | | |
|---|---|---|---|
| C | -3.07213700 | 0.00181300 | 0.02900900 |
| C | -5.22676700 | -0.05035800 | -0.63248000 |
| C | -5.21460700 | 0.17877700 | 0.70810100 |
| N | -3.87854800 | 0.21335500 | 1.09390800 |
| N | -3.89820800 | -0.16174200 | -1.02923200 |
| H | -6.02268800 | 0.31389700 | 1.41949300 |
| H | -6.04697600 | -0.13974200 | -1.33706200 |
| C | -3.40408300 | 0.42741200 | 2.43901900 |
| C | -3.11008100 | -0.70413000 | 3.22859300 |
| C | -3.25072400 | 1.75293300 | 2.89583200 |
| C | -2.67326100 | -0.47162900 | 4.54053800 |
| C | -2.81595700 | 1.92510600 | 4.21769800 |
| C | -2.53471900 | 0.82706800 | 5.03087700 |
| H | -2.43746600 | -1.31722300 | 5.18830800 |
| H | -2.68679200 | 2.93285800 | 4.61524600 |
| H | -2.19431400 | 0.98573600 | 6.05735700 |
| C | -3.44758900 | -0.40676200 | -2.37702400 |
| C | -3.08768100 | 0.70217200 | -3.17128300 |
| C | -3.38157600 | -1.74001800 | -2.83175800 |
| C | -2.66941100 | 0.43933800 | -4.48344800 |
| C | -2.96048300 | -1.94300400 | -4.15356500 |
| C | -2.61159200 | -0.86700900 | -4.96993900 |
| H | -2.38472700 | 1.26710900 | -5.13460700 |
| H | -2.89723900 | -2.95815000 | -4.54849500 |
| H | -2.28337700 | -1.04934600 | -5.99644700 |
| Ni | -1.18803100 | -0.05196600 | 0.02488600 |
| Cl | -0.70160200 | 2.07325600 | 0.00343400 |
| Cl | -0.82313300 | -2.20201000 | 0.04777000 |
| C | -3.30537300 | -2.12002900 | 2.69820700 |
| C | -4.72366900 | -2.62377100 | 3.02196300 |
| C | -2.23945500 | -3.10445200 | 3.19415700 |
| H | -3.19744700 | -2.08256100 | 1.60550000 |
| H | -5.49615600 | -1.95577900 | 2.61091500 |
| H | -4.88339200 | -3.62808800 | 2.59709400 |
| H | -4.87719200 | -2.68521200 | 4.11208500 |
| H | -1.22966500 | -2.73250800 | 2.96942600 |
| H | -2.32019400 | -3.29691800 | 4.27623500 |
| H | -2.35918900 | -4.06967900 | 2.67791300 |
| C | -3.56856500 | 2.95139500 | 2.00853600 |
| C | -2.59313900 | 4.11960000 | 2.20731300 |
| C | -5.02175500 | 3.41626200 | 2.21784000 |
| H | -3.45581000 | 2.62413500 | 0.96437600 |
| H | -1.55298200 | 3.78322500 | 2.09815600 |
| H | -2.78057700 | 4.89313900 | 1.44574500 |
| H | -2.71546200 | 4.59649100 | 3.19325400 |
| H | -5.74501600 | 2.61181800 | 2.01885800 |
| H | -5.17537900 | 3.75571200 | 3.25552900 |
| H | -5.25838800 | 4.25713300 | 1.54594700 |
| C | -3.19901600 | 2.12906200 | -2.64626900 |
| C | -4.58612700 | 2.71227800 | -2.97224800 |
| C | -2.07765900 | 3.04753900 | -3.14622300 |
| H | -3.09390300 | 2.08965500 | -1.55338000 |
| H | -5.39549800 | 2.09160800 | -2.55785900 |
| H | -4.68788000 | 3.72612500 | -2.55223100 |
| H | -4.73646800 | 2.77689300 | -4.06262200 |
| H | -1.09142400 | 2.61989500 | -2.91591800 |
| H | -2.14475700 | 3.23651400 | -4.22984300 |
| H | -2.14314500 | 4.02188800 | -2.63738200 |
| C | -3.78143900 | -2.91282700 | -1.94406400 |
| C | -2.87102600 | -4.13611600 | -2.11927100 |
| C | -5.25519700 | -3.29397000 | -2.17818600 |
| H | -3.67196400 | -2.58507900 | -0.89974400 |
| H | -1.81585500 | -3.85921300 | -1.99000100 |
| H | -3.11829100 | -4.89457100 | -1.35960600 |
| H | -3.00074600 | -4.60888400 | -3.10629700 |
| H | -5.93397500 | -2.44702400 | -1.99864100 |
| H | -5.40884100 | -3.63148600 | -3.21647500 |
| H | -5.55314300 | -4.11469800 | -1.50574200 |

**A'**

Zero-point correction= 0.690860 (Hartree/Particle)
Thermal correction to Energy= 0.735666
Thermal correction to Enthalpy= 0.736610
Thermal correction to Gibbs Free Energy= 0.613030
Sum of electronic and zero-point Energies= -3859.203489
Sum of electronic and thermal Energies= -3859.158683
Sum of electronic and thermal Enthalpies= -3859.157739
Sum of electronic and thermal Free Energies= -3859.281319

| | | | |
|---|---|---|---|
| Ni | 7.49409700 | -2.50239600 | -0.59757000 |
| C | 8.50222200 | -1.21262900 | 0.30921900 |
| C | 9.66047400 | 0.70688800 | 0.74178100 |

| | | | |
|---|---|---|---|
| C | 9.54353400 | 0.03003200 | 1.91437900 |
| N | 8.82837000 | -1.13261800 | 1.63494600 |
| N | 9.01746600 | -0.06465100 | -0.22228000 |
| H | 9.90920200 | 0.26055300 | 2.90972200 |
| H | 10.14146900 | 1.65091800 | 0.50372000 |
| C | 8.40541800 | -2.09237700 | 2.61764600 |
| C | 9.04950600 | -3.34915100 | 2.67377300 |
| C | 7.33036400 | -1.75021200 | 3.46328100 |
| C | 8.64357500 | -4.23454100 | 3.68028400 |
| C | 6.97112300 | -2.66952200 | 4.46114100 |
| C | 7.63091500 | -3.89116800 | 4.57878200 |
| H | 9.11433700 | -5.21470600 | 3.76028900 |
| H | 6.15031600 | -2.43367000 | 5.14102500 |
| H | 7.33608400 | -4.59649500 | 5.36001000 |
| C | 8.88316600 | 0.27858100 | -1.61037000 |
| C | 7.65169200 | 0.80273600 | -2.06481900 |
| C | 9.98160000 | 0.04820200 | -2.46390100 |
| C | 7.57292900 | 1.16451400 | -3.41720000 |
| C | 9.84936000 | 0.42970100 | -3.80704900 |
| C | 8.66248800 | 0.99518200 | -4.27385800 |
| H | 6.64417800 | 1.57771100 | -3.81243500 |
| H | 10.67650500 | 0.27208800 | -4.50099100 |
| H | 8.57783100 | 1.29002700 | -5.32307300 |
| C | 6.33840500 | -5.25755700 | 0.86844500 |
| C | 6.70672600 | -5.70569600 | -0.42940500 |
| C | 6.53571700 | -4.86997600 | -1.52341800 |
| C | 6.01959100 | -3.54572200 | -1.38382800 |
| C | 5.77018400 | -3.07500900 | -0.03661600 |
| C | 5.85164900 | -3.98194600 | 1.06837600 |
| H | 6.45235800 | -5.92419200 | 1.72637900 |
| H | 7.10314400 | -6.71424800 | -0.56570700 |
| H | 6.75556100 | -5.23901300 | -2.52923800 |
| H | 5.60853100 | -3.01995700 | -2.25131200 |
| H | 5.57550700 | -3.63356900 | 2.06250700 |
| O | 4.95529900 | -1.88721000 | 0.12012300 |
| S | 3.36065100 | -1.94890000 | 0.40290200 |
| O | 3.00844400 | -2.99368600 | 1.35420300 |
| O | 2.93849700 | -0.56771500 | 0.57381400 |
| C | 2.68821100 | -2.51610100 | -1.26906000 |
| F | 1.38746900 | -2.26078000 | -1.29815500 |
| F | 2.89206500 | -3.81687200 | -1.41661600 |
| F | 3.29110900 | -1.85589000 | -2.25294500 |
| C | 6.54087000 | -0.45696500 | 3.28040400 |
| C | 7.00598200 | 0.64315100 | 4.25077600 |
| C | 5.02483900 | -0.67359000 | 3.41927700 |
| H | 6.72407600 | -0.10653100 | 2.25310500 |
| H | 8.07194700 | 0.88079900 | 4.12747500 |
| H | 6.43156400 | 1.56930000 | 4.08677800 |
| H | 6.84978900 | 0.32665900 | 5.29528500 |
| H | 4.68438800 | -1.55816800 | 2.86722000 |
| H | 4.72702300 | -0.80509100 | 4.47195100 |
| H | 4.47743100 | 0.19633600 | 3.02602300 |
| C | 10.10710200 | -3.73105500 | 1.64094900 |
| C | 10.28310000 | -5.24351800 | 1.47054700 |
| C | 11.45813600 | -3.05068000 | 1.92047200 |
| H | 9.72663500 | -3.35551100 | 0.67744300 |
| H | 9.31992900 | -5.73649100 | 1.26831800 |
| H | 10.95226500 | -5.44408400 | 0.61888000 |
| H | 10.73576000 | -5.71451500 | 2.35861900 |
| H | 11.36441700 | -1.95653000 | 1.97518000 |
| H | 11.88063000 | -3.40404200 | 2.87585200 |
| H | 12.17956400 | -3.28609900 | 1.12102400 |
| C | 6.45374900 | 0.92596000 | -1.12574000 |
| C | 5.10271700 | 0.88390700 | -1.84751200 |
| C | 6.55012300 | 2.16950900 | -0.22469800 |
| H | 6.47850400 | 0.03605600 | -0.47947200 |
| H | 5.03747300 | 0.01987400 | -2.52542700 |
| H | 4.29438900 | 0.78555800 | -1.10868800 |
| H | 4.91517400 | 1.79826500 | -2.43449500 |
| H | 7.48004100 | 2.18252300 | 0.36210100 |
| H | 6.51383900 | 3.09301300 | -0.82648000 |
| H | 5.70594100 | 2.18994900 | 0.48351600 |
| C | 11.21392400 | -0.69842600 | -1.96195100 |
| C | 12.51529500 | -0.29590600 | -2.66635100 |
| C | 10.97443400 | -2.21817100 | -2.06986200 |
| H | 11.33863200 | -0.46596900 | -0.89335900 |
| H | 13.37450800 | -0.77876600 | -2.17476100 |
| H | 12.52688900 | -0.61282500 | -3.72162900 |
| H | 12.67145200 | 0.79400600 | -2.63739200 |
| H | 10.06286300 | -2.51745300 | -1.52945700 |
| H | 10.85630600 | -2.51742000 | -3.12413600 |
| H | 11.82213100 | -2.77894200 | -1.64348200 |

**TS-A'-B'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.690006 (Hartree/Particle)
Thermal correction to Energy= 0.734506
Thermal correction to Enthalpy= 0.735450
Thermal correction to Gibbs Free Energy= 0.612573
Sum of electronic and zero-point Energies= -3859.191840
Sum of electronic and thermal Energies= -3859.147340
Sum of electronic and thermal Enthalpies= -3859.146396
Sum of electronic and thermal Free Energies= -3859.269274

| | | | |
|---|---|---|---|
| Ni | 7.65057500 | -2.58251100 | -0.67482000 |
| C | 8.48044000 | -1.18787200 | 0.29225900 |
| C | 9.62071500 | 0.73077300 | 0.72712000 |
| C | 9.49514500 | 0.05427600 | 1.89925400 |
| N | 8.78557400 | -1.10929300 | 1.61756600 |
| N | 8.99198600 | -0.04521800 | -0.24025900 |
| H | 9.85097300 | 0.28586100 | 2.89744900 |
| H | 10.09577000 | 1.67831300 | 0.49172100 |
| C | 8.39010500 | -2.07808400 | 2.60814000 |
| C | 9.07381500 | -3.31323600 | 2.66906300 |
| C | 7.31621000 | -1.75532600 | 3.46387500 |
| C | 8.69645900 | -4.20692300 | 3.67951600 |
| C | 6.98891800 | -2.68307200 | 4.46539600 |
| C | 7.67868200 | -3.88822600 | 4.58043900 |
| H | 9.19684700 | -5.17199600 | 3.76226800 |
| H | 6.16668300 | -2.46733900 | 5.14931000 |
| H | 7.40481400 | -4.59940300 | 5.36381200 |
| C | 8.88406700 | 0.28974800 | -1.63551500 |
| C | 7.65057900 | 0.78333900 | -2.11838500 |
| C | 10.01216600 | 0.08895600 | -2.45777000 |
| C | 7.59396300 | 1.12716000 | -3.47682500 |
| C | 9.89792700 | 0.45052600 | -3.80809600 |
| C | 8.70522500 | 0.97395800 | -4.30768100 |
| H | 6.66511500 | 1.51540800 | -3.89571800 |
| H | 10.74564800 | 0.31419900 | -4.48103900 |
| H | 8.63564600 | 1.25330500 | -5.36215600 |
| C | 5.97838400 | -5.54086800 | 0.74477900 |
| C | 5.97535600 | -6.02955400 | -0.58817300 |
| C | 6.00545900 | -5.14505900 | -1.65098700 |
| C | 6.09326200 | -3.73956700 | -1.42574300 |
| C | 6.13028900 | -3.29005200 | -0.06992300 |
| C | 6.01153600 | -4.18545900 | 1.01943000 |
| H | 5.95393600 | -6.24855900 | 1.57816200 |
| H | 5.91520800 | -7.10540200 | -0.76791000 |
| H | 5.92117900 | -5.51211400 | -2.67782700 |
| H | 5.84143000 | -3.05581600 | -2.24301700 |
| H | 6.00378600 | -3.80542900 | 2.04047300 |
| O | 5.10615500 | -1.75110100 | 0.25178300 |
| S | 3.59076400 | -1.80666100 | 0.51382100 |
| O | 3.19876400 | -2.82396200 | 1.49548000 |
| O | 3.04536900 | -0.44921400 | 0.63418500 |
| C | 2.89510300 | -2.46556400 | -1.10782800 |
| F | 1.59443500 | -2.18942600 | -1.17114000 |
| F | 3.05870000 | -3.78523600 | -1.18166100 |
| F | 3.50316500 | -1.90173000 | -2.15732300 |
| C | 6.49564100 | -0.47995100 | 3.29225100 |
| C | 6.99716400 | 0.65896100 | 4.19896800 |

| | | | |
|---|---|---|---|
| C | 4.99626300 | -0.71398900 | 3.53833100 |
| H | 6.60633300 | -0.16567700 | 2.24300300 |
| H | 8.04559000 | 0.92406600 | 4.00616000 |
| H | 6.38740800 | 1.56370200 | 4.04436900 |
| H | 6.91233700 | 0.37040800 | 5.25971400 |
| H | 4.64463100 | -1.64593800 | 3.08073800 |
| H | 4.76569400 | -0.75931900 | 4.61527900 |
| H | 4.40761000 | 0.10824800 | 3.10530300 |
| C | 10.16025800 | -3.66538800 | 1.65637100 |
| C | 10.34550100 | -5.17333800 | 1.45315600 |
| C | 11.49750800 | -2.98536000 | 1.99632900 |
| H | 9.81571500 | -3.26918700 | 0.68905400 |
| H | 9.38730800 | -5.66695500 | 1.22740700 |
| H | 11.02938300 | -5.35238200 | 0.60852900 |
| H | 10.78578600 | -5.66242600 | 2.33725000 |
| H | 11.39384400 | -1.89305900 | 2.07288800 |
| H | 11.88820700 | -3.35724400 | 2.95796200 |
| H | 12.24763200 | -3.19870600 | 1.21744400 |
| C | 6.43348600 | 0.90108200 | -1.20494100 |
| C | 5.09650600 | 0.88262800 | -1.95280500 |
| C | 6.51495200 | 2.13354000 | -0.28605000 |
| H | 6.43075500 | 0.00603900 | -0.56704500 |
| H | 5.03656800 | 0.03595200 | -2.65211800 |
| H | 4.27842500 | 0.76820600 | -1.22745000 |
| H | 4.92453400 | 1.81293200 | -2.51964900 |
| H | 7.42827100 | 2.13848100 | 0.32616900 |
| H | 6.49619400 | 3.06478900 | -0.87658400 |
| H | 5.65241900 | 2.14530300 | 0.39934500 |
| C | 11.27072900 | -0.58535700 | -1.91717000 |
| C | 12.56180100 | -0.13227700 | -2.61078600 |
| C | 11.12102300 | -2.11778400 | -1.98976200 |
| H | 11.36752800 | -0.32083000 | -0.85320700 |
| H | 13.43612800 | -0.55141300 | -2.08864000 |
| H | 12.61157200 | -0.47951800 | -3.65521500 |
| H | 12.65632100 | 0.96484200 | -2.61269900 |
| H | 10.24336900 | -2.46268100 | -1.42231600 |
| H | 11.00164900 | -2.44904000 | -3.03382200 |
| H | 12.00640000 | -2.61844000 | -1.56585900 |

**B’**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.691598 (Hartree/Particle)
Thermal correction to Energy= 0.737000
Thermal correction to Enthalpy= 0.737945
Thermal correction to Gibbs Free Energy= 0.610514
Sum of electronic and zero-point Energies= -3859.265908
Sum of electronic and thermal Energies= -3859.220506
Sum of electronic and thermal Enthalpies= -3859.219562
Sum of electronic and thermal Free Energies= -3859.346992

| | | | |
|---|---|---|---|
| C | 1.12900200 | 1.05792300 | 0.89094400 |
| C | 2.46030700 | 2.46967100 | -0.27186000 |
| C | 2.89507600 | 2.48210900 | 1.01750600 |
| N | 2.06477300 | 1.61370400 | 1.71094600 |
| N | 1.38175000 | 1.58978000 | -0.32915400 |
| H | 3.70439900 | 3.02283800 | 1.49895300 |
| H | 2.82407100 | 2.98354600 | -1.15612800 |
| C | 2.13383700 | 1.22762800 | 3.09875400 |
| C | 1.55033400 | 2.08105900 | 4.06076900 |
| C | 2.72147300 | -0.01891700 | 3.42151400 |
| C | 1.57308000 | 1.65300900 | 5.39394700 |
| C | 2.70096200 | -0.40089900 | 4.77088900 |
| C | 2.13796800 | 0.42479600 | 5.74246200 |
| H | 1.12935500 | 2.27627800 | 6.17129600 |
| H | 3.12424600 | -1.36046000 | 5.06723300 |
| H | 2.13186200 | 0.10345600 | 6.78682800 |
| C | 0.73839900 | 1.19948100 | -1.55631400 |
| C | -0.40200400 | 1.90836900 | -1.97884500 |
| C | 1.28629300 | 0.11393800 | -2.26703400 |
| C | -0.98934900 | 1.51038000 | -3.18646800 |
| C | 0.65098900 | -0.25265800 | -3.46240900 |
| C | -0.46829500 | 0.44311000 | -3.91981600 |
| H | -1.87843300 | 2.02664700 | -3.55038700 |
| H | 1.03305400 | -1.09730100 | -4.03886200 |
| H | -0.94889500 | 0.14222600 | -4.85417500 |
| C | -3.86067100 | 0.29992300 | 0.79988700 |
| C | -4.02107000 | -0.34990800 | -0.42858500 |
| C | -2.90469100 | -0.89617800 | -1.06968700 |
| C | -1.63464200 | -0.79621100 | -0.48918700 |
| C | -1.47333200 | -0.14172300 | 0.73531400 |
| C | -2.59114100 | 0.40273000 | 1.38215900 |
| H | -4.72753000 | 0.72516900 | 1.31400600 |
| H | -5.01214400 | -0.43174300 | -0.88261500 |
| H | -3.01758900 | -1.40984900 | -2.02855000 |
| H | -0.77873300 | -1.24175200 | -0.99486700 |
| H | -2.48714700 | 0.88981700 | 2.35444600 |
| Ni | 0.08832400 | -0.24211500 | 1.72515900 |
| C | 2.47528800 | -0.68046900 | -1.73517100 |
| C | 3.53419300 | -0.95521700 | -2.81303700 |
| C | 2.00501800 | -1.98353200 | -1.06502300 |
| H | 2.96500800 | -0.07695700 | -0.95625900 |
| H | 3.86047100 | -0.02479700 | -3.30418600 |
| H | 4.41770400 | -1.43320700 | -2.36097800 |
| H | 3.15852200 | -1.63679500 | -3.59266300 |
| H | 1.30663200 | -1.79878100 | -0.23696100 |
| H | 1.49362400 | -2.63829900 | -1.78902500 |
| H | 2.86340900 | -2.53867400 | -0.65397200 |
| C | -0.97166300 | 3.05129100 | -1.14704200 |
| C | -2.50119400 | 3.14052100 | -1.21740900 |
| C | -0.32575000 | 4.39359000 | -1.53716100 |
| H | -0.71386500 | 2.84397300 | -0.09684100 |
| H | -2.96570400 | 2.17031500 | -0.99474200 |
| H | -2.86647800 | 3.87304500 | -0.48025600 |
| H | -2.84798400 | 3.47615300 | -2.20834000 |
| H | 0.76839700 | 4.37283400 | -1.42380700 |
| H | -0.55062800 | 4.64048100 | -2.58787900 |
| H | -0.71559700 | 5.20792800 | -0.90506400 |
| C | 3.38262100 | -0.89718700 | 2.35919000 |
| C | 3.40009300 | -2.38827600 | 2.71476600 |
| C | 4.80324800 | -0.39378800 | 2.04398900 |
| H | 2.78981700 | -0.80653900 | 1.43629500 |
| H | 2.40601500 | -2.75653300 | 2.99970400 |
| H | 3.73593700 | -2.96979900 | 1.84257300 |
| H | 4.09743400 | -2.60397000 | 3.54003300 |
| H | 4.80514300 | 0.65622500 | 1.71682300 |
| H | 5.44657900 | -0.47388200 | 2.93540900 |
| H | 5.25355000 | -0.99899300 | 1.24087700 |
| C | 0.84942900 | 3.37043500 | 3.64515100 |
| C | 0.90614700 | 4.47162300 | 4.71130700 |
| C | -0.60570900 | 3.07326100 | 3.23427000 |
| H | 1.36555600 | 3.75933200 | 2.75349700 |
| H | 1.93743200 | 4.65652800 | 5.05061200 |
| H | 0.50620600 | 5.41158100 | 4.30015600 |
| H | 0.29688000 | 4.22029400 | 5.59411200 |
| H | -0.65061100 | 2.31552400 | 2.44001800 |
| H | -1.17911000 | 2.68945300 | 4.09373100 |
| H | -1.10221400 | 3.98603700 | 2.86777900 |
| S | -0.40254100 | -3.04471600 | 2.70756300 |
| O | 0.13682500 | -3.35689500 | 1.37678100 |
| O | 0.13338500 | -3.76501500 | 3.86546300 |
| O | -0.50138700 | -1.53752800 | 2.97920500 |
| C | -2.21286200 | -3.51624400 | 2.63602400 |
| F | -2.83089100 | -3.14541300 | 3.75682500 |
| F | -2.80983000 | -2.93247500 | 1.60019900 |
| F | -2.31710100 | -4.83927200 | 2.50333600 |

**K’**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.804093 (Hartree/Particle)
Thermal correction to Energy= 0.854561
Thermal correction to Enthalpy= 0.855505

Thermal correction to Gibbs Free Energy= 0.720707
Sum of electronic and zero-point Energies= -4016.277585
Sum of electronic and thermal Energies= -4016.227117
Sum of electronic and thermal Enthalpies= -4016.226172
Sum of electronic and thermal Free Energies= -4016.360970

| | | | |
|---|---|---|---|
| C | 0.85286100 | 0.60703700 | 0.73496800 |
| C | 2.70789200 | 1.55623700 | -0.17706200 |
| C | 2.91028100 | 1.47689200 | 1.16006700 |
| N | 1.76220200 | 0.90548000 | 1.70401400 |
| N | 1.44612700 | 1.02453300 | -0.42010900 |
| H | 3.75399500 | 1.76640800 | 1.77739700 |
| H | 3.32853000 | 1.95308600 | -0.97297300 |
| C | 1.58943800 | 0.78523600 | 3.13112400 |
| C | 1.26667600 | 1.95378400 | 3.85409100 |
| C | 1.78304900 | -0.47026400 | 3.74625800 |
| C | 1.16767500 | 1.84423500 | 5.24884800 |
| C | 1.66094400 | -0.52337100 | 5.14210700 |
| C | 1.36619000 | 0.62051600 | 5.88593000 |
| H | 0.92541400 | 2.72735000 | 5.84328900 |
| H | 1.79758100 | -1.47378700 | 5.65840000 |
| H | 1.28244000 | 0.55372900 | 6.97365500 |
| C | 0.86029100 | 1.00333300 | -1.73953800 |
| C | -0.10880600 | 1.98240200 | -2.06452600 |
| C | 1.32010500 | 0.04636100 | -2.66617800 |
| C | -0.60070100 | 1.98964100 | -3.37640500 |
| C | 0.79563500 | 0.10548800 | -3.96699200 |
| C | -0.14803500 | 1.06602600 | -4.32045000 |
| H | -1.35065500 | 2.72367000 | -3.67145800 |
| H | 1.12673900 | -0.62099500 | -4.71084500 |
| H | -0.54467000 | 1.09211800 | -5.33853700 |
| C | -4.03724900 | -2.97161300 | -0.53256800 |
| C | -4.28169000 | -2.46835300 | -1.81405200 |
| C | -3.61787700 | -1.31084700 | -2.23618200 |
| C | -2.72634100 | -0.65901200 | -1.37739500 |
| C | -2.47417100 | -1.16403600 | -0.09260600 |
| C | -3.14007800 | -2.32105200 | 0.32393400 |
| H | -4.53868100 | -3.88401800 | -0.19732700 |
| H | -4.98143700 | -2.97729900 | -2.48234300 |
| H | -3.79110200 | -0.91189300 | -3.24015400 |
| H | -2.21711000 | 0.24246700 | -1.73040100 |
| H | -2.93485100 | -2.73899900 | 1.31138700 |
| C | -1.49282700 | 0.93185000 | 2.10982300 |
| H | -0.95979900 | 0.56471300 | 2.98938600 |
| H | -1.30579300 | 1.97705300 | 1.84995800 |
| C | -2.68528500 | 0.33607800 | 1.71845700 |
| H | -3.02212400 | -0.53344900 | 2.29021800 |
| C | -3.77825100 | 1.13256400 | 1.04378000 |
| H | -3.33647100 | 1.76676100 | 0.26245500 |
| H | -4.48405200 | 0.45754500 | 0.54083000 |
| C | -4.52032800 | 2.00330100 | 2.06726200 |
| H | -3.84113500 | 2.73120800 | 2.53979700 |
| H | -5.33623800 | 2.56195900 | 1.58186700 |
| H | -4.96296100 | 1.38920400 | 2.86858100 |
| Ni | -0.87879700 | -0.33248900 | 0.65641800 |
| C | 2.34105700 | -1.02448400 | -2.30263500 |
| C | 3.76117100 | -0.63064900 | -2.74663300 |
| C | 1.96455200 | -2.39556500 | -2.88686500 |
| H | 2.32879900 | -1.13330600 | -1.21036600 |
| H | 4.10190300 | 0.30696600 | -2.28374500 |
| H | 4.47790600 | -1.42091500 | -2.47072800 |
| H | 3.80561200 | -0.49990500 | -3.84062300 |
| H | 0.89103500 | -2.58481300 | -2.77462800 |
| H | 2.21221800 | -2.46613100 | -3.95888400 |
| H | 2.50617500 | -3.19092300 | -2.35632100 |
| C | -0.60869600 | 2.98687600 | -1.02756100 |
| C | -1.98623200 | 3.57547500 | -1.35757100 |
| C | 0.40389800 | 4.12102100 | -0.78181600 |
| H | -0.71969200 | 2.42830900 | -0.08796000 |
| H | -2.71785600 | 2.79225600 | -1.60657700 |
| H | -2.36943300 | 4.13664500 | -0.49117900 |
| H | -1.93946400 | 4.27668200 | -2.20614000 |
| H | 1.38554800 | 3.74270400 | -0.46563600 |
| H | 0.54803100 | 4.71449600 | -1.69934800 |
| H | 0.03676800 | 4.79715900 | 0.00751100 |
| C | 2.10909100 | -1.70698000 | 2.91969700 |
| C | 1.73996100 | -3.02516400 | 3.60639300 |
| C | 3.58359200 | -1.73630000 | 2.47819000 |
| H | 1.50086300 | -1.63754100 | 2.00959300 |
| H | 0.69722300 | -3.02207500 | 3.95489600 |
| H | 1.83886000 | -3.84453100 | 2.88211900 |
| H | 2.40153100 | -3.23687900 | 4.46277800 |
| H | 3.87454200 | -0.82683600 | 1.93372600 |
| H | 4.24982100 | -1.83938600 | 3.35084500 |
| H | 3.74361700 | -2.59343600 | 1.80681300 |
| C | 1.02772000 | 3.29752900 | 3.17072400 |
| C | 2.24822200 | 4.22297800 | 3.32434200 |
| C | -0.24319800 | 4.00221300 | 3.67497600 |
| H | 0.88788000 | 3.11066000 | 2.09532500 |
| H | 3.16215600 | 3.76393700 | 2.92015300 |
| H | 2.08213000 | 5.17414200 | 2.79328800 |
| H | 2.42964100 | 4.45246200 | 4.38706000 |
| H | -1.12010800 | 3.33907400 | 3.63870100 |
| H | -0.13079600 | 4.35355400 | 4.71275100 |
| H | -0.45543200 | 4.88603700 | 3.05225800 |
| S | 0.28892000 | -3.16450100 | 0.22709700 |
| O | 1.69527100 | -3.59355000 | 0.17537200 |
| O | -0.45308200 | -3.41059500 | 1.47278300 |
| O | 0.11143400 | -1.75533000 | -0.31781200 |
| C | -0.58190900 | -4.25139200 | -1.07862000 |
| F | -1.49491100 | -5.01628800 | -0.48576500 |
| F | -1.18086800 | -3.51024400 | -2.00912900 |
| F | 0.31060100 | -5.04021800 | -1.67751000 |

**TS-K'-C'**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.803915 (Hartree/Particle)
Thermal correction to Energy= 0.853564
Thermal correction to Enthalpy= 0.854508
Thermal correction to Gibbs Free Energy= 0.721825
Sum of electronic and zero-point Energies= -4016.277665
Sum of electronic and thermal Energies= -4016.228016
Sum of electronic and thermal Enthalpies= -4016.227072
Sum of electronic and thermal Free Energies= -4016.359755

| | | | |
|---|---|---|---|
| C | 0.86253900 | 0.60142100 | 0.72795500 |
| C | 2.72504800 | 1.54582300 | -0.17284200 |
| C | 2.91845400 | 1.46649900 | 1.16596000 |
| N | 1.76545700 | 0.89804800 | 1.70283200 |
| N | 1.46366000 | 1.01720100 | -0.42364300 |
| H | 3.75903100 | 1.75383300 | 1.78860500 |
| H | 3.35246300 | 1.94026600 | -0.96466400 |
| C | 1.57707500 | 0.78318300 | 3.12812200 |
| C | 1.23920600 | 1.95333700 | 3.84134500 |
| C | 1.76988200 | -0.46833200 | 3.75104100 |
| C | 1.12974500 | 1.85097500 | 5.23586600 |
| C | 1.63712900 | -0.51467300 | 5.14615900 |
| C | 1.33126500 | 0.63197000 | 5.88127000 |
| H | 0.87628100 | 2.73553900 | 5.82342400 |
| H | 1.77331700 | -1.46191200 | 5.66846800 |
| H | 1.23968200 | 0.57084200 | 6.96871200 |
| C | 0.87076100 | 1.00701900 | -1.73952200 |
| C | -0.08859700 | 1.99929600 | -2.05219200 |
| C | 1.30535500 | 0.04306800 | -2.67071200 |
| C | -0.60143900 | 2.01061600 | -3.35590100 |
| C | 0.76148700 | 0.10655000 | -3.96330300 |
| C | -0.17617300 | 1.07806000 | -4.30396500 |
| H | -1.34564500 | 2.75489700 | -3.64043100 |
| H | 1.07155400 | -0.62530600 | -4.71092200 |
| H | -0.58859600 | 1.10621100 | -5.31573500 |
| C | -3.97642000 | -2.97848500 | -0.56026500 |
| C | -4.20759000 | -2.46588800 | -1.84057900 |

| | | | |
|---|---|---|---|
| C | -3.58473000 | -1.27405300 | -2.22805300 |
| C | -2.75013700 | -0.59486600 | -1.33479300 |
| C | -2.50716100 | -1.11214700 | -0.05263700 |
| C | -3.13163400 | -2.30431400 | 0.32929700 |
| H | -4.44508100 | -3.91740900 | -0.25281400 |
| H | -4.86627600 | -2.99408600 | -2.53500100 |
| H | -3.74848200 | -0.86743900 | -3.23033100 |
| H | -2.27830100 | 0.33769500 | -1.65684300 |
| H | -2.93302000 | -2.72821000 | 1.31532700 |
| C | -1.52324600 | 0.94019000 | 2.04978300 |
| H | -0.99655100 | 0.62734700 | 2.95467900 |
| H | -1.39381500 | 1.99267500 | 1.78081700 |
| C | -2.71010800 | 0.29205600 | 1.68113600 |
| H | -3.01784700 | -0.55719900 | 2.29867100 |
| C | -3.85009200 | 1.07799800 | 1.06760000 |
| H | -3.45686300 | 1.72448600 | 0.26956100 |
| H | -4.57366300 | 0.39780200 | 0.59747400 |
| C | -4.54792800 | 1.93229200 | 2.13449300 |
| H | -3.85477300 | 2.66561800 | 2.57717000 |
| H | -5.39424800 | 2.48392200 | 1.69538200 |
| H | -4.94213800 | 1.30763600 | 2.95287700 |
| Ni | -0.86449800 | -0.31213800 | 0.65859100 |
| C | 2.32068600 | -1.03635500 | -2.31787500 |
| C | 3.74131700 | -0.64608100 | -2.76357500 |
| C | 1.93643700 | -2.40229200 | -2.90818900 |
| H | 2.31133400 | -1.15136100 | -1.22615100 |
| H | 4.08679300 | 0.28780000 | -2.29667100 |
| H | 4.45564800 | -1.44056900 | -2.49359900 |
| H | 3.78329000 | -0.50967100 | -3.85698700 |
| H | 0.86266300 | -2.58795800 | -2.79230600 |
| H | 2.17982200 | -2.46830400 | -3.98152500 |
| H | 2.47738100 | -3.20239100 | -2.38396800 |
| C | -0.55004100 | 3.01742200 | -1.01153300 |
| C | -1.94076200 | 3.59907900 | -1.29471300 |
| C | 0.47224600 | 4.15357200 | -0.82350000 |
| H | -0.62211600 | 2.47392000 | -0.06008200 |
| H | -2.67854000 | 2.81118100 | -1.50841200 |
| H | -2.29323500 | 4.16736400 | -0.41984000 |
| H | -1.92936500 | 4.29191500 | -2.15134500 |
| H | 1.46411700 | 3.77548300 | -0.54004600 |
| H | 0.58194900 | 4.73335800 | -1.75450400 |
| H | 0.13797400 | 4.84181300 | -0.02996400 |
| C | 2.10287400 | -1.70798700 | 2.93188300 |
| C | 1.72491800 | -3.02335300 | 3.61910200 |
| C | 3.58118000 | -1.74088700 | 2.50394200 |
| H | 1.50273100 | -1.64099500 | 2.01614000 |
| H | 0.67936800 | -3.01637600 | 3.95897900 |
| H | 1.82706400 | -3.84479200 | 2.89756500 |
| H | 2.37887400 | -3.23468100 | 4.48145200 |
| H | 3.87898100 | -0.83257400 | 1.96128000 |
| H | 4.23931700 | -1.84440800 | 3.38269100 |
| H | 3.74568600 | -2.59897200 | 1.83483000 |
| C | 0.99188000 | 3.28938300 | 3.14594600 |
| C | 2.20551100 | 4.22509100 | 3.29047600 |
| C | -0.28446700 | 3.98892400 | 3.64331200 |
| H | 0.85281300 | 3.09099600 | 2.07257200 |
| H | 3.12232500 | 3.76944200 | 2.88909900 |
| H | 2.03181800 | 5.17029100 | 2.75121000 |
| H | 2.38607500 | 4.46513700 | 4.35102700 |
| H | -1.15452400 | 3.31651900 | 3.61726200 |
| H | -0.17337200 | 4.35540800 | 4.67603100 |
| H | -0.50625100 | 4.86219400 | 3.00912600 |
| S | 0.28600900 | -3.16283500 | 0.22378700 |
| O | 1.69705600 | -3.57840800 | 0.17725200 |
| O | -0.45342700 | -3.40884600 | 1.47175600 |
| O | 0.08655100 | -1.76467300 | -0.33447800 |
| C | -0.57312600 | -4.27067500 | -1.07117300 |
| F | -1.48081200 | -5.03803200 | -0.47208500 |
| F | -1.17931600 | -3.54285200 | -2.00837300 |
| F | 0.32495000 | -5.05785300 | -1.66375900 |

**C'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.804892 (Hartree/Particle)
Thermal correction to Energy= 0.854971
Thermal correction to Enthalpy= 0.855915
Thermal correction to Gibbs Free Energy= 0.719594
Sum of electronic and zero-point Energies= -4016.326277
Sum of electronic and thermal Energies= -4016.276199
Sum of electronic and thermal Enthalpies= -4016.275254
Sum of electronic and thermal Free Energies= -4016.411575

| | | | |
|---|---|---|---|
| C | 1.01994200 | 0.80002800 | 0.72702800 |
| C | 2.76986900 | 1.86671500 | -0.23521200 |
| C | 3.01184500 | 1.80737600 | 1.10142600 |
| N | 1.92543300 | 1.15029700 | 1.67463100 |
| N | 1.54711200 | 1.23715300 | -0.44609000 |
| H | 3.85461300 | 2.15312200 | 1.69063700 |
| H | 3.35051400 | 2.29028900 | -1.04805200 |
| C | 1.75992400 | 0.85163000 | 3.07376400 |
| C | 1.31281600 | 1.87871900 | 3.92996400 |
| C | 2.01218900 | -0.46747800 | 3.51525800 |
| C | 1.15897200 | 1.56454200 | 5.28852100 |
| C | 1.83320900 | -0.72585000 | 4.88139300 |
| C | 1.42030100 | 0.27847300 | 5.75872600 |
| H | 0.82138900 | 2.33292900 | 5.98617000 |
| H | 2.01022000 | -1.72956700 | 5.26790500 |
| H | 1.28946600 | 0.05086300 | 6.81968400 |
| C | 0.89198600 | 1.04644600 | -1.71597500 |
| C | -0.01980300 | 2.02985700 | -2.15192300 |
| C | 1.15678200 | -0.13620500 | -2.43974400 |
| C | -0.67253100 | 1.80783200 | -3.37247500 |
| C | 0.47355900 | -0.30780700 | -3.65210700 |
| C | -0.42852000 | 0.65193300 | -4.11322000 |
| H | -1.39094600 | 2.54046500 | -3.74267700 |
| H | 0.64057900 | -1.21006100 | -4.24155600 |
| H | -0.95365400 | 0.49240700 | -5.05855400 |
| C | -3.95366900 | 0.65459800 | -2.17996500 |
| C | -5.04696500 | 1.51204000 | -2.02871000 |
| C | -5.39445400 | 1.96503100 | -0.75099100 |
| C | -4.65402900 | 1.56493300 | 0.36543000 |
| C | -3.55414700 | 0.70488200 | 0.22313800 |
| C | -3.21476000 | 0.25611600 | -1.06275600 |
| H | -3.66283100 | 0.29854000 | -3.17102200 |
| H | -5.62510000 | 1.82814300 | -2.90068900 |
| H | -6.24595200 | 2.63836900 | -0.62195900 |
| H | -4.93032000 | 1.93809700 | 1.35412100 |
| H | -2.35530500 | -0.40541600 | -1.19562900 |
| C | -1.56827700 | 1.33590600 | 1.63494900 |
| H | -1.32797000 | 1.55338900 | 2.68360500 |
| H | -1.64180400 | 2.25692200 | 1.04551400 |
| C | -2.68390200 | 0.34087200 | 1.41663200 |
| H | -2.20639300 | -0.67140600 | 1.09904400 |
| C | -3.44878500 | -0.07878000 | 2.69289600 |
| H | -3.95386300 | 0.81198500 | 3.10128100 |
| H | -4.24169400 | -0.78884300 | 2.40424000 |
| C | -2.55261900 | -0.71331000 | 3.75695000 |
| H | -1.77122600 | -0.01966300 | 4.10647100 |
| H | -3.14547200 | -1.01284400 | 4.63522300 |
| H | -2.05072100 | -1.60771300 | 3.35782100 |
| Ni | -0.58946800 | -0.09284200 | 0.92254100 |
| C | 2.15953500 | -1.17173600 | -1.94315100 |
| C | 3.58724900 | -0.81703300 | -2.40013900 |
| C | 1.80884200 | -2.60470900 | -2.36169800 |
| H | 2.13119700 | -1.14579500 | -0.84484400 |
| H | 3.90005000 | 0.17921800 | -2.05568200 |
| H | 4.30818600 | -1.55108500 | -2.00510900 |
| H | 3.65684300 | -0.82988000 | -3.50046000 |
| H | 0.76651000 | -2.84508900 | -2.12400900 |
| H | 1.97623500 | -2.76825100 | -3.43904400 |
| H | 2.44219900 | -3.31864000 | -1.81467000 |

| | | | |
|---|---|---|---|
| C | -0.26313900 | 3.30361000 | -1.35085400 |
| C | -1.72666800 | 3.76733100 | -1.38140500 |
| C | 0.67906400 | 4.42633300 | -1.82305800 |
| H | -0.01515000 | 3.08467900 | -0.30162700 |
| H | -2.41610800 | 2.94963800 | -1.12825600 |
| H | -1.87655700 | 4.58435300 | -0.65803200 |
| H | -2.01271300 | 4.15477800 | -2.37222800 |
| H | 1.73610100 | 4.13164200 | -1.73854600 |
| H | 0.48302800 | 4.67886100 | -2.87806500 |
| H | 0.53071900 | 5.33722200 | -1.22041300 |
| C | 2.46031000 | -1.56173300 | 2.54809700 |
| C | 2.16516400 | -2.98227800 | 3.04434800 |
| C | 3.95241800 | -1.42329200 | 2.19177600 |
| H | 1.87933900 | -1.42855000 | 1.62349700 |
| H | 1.11530400 | -3.09304800 | 3.34779300 |
| H | 2.33865500 | -3.69770900 | 2.22727700 |
| H | 2.81511400 | -3.26558000 | 3.88852500 |
| H | 4.19112900 | -0.44115600 | 1.75993600 |
| H | 4.57847200 | -1.56177600 | 3.08879600 |
| H | 4.23798600 | -2.19109000 | 1.45487500 |
| C | 1.01772300 | 3.28417300 | 3.41423000 |
| C | 2.23004000 | 4.21166800 | 3.62012600 |
| C | -0.23735300 | 3.90776800 | 4.04441400 |
| H | 0.83097500 | 3.20455500 | 2.33165800 |
| H | 3.13401200 | 3.82331100 | 3.12938300 |
| H | 2.02596000 | 5.21432100 | 3.21090700 |
| H | 2.45372200 | 4.32057200 | 4.69403000 |
| H | -1.10868200 | 3.24168600 | 3.96295900 |
| H | -0.08746000 | 4.14230400 | 5.11011400 |
| H | -0.48260100 | 4.85299200 | 3.53490600 |
| S | -0.45353000 | -3.20429900 | 0.63570700 |
| O | 0.54431800 | -4.21318200 | 0.27279300 |
| O | -0.99005200 | -3.20826100 | 2.00607800 |
| O | -0.08737300 | -1.81846900 | 0.12776500 |
| C | -1.94984100 | -3.58257600 | -0.42974100 |
| F | -2.34437400 | -4.83912900 | -0.24761400 |
| F | -2.95862000 | -2.76350000 | -0.09888000 |
| F | -1.67288300 | -3.39950000 | -1.72360600 |

**TS-C'-D'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.802737 (Hartree/Particle)
Thermal correction to Energy= 0.852474
Thermal correction to Enthalpy= 0.853419
Thermal correction to Gibbs Free Energy= 0.718063
Sum of electronic and zero-point Energies= -4016.328355
Sum of electronic and thermal Energies= -4016.278617
Sum of electronic and thermal Enthalpies= -4016.277673
Sum of electronic and thermal Free Energies= -4016.413028

| | | | |
|---|---|---|---|
| C | 0.96775600 | 0.77989300 | 0.72759600 |
| C | 2.70509200 | 1.86908000 | -0.23186900 |
| C | 2.94734100 | 1.80988700 | 1.10478900 |
| N | 1.86857900 | 1.13914800 | 1.67648500 |
| N | 1.48995200 | 1.22566200 | -0.44455600 |
| H | 3.78577500 | 2.16454700 | 1.69491800 |
| H | 3.28123300 | 2.30086400 | -1.04359200 |
| C | 1.70475600 | 0.83663000 | 3.07500500 |
| C | 1.24891200 | 1.85848100 | 3.93281900 |
| C | 1.96578900 | -0.48165900 | 3.51388700 |
| C | 1.09582000 | 1.54022600 | 5.29052000 |
| C | 1.78676300 | -0.74440200 | 4.87914400 |
| C | 1.36562800 | 0.25500800 | 5.75820700 |
| H | 0.75184500 | 2.30468600 | 5.98938700 |
| H | 1.97024600 | -1.74775700 | 5.26360600 |
| H | 1.23500900 | 0.02409000 | 6.81847200 |
| C | 0.83655500 | 1.02769100 | -1.71421600 |
| C | -0.08505500 | 2.00172500 | -2.15049700 |
| C | 1.11110900 | -0.15427300 | -2.43567200 |
| C | -0.73824800 | 1.77062200 | -3.36916500 |
| C | 0.42694500 | -0.33516400 | -3.64609200 |
| C | -0.48511100 | 0.61507600 | -4.10744900 |
| H | -1.46417700 | 2.49560500 | -3.73984100 |
| H | 0.60076800 | -1.23726800 | -4.23380600 |
| H | -1.01084800 | 0.44826300 | -5.05118800 |
| C | -4.02885300 | 0.61892500 | -2.16334400 |
| C | -5.12591500 | 1.47042600 | -2.00483200 |
| C | -5.47316600 | 1.91392200 | -0.72379900 |
| C | -4.72881900 | 1.51066100 | 0.38905900 |
| C | -3.62512000 | 0.65697500 | 0.23947000 |
| C | -3.28618900 | 0.21744500 | -1.04983700 |
| H | -3.73853000 | 0.26986800 | -3.15706700 |
| H | -5.70731100 | 1.78889400 | -2.87377700 |
| H | -6.32788300 | 2.58207400 | -0.58915200 |
| H | -5.00579800 | 1.87580900 | 1.38052000 |
| H | -2.42431500 | -0.44006500 | -1.18737400 |
| C | -1.62387500 | 1.28265400 | 1.63261300 |
| H | -1.38226700 | 1.50538000 | 2.68015100 |
| H | -1.70632100 | 2.20368300 | 1.04390100 |
| C | -2.74845600 | 0.28863900 | 1.42665100 |
| H | -2.28381900 | -0.72504500 | 1.10938700 |
| C | -3.50215500 | -0.11419300 | 2.71454000 |
| H | -3.98388400 | 0.78611900 | 3.13039700 |
| H | -4.31269000 | -0.80976200 | 2.43976700 |
| C | -2.60006100 | -0.76411600 | 3.76439200 |
| H | -1.80126100 | -0.08373000 | 4.10067000 |
| H | -3.18315400 | -1.05344000 | 4.65256700 |
| H | -2.11893000 | -1.66666900 | 3.35766900 |
| Ni | -0.62727800 | -0.13424200 | 0.92184800 |
| C | 2.12496600 | -1.17858800 | -1.93815900 |
| C | 3.54903800 | -0.80728800 | -2.39327700 |
| C | 1.79200100 | -2.61564200 | -2.35704800 |
| H | 2.09496400 | -1.15313800 | -0.83986400 |
| H | 3.84952900 | 0.19264700 | -2.04866200 |
| H | 4.27793500 | -1.53273700 | -1.99699000 |
| H | 3.62015800 | -0.81974200 | -3.49349900 |
| H | 0.75282900 | -2.86932300 | -2.11950200 |
| H | 1.96172500 | -2.77691500 | -3.43436600 |
| H | 2.43457600 | -3.32162600 | -1.81031500 |
| C | -0.33813900 | 3.27513700 | -1.35181200 |
| C | -1.80568200 | 3.72616200 | -1.37954400 |
| C | 0.59275300 | 4.40507200 | -1.82934800 |
| H | -0.08546300 | 3.06116200 | -0.30261900 |
| H | -2.48755700 | 2.90363500 | -1.12169300 |
| H | -1.96025100 | 4.54428000 | -0.65841500 |
| H | -2.09784600 | 4.10795000 | -2.37077300 |
| H | 1.65264700 | 4.12008600 | -1.74735400 |
| H | 0.39138800 | 4.65325100 | -2.88437300 |
| H | 0.43804700 | 5.31606600 | -1.22847200 |
| C | 2.42310600 | -1.57028100 | 2.54481700 |
| C | 2.13423600 | -2.99397700 | 3.03552700 |
| C | 3.91521500 | -1.42105400 | 2.19315100 |
| H | 1.84390900 | -1.43821900 | 1.61903300 |
| H | 1.08395300 | -3.11136300 | 3.33530800 |
| H | 2.31398100 | -3.70594600 | 2.21679300 |
| H | 2.78273000 | -3.27674200 | 3.88099600 |
| H | 4.14849800 | -0.43541800 | 1.76611200 |
| H | 4.53981700 | -1.55908400 | 3.09125100 |
| H | 4.20772700 | -2.18389900 | 1.45383100 |
| C | 0.94333200 | 3.26275100 | 3.42003500 |
| C | 2.14622400 | 4.20049000 | 3.63443800 |
| C | -0.32045400 | 3.87273700 | 4.04621700 |
| H | 0.76222200 | 3.18502900 | 2.33638500 |
| H | 3.05606700 | 3.82142000 | 3.14720600 |
| H | 1.93524700 | 5.20240100 | 3.22690600 |
| H | 2.36360800 | 4.30847200 | 4.70973200 |
| H | -1.18556100 | 3.19956600 | 3.95694300 |
| H | -0.17835700 | 4.10378000 | 5.11373800 |
| H | -0.57103900 | 4.81804600 | 3.53947800 |
| S | -0.48242000 | -3.25341700 | 0.63161800 |
| O | 0.52109700 | -4.25913800 | 0.27540300 |

| | | | |
|---|---|---|---|
| O | -1.02978200 | -3.26020900 | 1.99786000 |
| O | -0.11720300 | -1.86591400 | 0.12787100 |
| C | -1.96857100 | -3.63504300 | -0.44649000 |
| F | -2.36612400 | -4.89043100 | -0.26230400 |
| F | -2.97998600 | -2.81358600 | -0.12969100 |
| F | -1.67875700 | -3.45845000 | -1.73835200 |

**D'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.800802 (Hartree/Particle)
Thermal correction to Energy= 0.852141
Thermal correction to Enthalpy= 0.853085
Thermal correction to Gibbs Free Energy= 0.712639
Sum of electronic and zero-point Energies= -4016.289525
Sum of electronic and thermal Energies= -4016.238187
Sum of electronic and thermal Enthalpies= -4016.237243
Sum of electronic and thermal Free Energies= -4016.377689

| | | | |
|---|---|---|---|
| Ni | 1.15960200 | 0.96125700 | -0.49178100 |
| N | 1.71331000 | 2.29280300 | 1.87385100 |
| N | -0.37975300 | 1.78208600 | 1.89917700 |
| C | 3.99913400 | 1.41671800 | 1.77299100 |
| C | 5.29274700 | 1.51615100 | 1.24524700 |
| C | 5.63219300 | 2.54713900 | 0.36815600 |
| C | 4.68615400 | 3.49941500 | -0.00324300 |
| C | 3.37760700 | 3.45148000 | 0.49680200 |
| C | 3.06441600 | 2.40186800 | 1.38560900 |
| C | 1.21025700 | 2.77611200 | 3.07324100 |
| C | -0.11075300 | 2.44723100 | 3.09191400 |
| C | 0.74432900 | 1.67761800 | 1.14285900 |
| C | -1.67263300 | 1.26942600 | 1.52726100 |
| C | -1.93831400 | -0.09731900 | 1.73346500 |
| C | -3.20164700 | -0.57178400 | 1.35031300 |
| C | -4.15043600 | 0.28594600 | 0.79761200 |
| C | -3.85781800 | 1.63780000 | 0.60548700 |
| C | -2.61078300 | 2.16373300 | 0.96709200 |
| H | 6.04194600 | 0.76705000 | 1.50732500 |
| H | 6.64215600 | 2.59589000 | -0.04560200 |
| H | 4.96133500 | 4.28343700 | -0.71132300 |
| H | 1.83333400 | 3.29982800 | 3.79211800 |
| H | -0.88318200 | 2.62295700 | 3.83453000 |
| H | -3.44219400 | -1.62885500 | 1.48001200 |
| H | -5.12926900 | -0.10287300 | 0.50698800 |
| H | -4.61119900 | 2.28776600 | 0.15961800 |
| C | -1.16993500 | -1.33176700 | -2.28135900 |
| H | -1.26266500 | -2.34554200 | -1.88285300 |
| H | -0.15667900 | -0.94890900 | -2.40080200 |
| C | -3.63887300 | -1.26136000 | -2.40856400 |
| H | -4.31050700 | -0.57358800 | -1.87025200 |
| H | -3.53159800 | -2.14022800 | -1.75351200 |
| C | -2.20561800 | 0.76311000 | -3.14143900 |
| C | -3.36586000 | 1.55071500 | -3.29516000 |
| C | -0.98020900 | 1.34008700 | -3.53827100 |
| C | -3.30727300 | 2.84057400 | -3.83310000 |
| H | -4.33786200 | 1.16086000 | -2.99145200 |
| C | -0.91686700 | 2.62905600 | -4.06507600 |
| H | -0.05110900 | 0.78544100 | -3.44048200 |
| C | -2.08251800 | 3.38733300 | -4.22449200 |
| H | -4.22793200 | 3.42044200 | -3.94117100 |
| H | 0.06026600 | 3.02528300 | -4.34795100 |
| H | -2.03506300 | 4.39591000 | -4.64330600 |
| C | -4.29003500 | -1.69245100 | -3.73165900 |
| H | -4.41970100 | -0.84044800 | -4.41685300 |
| H | -3.66368600 | -2.43846200 | -4.24632000 |
| H | -5.28182500 | -2.14046400 | -3.55712500 |
| C | -2.27385500 | -0.62184800 | -2.58812900 |
| H | -0.22570700 | 0.86524000 | -0.71023600 |
| C | 2.34352000 | 4.47271100 | 0.03841300 |
| C | 2.02220600 | 4.28674700 | -1.45319400 |
| C | 2.78393900 | 5.91180400 | 0.34925500 |
| H | 1.41174100 | 4.29152500 | 0.59450800 |
| H | 1.64044800 | 3.27689300 | -1.65735900 |
| H | 1.25394600 | 5.00553300 | -1.77798700 |
| H | 2.91442700 | 4.42487000 | -2.08304800 |
| H | 2.99721300 | 6.04359200 | 1.42198400 |
| H | 3.69066000 | 6.18873100 | -0.21213900 |
| H | 1.99020700 | 6.62204000 | 0.06730800 |
| C | 3.59616500 | 0.23790800 | 2.65163800 |
| C | 4.65398700 | -0.12185200 | 3.70414400 |
| C | 3.24781000 | -0.97579600 | 1.77033200 |
| H | 2.68178500 | 0.51797400 | 3.19655700 |
| H | 4.92619400 | 0.75209400 | 4.31660000 |
| H | 4.26789100 | -0.90507700 | 4.37564700 |
| H | 5.57492200 | -0.51359200 | 3.24391000 |
| H | 2.44764800 | -0.72864800 | 1.05654500 |
| H | 4.12513300 | -1.30332900 | 1.18983500 |
| H | 2.90110000 | -1.82189700 | 2.38496500 |
| C | -0.89481400 | -1.05087600 | 2.30278300 |
| C | -0.32551500 | -1.94568400 | 1.18912800 |
| C | -1.43504100 | -1.88049100 | 3.47733500 |
| H | -0.05978000 | -0.44898100 | 2.69155500 |
| H | 0.09942200 | -1.32898300 | 0.38448600 |
| H | 0.46683900 | -2.60147200 | 1.58286500 |
| H | -1.11218700 | -2.57835300 | 0.74807900 |
| H | -1.84342800 | -1.23522500 | 4.27126700 |
| H | -2.23265000 | -2.57075700 | 3.15883500 |
| H | -0.62811000 | -2.49136500 | 3.91292800 |
| C | -2.25200000 | 3.62450200 | 0.71250400 |
| C | -3.45919700 | 4.56982400 | 0.75547200 |
| C | -1.50021900 | 3.76596900 | -0.62321900 |
| H | -1.56677500 | 3.94231100 | 1.51449100 |
| H | -4.04467100 | 4.44661500 | 1.68032100 |
| H | -3.11679800 | 5.61511500 | 0.70165700 |
| H | -4.13300700 | 4.40716200 | -0.10078100 |
| H | -0.62066200 | 3.11220700 | -0.66997900 |
| H | -2.15159400 | 3.48932800 | -1.46403700 |
| H | -1.16673600 | 4.80553000 | -0.77233300 |
| S | 2.86937100 | 0.88569400 | -3.02969400 |
| O | 1.89583900 | 0.19280000 | -2.06539600 |
| O | 2.24053200 | 1.93412000 | -3.84231500 |
| O | 4.17056700 | 1.17075900 | -2.41846300 |
| C | 3.14270200 | -0.54197000 | -4.20482200 |
| F | 3.96747600 | -0.16124500 | -5.17887100 |
| F | 1.98306000 | -0.92087200 | -4.74372700 |
| F | 3.68017800 | -1.57892100 | -3.56415200 |

**E'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.762557 (Hartree/Particle)
Thermal correction to Energy= 0.804108
Thermal correction to Enthalpy= 0.805052
Thermal correction to Gibbs Free Energy= 0.687811
Sum of electronic and zero-point Energies= -3054.806579
Sum of electronic and thermal Energies= -3054.765029
Sum of electronic and thermal Enthalpies= -3054.764084
Sum of electronic and thermal Free Energies= -3054.881325

| | | | |
|---|---|---|---|
| Ni | 0.08588200 | -0.08649700 | -0.86078700 |
| C | -0.77147800 | -0.39261500 | -2.59467700 |
| C | 0.37355700 | 0.42738500 | -2.73270800 |
| H | 1.28057200 | 0.01104200 | -3.19026000 |
| H | 0.29429900 | 1.51750500 | -2.82644000 |
| C | -0.70539600 | -1.85252400 | -3.03018100 |
| H | -1.28805100 | -2.48703000 | -2.34292400 |
| H | 0.33619600 | -2.20108400 | -2.94493000 |
| C | -2.12559200 | 0.19362200 | -2.38731900 |
| C | -3.11143000 | -0.51584400 | -1.66410800 |
| C | -2.47562300 | 1.47474900 | -2.86597300 |
| C | -4.37177900 | 0.03185700 | -1.42177600 |
| H | -2.87269800 | -1.49897700 | -1.25330900 |
| C | -3.73728900 | 2.02188100 | -2.62721200 |
| H | -1.74550200 | 2.04326600 | -3.44588900 |

| | | | |
|---|---|---|---|
| C | -4.69678900 | 1.30517600 | -1.90229000 |
| H | -5.10070400 | -0.53829200 | -0.84045800 |
| H | -3.97662200 | 3.01564700 | -3.01647000 |
| H | -5.68465100 | 1.73376700 | -1.71461300 |
| C | -1.21022900 | -2.06607500 | -4.46370300 |
| H | -2.26098100 | -1.74832000 | -4.56269200 |
| H | -0.61534500 | -1.47416500 | -5.17843500 |
| H | -1.14699500 | -3.12619100 | -4.76078700 |
| C | 0.71052700 | 0.00277100 | 0.93309400 |
| N | -0.00364500 | -0.26329500 | 2.07131300 |
| N | 1.95990500 | 0.29786700 | 1.40620100 |
| C | -1.39817600 | -0.60956300 | 2.06446100 |
| C | 0.77803200 | -0.13640600 | 3.21575300 |
| C | 2.02037600 | 0.22081600 | 2.79499100 |
| C | 3.06697900 | 0.65192700 | 0.56204000 |
| C | -2.35227200 | 0.42754100 | 2.09785200 |
| C | -1.75644700 | -1.97292000 | 2.00829500 |
| H | 0.37879600 | -0.31005100 | 4.21076900 |
| H | 2.93360600 | 0.42719500 | 3.34539800 |
| C | 3.89251700 | -0.37482200 | 0.06047700 |
| C | 3.27557100 | 2.01314800 | 0.25912100 |
| C | -3.70578700 | 0.06350000 | 2.07156500 |
| C | -1.94277400 | 1.89468700 | 2.07380900 |
| C | -3.12334400 | -2.28387000 | 1.98539500 |
| C | -0.70043300 | -3.06531100 | 1.88872400 |
| C | 4.96189200 | -0.00124500 | -0.76639400 |
| C | 3.58994500 | -1.84454200 | 0.32613200 |
| C | 4.35879100 | 2.33457600 | -0.57117000 |
| C | 2.30929300 | 3.09112600 | 0.73494700 |
| C | -4.08805000 | -1.27612100 | 2.01975900 |
| H | -4.47188500 | 0.84095500 | 2.07297300 |
| C | -2.71911600 | 2.75008700 | 3.08530300 |
| C | -2.07659400 | 2.44390700 | 0.64317200 |
| H | -0.87847200 | 1.95269000 | 2.34800200 |
| H | -3.43998700 | -3.32714600 | 1.93171200 |
| C | -0.48045800 | -3.41002100 | 0.40550400 |
| C | -1.02260300 | -4.31771100 | 2.71510900 |
| H | 0.24796500 | -2.65771600 | 2.27075300 |
| C | 5.19553400 | 1.33886200 | -1.07634900 |
| H | 5.61600300 | -0.77006500 | -1.18237500 |
| C | 4.83895300 | -2.66537800 | 0.67595500 |
| C | 2.83667500 | -2.44027500 | -0.87686600 |
| H | 2.91175900 | -1.89642000 | 1.19145300 |
| H | 4.54479400 | 3.37727700 | -0.83604700 |
| C | 1.30188900 | 3.40923100 | -0.38433400 |
| C | 3.01425800 | 4.35725900 | 1.24095300 |
| H | 1.73531600 | 2.67936500 | 1.57879900 |
| H | -5.14891400 | -1.53843600 | 1.99526000 |
| H | -2.64176800 | 2.34149700 | 4.10564600 |
| H | -2.32013700 | 3.77705600 | 3.09609100 |
| H | -3.78836800 | 2.82020300 | 2.82866100 |
| H | -1.44954600 | 1.86266500 | -0.04924900 |
| H | -3.11552400 | 2.37457100 | 0.28631700 |
| H | -1.75999200 | 3.49817500 | 0.59826100 |
| H | -0.19189200 | -2.51060900 | -0.16021700 |
| H | 0.31836700 | -4.15950000 | 0.28806000 |
| H | -1.40314700 | -3.81330400 | -0.04318500 |
| H | -1.21721000 | -4.06723700 | 3.77000300 |
| H | -1.90392500 | -4.85165100 | 2.32529000 |
| H | -0.17583700 | -5.02152800 | 2.67961800 |
| H | 6.03353000 | 1.60933600 | -1.72402800 |
| H | 5.39058000 | -2.22175100 | 1.52009000 |
| H | 4.55109000 | -3.69153200 | 0.95520900 |
| H | 5.53124000 | -2.74334700 | -0.17758600 |
| H | 1.90927500 | -1.87376100 | -1.05807300 |
| H | 3.45463600 | -2.39263400 | -1.78867900 |
| H | 2.57191700 | -3.49366500 | -0.69233600 |
| H | 0.76261800 | 2.49744100 | -0.68096600 |
| H | 0.56603200 | 4.15673700 | -0.04773600 |
| H | 1.81931800 | 3.80784800 | -1.27264800 |
| H | 3.75683700 | 4.12235500 | 2.02010300 |
| H | 3.53241200 | 4.89277600 | 0.42928200 |
| H | 2.27635400 | 5.05429100 | 1.66918900 |

**(*E*)-TS-E'-F'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.757699 (Hartree/Particle)

Thermal correction to Energy= 0.798845

Thermal correction to Enthalpy= 0.799789

Thermal correction to Gibbs Free Energy= 0.684585

Sum of electronic and zero-point Energies= -3054.785904

Sum of electronic and thermal Energies= -3054.744758

Sum of electronic and thermal Enthalpies= -3054.743814

Sum of electronic and thermal Free Energies= -3054.859018

| | | | |
|---|---|---|---|
| Ni | 0.26454900 | -0.26301800 | -1.08770900 |
| C | -0.61447000 | 0.29439100 | -2.75481400 |
| C | 0.35257000 | 1.29118900 | -2.48583300 |
| H | 1.37431200 | 1.21502700 | -2.87282500 |
| H | 0.01649600 | 2.31140400 | -2.28857000 |
| C | -0.21318600 | -1.10769400 | -2.86430500 |
| H | 0.02326500 | -1.72507200 | -1.43786300 |
| C | -2.06280300 | 0.62141100 | -2.58508700 |
| C | -2.93039300 | -0.21931300 | -1.85993100 |
| C | -2.58867600 | 1.81454800 | -3.11396400 |
| C | -4.26925400 | 0.12562000 | -1.66614900 |
| H | -2.54129500 | -1.12844300 | -1.39632600 |
| C | -3.92925900 | 2.15939300 | -2.92255100 |
| H | -1.93352600 | 2.47590800 | -3.68566800 |
| C | -4.77761900 | 1.31637900 | -2.19622600 |
| H | -4.91156900 | -0.53335400 | -1.07715600 |
| H | -4.31427000 | 3.09142100 | -3.34549500 |
| H | -5.82566700 | 1.58664500 | -2.04285600 |
| C | 0.90423100 | -0.10674500 | 0.64887700 |
| N | 0.17455100 | -0.33893600 | 1.78639400 |
| N | 2.15013700 | 0.20173800 | 1.12543300 |
| C | -1.20318900 | -0.73911000 | 1.75095900 |
| C | 0.94851400 | -0.19362600 | 2.93488000 |
| C | 2.19594200 | 0.14765300 | 2.51901700 |
| C | 3.26372600 | 0.51296400 | 0.27460300 |
| C | -2.20217100 | 0.24791800 | 1.87305300 |
| C | -1.49862200 | -2.10532400 | 1.55654600 |
| H | 0.53883100 | -0.33545200 | 3.93048800 |
| H | 3.10552400 | 0.35361700 | 3.07525700 |
| C | 4.18969000 | -0.50872200 | -0.02068400 |
| C | 3.37001700 | 1.81865000 | -0.25432900 |
| C | -3.53823100 | -0.17400000 | 1.82128800 |
| C | -1.84318400 | 1.72636000 | 1.97005400 |
| C | -2.84988200 | -2.47518300 | 1.51071300 |
| C | -0.38671800 | -3.13973600 | 1.43167600 |
| C | 5.27581100 | -0.18148100 | -0.84651600 |
| C | 3.96426300 | -1.93883700 | 0.45909300 |
| C | 4.47255300 | 2.09232000 | -1.07574200 |
| C | 2.31437600 | 2.87520400 | 0.05679400 |
| C | -3.85882900 | -1.52007000 | 1.64665200 |
| H | -4.34052400 | 0.56126900 | 1.89982900 |
| C | -2.77291100 | 2.52050200 | 2.89722800 |
| C | -1.79491000 | 2.34556200 | 0.56092000 |
| H | -0.82794100 | 1.79522900 | 2.39088000 |
| H | -3.11943300 | -3.52289100 | 1.36570900 |
| C | -0.68630500 | -4.22647500 | 0.39176300 |
| C | -0.06003300 | -3.75238900 | 2.80504000 |
| H | 0.50723000 | -2.61038900 | 1.07516100 |
| C | 5.41880300 | 1.10620100 | -1.36223200 |
| H | 6.01359300 | -0.94468900 | -1.10036700 |
| C | 5.25970100 | -2.68303100 | 0.80785100 |
| C | 3.13751600 | -2.71164900 | -0.58652900 |
| H | 3.36049500 | -1.89365700 | 1.37807000 |
| H | 4.59580500 | 3.08748800 | -1.50490500 |
| C | 2.21665100 | 3.97712900 | -1.00532000 |
| C | 2.53150200 | 3.49760000 | 1.44833300 |

| | | | |
|---|---|---|---|
| H | 1.34802100 | 2.34841700 | 0.05768100 |
| H | -4.90710400 | -1.82759000 | 1.60562300 |
| H | -2.84948800 | 2.05555000 | 3.89311700 |
| H | -2.39045900 | 3.54565200 | 3.02534000 |
| H | -3.79035800 | 2.60552900 | 2.48269300 |
| H | -1.08951100 | 1.79891000 | -0.07970400 |
| H | -2.78301400 | 2.29863900 | 0.07560200 |
| H | -1.47778500 | 3.40052000 | 0.61016100 |
| H | -0.93515900 | -3.77630400 | -0.58164400 |
| H | 0.20002900 | -4.86624100 | 0.25334300 |
| H | -1.51807500 | -4.88219200 | 0.69659000 |
| H | 0.22276100 | -2.97627300 | 3.53307900 |
| H | -0.93030300 | -4.29508800 | 3.21036100 |
| H | 0.77845000 | -4.46367100 | 2.72418600 |
| H | 6.27122900 | 1.34262700 | -2.00453000 |
| H | 5.87473400 | -2.11481800 | 1.52374200 |
| H | 5.02262600 | -3.65973500 | 1.25884000 |
| H | 5.87393600 | -2.88069100 | -0.08532400 |
| H | 2.19287000 | -2.19140500 | -0.80357000 |
| H | 3.69931200 | -2.80769800 | -1.53056500 |
| H | 2.89882500 | -3.72502700 | -0.22327000 |
| H | 2.12287100 | 3.55894200 | -2.01801900 |
| H | 1.32899300 | 4.59997100 | -0.81214000 |
| H | 3.09311200 | 4.64593900 | -0.99023600 |
| H | 2.53206600 | 2.73940900 | 2.24395900 |
| H | 3.49443600 | 4.03367200 | 1.48847100 |
| H | 1.73016400 | 4.22002400 | 1.67465300 |
| H | -1.05725900 | -1.77345300 | -3.07668700 |
| C | 1.03580700 | -1.51109200 | -3.63395400 |
| H | 1.27358500 | -2.57115100 | -3.45777300 |
| H | 0.88376900 | -1.36648700 | -4.71749400 |
| H | 1.91852700 | -0.92733000 | -3.33573500 |

**(*E*)-F'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.759289 (Hartree/Particle)
Thermal correction to Energy= 0.800619
Thermal correction to Enthalpy= 0.801563
Thermal correction to Gibbs Free Energy= 0.686660
Sum of electronic and zero-point Energies= -3054.797212
Sum of electronic and thermal Energies= -3054.755883
Sum of electronic and thermal Enthalpies= -3054.754939
Sum of electronic and thermal Free Energies= -3054.869842

| | | | |
|---|---|---|---|
| Ni | 0.58095300 | 0.15819000 | -0.77079300 |
| N | 0.48162300 | 0.45376800 | 2.14930900 |
| N | -1.45642900 | 0.05728200 | 1.30078200 |
| C | 2.75073400 | -0.30267200 | 2.65825400 |
| C | 4.11188300 | 0.00343000 | 2.80542200 |
| C | 4.58706300 | 1.28786300 | 2.54272500 |
| C | 3.71756200 | 2.28509300 | 2.09669100 |
| C | 2.34861200 | 2.03226100 | 1.93456800 |
| C | 1.88634300 | 0.73648500 | 2.25899600 |
| C | -0.41852400 | 0.41752000 | 3.21383800 |
| C | -1.64268500 | 0.17033800 | 2.67740900 |
| C | -0.14195600 | 0.21942500 | 0.95596300 |
| C | -2.49266400 | -0.18674800 | 0.33511000 |
| C | -2.95733800 | -1.50707700 | 0.16709600 |
| C | -4.00116000 | -1.71726900 | -0.74489800 |
| C | -4.53553300 | -0.65814300 | -1.47705200 |
| C | -4.01757300 | 0.63025100 | -1.33541800 |
| C | -2.98000600 | 0.89639200 | -0.43112500 |
| H | 4.81199500 | -0.77457400 | 3.11413200 |
| H | 5.65040200 | 1.50995500 | 2.66471500 |
| H | 4.11793700 | 3.27153400 | 1.86005800 |
| H | -0.10597600 | 0.57369400 | 4.24213400 |
| H | -2.61973600 | 0.06702100 | 3.14020400 |
| H | -4.38539400 | -2.72582500 | -0.90385000 |
| H | -5.34773300 | -0.84162600 | -2.18524200 |
| H | -4.42509300 | 1.43774200 | -1.94440900 |
| C | 1.10227000 | 0.14076600 | -2.65126300 |
| C | 2.23151700 | -0.05926000 | -1.81540900 |
| C | 0.81275000 | 1.48033800 | -3.30341000 |
| H | -0.26828100 | 1.65623600 | -3.40316600 |
| H | 1.21756800 | 2.31576400 | -2.71580700 |
| H | 1.24449800 | 1.53945400 | -4.32078800 |
| C | 0.30467100 | -1.03100200 | -3.11261600 |
| C | -1.09868400 | -0.93182900 | -3.26434400 |
| C | 0.88966300 | -2.29039700 | -3.37130700 |
| C | -1.87158800 | -2.03081200 | -3.63854900 |
| H | -1.59877500 | 0.01341300 | -3.04539700 |
| C | 0.11631500 | -3.39128600 | -3.74498300 |
| H | 1.97308700 | -2.40027800 | -3.28722800 |
| C | -1.27147300 | -3.27141900 | -3.88251700 |
| H | -2.95507800 | -1.91723100 | -3.72148400 |
| H | 0.60409900 | -4.35055200 | -3.94115000 |
| H | -1.87662100 | -4.13310000 | -4.17598800 |
| C | 3.35788300 | 0.92367100 | -1.60339900 |
| H | 3.76575700 | 0.83240500 | -0.58359300 |
| H | 4.19108700 | 0.74230100 | -2.30998800 |
| H | 3.04167400 | 1.96808300 | -1.73434100 |
| H | 2.54130400 | -1.09854300 | -1.63385400 |
| C | -2.37776200 | 2.29230700 | -0.29166300 |
| C | -2.92742600 | 3.02602500 | 0.94396100 |
| C | -2.53674700 | 3.15785300 | -1.54713900 |
| H | -1.29490200 | 2.14420900 | -0.15217600 |
| H | -2.74376000 | 2.46336000 | 1.87014600 |
| H | -2.44924800 | 4.01284200 | 1.05116900 |
| H | -4.01482300 | 3.18217100 | 0.84843800 |
| H | -2.18111800 | 2.63386900 | -2.44750900 |
| H | -3.58379900 | 3.45711000 | -1.71690300 |
| H | -1.94675100 | 4.08150300 | -1.43851000 |
| C | -2.25651700 | -2.67553500 | 0.85028200 |
| C | -1.08469300 | -3.14328200 | -0.03576700 |
| C | -3.19010800 | -3.84124000 | 1.19907500 |
| H | -1.82746000 | -2.30822000 | 1.79516100 |
| H | -0.40003700 | -2.31090900 | -0.25780700 |
| H | -0.51265700 | -3.94115300 | 0.46508800 |
| H | -1.45305500 | -3.52681000 | -0.99984500 |
| H | -4.05976200 | -3.50552000 | 1.78637300 |
| H | -3.56510900 | -4.35041300 | 0.29662800 |
| H | -2.64618100 | -4.59432800 | 1.79086000 |
| C | 2.24034300 | -1.73313800 | 2.79043000 |
| C | 2.96579900 | -2.55734700 | 3.86099900 |
| C | 2.30814300 | -2.41904100 | 1.41132900 |
| H | 1.17907400 | -1.68867300 | 3.07877100 |
| H | 2.96194700 | -2.04836500 | 4.83807500 |
| H | 2.47260000 | -3.53487100 | 3.98161600 |
| H | 4.01414200 | -2.75717900 | 3.58655100 |
| H | 1.75846000 | -1.83736100 | 0.65554800 |
| H | 3.35523300 | -2.50663500 | 1.07676000 |
| H | 1.87335700 | -3.43059700 | 1.45556900 |
| C | 1.39557200 | 3.08795500 | 1.38061100 |
| C | 2.09157600 | 4.16561500 | 0.54141400 |
| C | 0.54491600 | 3.73642700 | 2.48651700 |
| H | 0.72501600 | 2.54455200 | 0.69462900 |
| H | 2.73041200 | 3.72188900 | -0.23682900 |
| H | 1.33550600 | 4.79275100 | 0.04299500 |
| H | 2.71525200 | 4.83493100 | 1.15655000 |
| H | -0.03695000 | 2.99368000 | 3.04974600 |
| H | 1.18678300 | 4.28021400 | 3.19955100 |
| H | -0.16647500 | 4.45678000 | 2.05173400 |

**(*E*)-G'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.759225 (Hartree/Particle)
Thermal correction to Energy= 0.800557
Thermal correction to Enthalpy= 0.801501
Thermal correction to Gibbs Free Energy= 0.686706
Sum of electronic and zero-point Energies= -3054.796568
Sum of electronic and thermal Energies= -3054.755235

Sum of electronic and thermal Enthalpies= -3054.754291
Sum of electronic and thermal Free Energies= -3054.869086

| | | | |
|---|---|---|---|
| Ni | 0.49214900 | 0.58416300 | -0.95602900 |
| N | 0.56158500 | 0.60498800 | 2.00792400 |
| N | -1.37569400 | 0.11786900 | 1.20883300 |
| C | 2.79634500 | -0.14064900 | 2.67398900 |
| C | 4.16515400 | 0.13894700 | 2.79305500 |
| C | 4.68438900 | 1.36864200 | 2.38714100 |
| C | 3.84461300 | 2.34956700 | 1.86125700 |
| C | 2.46609400 | 2.12765300 | 1.73038200 |
| C | 1.96904000 | 0.87066400 | 2.13613000 |
| C | -0.31993000 | 0.56749700 | 3.08894200 |
| C | -1.53964400 | 0.25373600 | 2.58413300 |
| C | -0.07995300 | 0.34078000 | 0.82685900 |
| C | -2.44578600 | -0.13913700 | 0.28493400 |
| C | -2.74249100 | -1.47474300 | -0.05178800 |
| C | -3.76955800 | -1.69657400 | -0.98008400 |
| C | -4.47664400 | -0.63045000 | -1.53461100 |
| C | -4.17700600 | 0.68226100 | -1.16630700 |
| C | -3.15641200 | 0.95844700 | -0.24593900 |
| H | 4.84012300 | -0.61611600 | 3.19737400 |
| H | 5.75584500 | 1.56333900 | 2.48136900 |
| H | 4.26972500 | 3.30482200 | 1.55060000 |
| H | 0.00755500 | 0.76204300 | 4.10577700 |
| H | -2.50115700 | 0.10918300 | 3.06696600 |
| H | -4.01129100 | -2.71670900 | -1.28283900 |
| H | -5.27102800 | -0.82369900 | -2.26034600 |
| H | -4.74787600 | 1.50490700 | -1.60100300 |
| C | 1.24980100 | -0.33408400 | -2.56735500 |
| C | 2.05131400 | -0.76103700 | -1.48140000 |
| C | 1.09099300 | 1.06170000 | -2.81346600 |
| H | -0.32297300 | 1.81638000 | -0.99694600 |
| H | 1.93304700 | 1.74673900 | -2.66928100 |
| H | 0.39245300 | 1.37628200 | -3.59233900 |
| C | 0.32557000 | -1.31377100 | -3.22236000 |
| C | -1.03657300 | -1.02278200 | -3.42132300 |
| C | 0.80695600 | -2.56812000 | -3.63313100 |
| C | -1.88935600 | -1.96010300 | -4.00655300 |
| H | -1.43859000 | -0.07056400 | -3.06869900 |
| C | -0.04490700 | -3.50595800 | -4.22429000 |
| H | 1.86320600 | -2.80706500 | -3.48780600 |
| C | -1.39810500 | -3.20625800 | -4.41229200 |
| H | -2.94879600 | -1.72112600 | -4.12613300 |
| H | 0.35056000 | -4.47576900 | -4.53819400 |
| H | -2.06700800 | -3.94098500 | -4.86810100 |
| C | 3.33219600 | -0.09466300 | -1.03569100 |
| H | 3.52932300 | -0.29032100 | 0.02736800 |
| H | 4.19834000 | -0.47865100 | -1.60833200 |
| H | 3.31681700 | 0.99735900 | -1.16015800 |
| H | 1.98871000 | -1.82433800 | -1.23213200 |
| C | -2.86943700 | 2.38669500 | 0.20136800 |
| C | -3.85426800 | 2.80880800 | 1.30688300 |
| C | -2.87369300 | 3.39315100 | -0.95676700 |
| H | -1.85692300 | 2.40050100 | 0.62742700 |
| H | -3.80896100 | 2.12630900 | 2.16960600 |
| H | -3.62279000 | 3.82513300 | 1.66562700 |
| H | -4.89073800 | 2.80755200 | 0.93063400 |
| H | -2.17814500 | 3.07707800 | -1.74824300 |
| H | -3.87655200 | 3.51687500 | -1.39680800 |
| H | -2.55231500 | 4.38311400 | -0.59483400 |
| C | -1.94270200 | -2.63692900 | 0.52378800 |
| C | -0.83059600 | -3.04255100 | -0.45606200 |
| C | -2.81727200 | -3.83733200 | 0.91133000 |
| H | -1.45277700 | -2.28105200 | 1.44332500 |
| H | -0.18703600 | -2.18253700 | -0.67626800 |
| H | -0.20805800 | -3.84642200 | -0.03142200 |
| H | -1.25217400 | -3.39212600 | -1.41134000 |
| H | -3.63668400 | -3.54275900 | 1.58632400 |
| H | -3.26293600 | -4.32210400 | 0.02784300 |
| H | -2.20662800 | -4.59783600 | 1.42388400 |
| C | 2.23372000 | -1.51272000 | 3.03937700 |
| C | 3.05536500 | -2.25996800 | 4.09658100 |
| C | 2.05508100 | -2.36947700 | 1.77305100 |
| H | 1.23080200 | -1.35972400 | 3.46665500 |
| H | 3.23198500 | -1.64111600 | 4.99045600 |
| H | 2.52012900 | -3.16986300 | 4.41042000 |
| H | 4.03439600 | -2.58043900 | 3.70529800 |
| H | 1.43589000 | -1.85463400 | 1.02771100 |
| H | 3.03205600 | -2.58198800 | 1.30877700 |
| H | 1.57537200 | -3.33078700 | 2.01849000 |
| C | 1.53270200 | 3.21481800 | 1.20876400 |
| C | 2.20099400 | 4.17749200 | 0.22121700 |
| C | 0.88209200 | 3.97779400 | 2.37647900 |
| H | 0.73449800 | 2.71392400 | 0.64461000 |
| H | 2.69703900 | 3.62878400 | -0.59478700 |
| H | 1.44018400 | 4.83423100 | -0.22914500 |
| H | 2.94899000 | 4.82681500 | 0.70503000 |
| H | 0.33385600 | 3.29862400 | 3.04716300 |
| H | 1.64347500 | 4.50534800 | 2.97514500 |
| H | 0.16614900 | 4.72539400 | 1.99727500 |

**(*E*)-TS-G'-P'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.757766 (Hartree/Particle)
Thermal correction to Energy= 0.798820
Thermal correction to Enthalpy= 0.799764
Thermal correction to Gibbs Free Energy= 0.685506
Sum of electronic and zero-point Energies= -3054.786444
Sum of electronic and thermal Energies= -3054.745390
Sum of electronic and thermal Enthalpies= -3054.744445
Sum of electronic and thermal Free Energies= -3054.858703

| | | | |
|---|---|---|---|
| Ni | 0.02506000 | 0.42123500 | -1.22040200 |
| N | 0.05945000 | 0.63143700 | 1.72348700 |
| N | -1.86998100 | 0.11831100 | 0.91646300 |
| C | 2.31729900 | -0.07559300 | 2.34331400 |
| C | 3.68042900 | 0.23350100 | 2.45696500 |
| C | 4.16697900 | 1.48084700 | 2.06502200 |
| C | 3.30272800 | 2.44339800 | 1.54259300 |
| C | 1.92981000 | 2.18904800 | 1.41450500 |
| C | 1.46092900 | 0.92456000 | 1.83387800 |
| C | -0.82709200 | 0.58472000 | 2.80117400 |
| C | -2.04247300 | 0.25856900 | 2.29108500 |
| C | -0.57174600 | 0.35008700 | 0.53829000 |
| C | -2.91733000 | -0.12871100 | -0.03263000 |
| C | -3.24522200 | -1.45987700 | -0.35686100 |
| C | -4.26371300 | -1.66567000 | -1.29851100 |
| C | -4.92185000 | -0.58814700 | -1.89007000 |
| C | -4.56747100 | 0.72203200 | -1.56218500 |
| C | -3.55377200 | 0.98114900 | -0.62960400 |
| H | 4.37599000 | -0.51238500 | 2.84382800 |
| H | 5.23354800 | 1.70153900 | 2.15810100 |
| H | 3.70667900 | 3.40631300 | 1.22748700 |
| H | -0.50774600 | 0.78362100 | 3.81991600 |
| H | -3.00489300 | 0.10974200 | 2.77131800 |
| H | -4.53283100 | -2.68294800 | -1.58788100 |
| H | -5.71192300 | -0.77008500 | -2.62342300 |
| H | -5.08625000 | 1.55390900 | -2.04222800 |
| C | 0.72374600 | -0.27044100 | -2.92991800 |
| C | 1.61776100 | -0.74339100 | -1.93714100 |
| C | 0.44685400 | 1.15979600 | -3.03803600 |
| H | -0.46197800 | 1.70588700 | -1.87385300 |
| H | 1.28999800 | 1.85720800 | -2.96460100 |
| H | -0.23792800 | 1.44696200 | -3.84155800 |
| C | -0.19376600 | -1.23593300 | -3.60643200 |
| C | -1.56909300 | -0.96614700 | -3.75464300 |
| C | 0.29282700 | -2.46589700 | -4.08628000 |
| C | -2.42390500 | -1.89634500 | -4.34837700 |
| H | -1.98477700 | -0.03890100 | -3.35385000 |
| C | -0.56199400 | -3.39735700 | -4.68181400 |
| H | 1.35827900 | -2.68902300 | -3.99364900 |

| | | | |
|---|---|---|---|
| C | -1.92636500 | -3.11789700 | -4.81552500 |
| H | -3.49009800 | -1.67053200 | -4.42619400 |
| H | -0.15882500 | -4.34590600 | -5.04718100 |
| H | -2.59642900 | -3.84654900 | -5.27925400 |
| C | 2.86822900 | -0.03176300 | -1.47312800 |
| H | 3.04877600 | -0.20674800 | -0.40195800 |
| H | 3.76082300 | -0.39153500 | -2.02108300 |
| H | 2.81627700 | 1.05795400 | -1.60988500 |
| H | 1.64491700 | -1.82917400 | -1.79736300 |
| C | -3.16880000 | 2.40721900 | -0.25335200 |
| C | -4.08288400 | 2.94197800 | 0.86303700 |
| C | -3.14189300 | 3.36035400 | -1.45508900 |
| H | -2.14270700 | 2.37292900 | 0.13700700 |
| H | -4.05076900 | 2.29458200 | 1.75277700 |
| H | -3.77091200 | 3.95416300 | 1.16880700 |
| H | -5.12984800 | 2.99525100 | 0.52094600 |
| H | -2.50109000 | 2.96080400 | -2.25598300 |
| H | -4.14713500 | 3.54050500 | -1.86933200 |
| H | -2.73503000 | 4.33786400 | -1.14967600 |
| C | -2.46262500 | -2.63232600 | 0.22114500 |
| C | -1.35857400 | -3.05263400 | -0.76561600 |
| C | -3.35140700 | -3.82083900 | 0.61204400 |
| H | -1.96353200 | -2.28107400 | 1.13733400 |
| H | -0.70375700 | -2.20063800 | -0.99311300 |
| H | -0.74421400 | -3.86301700 | -0.34087200 |
| H | -1.79096500 | -3.40124800 | -1.71700300 |
| H | -4.16119100 | -3.51589400 | 1.29413800 |
| H | -3.81124400 | -4.29627500 | -0.26936300 |
| H | -2.74875500 | -4.59214900 | 1.11784500 |
| C | 1.78881100 | -1.47222300 | 2.65928400 |
| C | 2.60567600 | -2.22277700 | 3.71759900 |
| C | 1.67573600 | -2.29290600 | 1.36012200 |
| H | 0.76962000 | -1.36226900 | 3.06045200 |
| H | 2.73303700 | -1.62606800 | 4.63477800 |
| H | 2.09629200 | -3.16129100 | 3.98742700 |
| H | 3.60721000 | -2.49487200 | 3.34708000 |
| H | 1.08523500 | -1.76211000 | 0.60036900 |
| H | 2.67624900 | -2.48002000 | 0.93609500 |
| H | 1.19933200 | -3.26732700 | 1.55626400 |
| C | 0.97183700 | 3.22845900 | 0.84093500 |
| C | 1.64080600 | 4.21956800 | -0.11720200 |
| C | 0.20949900 | 3.96638300 | 1.95543000 |
| H | 0.23937700 | 2.67250800 | 0.23811300 |
| H | 2.21021100 | 3.69519400 | -0.90081400 |
| H | 0.87198100 | 4.83387200 | -0.61206500 |
| H | 2.32660500 | 4.90953600 | 0.40146000 |
| H | -0.33758400 | 3.26705300 | 2.60494000 |
| H | 0.90194000 | 4.54787200 | 2.58703000 |
| H | -0.52548900 | 4.66437700 | 1.52171000 |

**(*E*)-P'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.761136 (Hartree/Particle)

Thermal correction to Energy= 0.803311

Thermal correction to Enthalpy= 0.804256

Thermal correction to Gibbs Free Energy= 0.686036

Sum of electronic and zero-point Energies= -3054.802803

Sum of electronic and thermal Energies= -3054.760628

Sum of electronic and thermal Enthalpies= -3054.759683

Sum of electronic and thermal Free Energies= -3054.877903

| | | | |
|---|---|---|---|
| Ni | 0.02572500 | -0.43178000 | -1.06719800 |
| C | -0.76312100 | 0.44572000 | -2.67485400 |
| C | 0.17381800 | 1.36598200 | -2.14570800 |
| H | 1.21538800 | 1.37216200 | -2.48080700 |
| H | -0.18881500 | 2.31738400 | -1.75470800 |
| C | -0.33588000 | -0.87249100 | -3.01085100 |
| H | -0.12495900 | -1.87543700 | -0.77688600 |
| C | -2.22566400 | 0.74279900 | -2.53802800 |
| C | -3.11506100 | -0.17831000 | -1.95353800 |
| C | -2.73071900 | 1.98556700 | -2.95503500 |
| C | -4.46405800 | 0.13874800 | -1.78541300 |
| H | -2.73113800 | -1.13217300 | -1.58607800 |
| C | -4.08327100 | 2.30139800 | -2.79406500 |
| H | -2.05087400 | 2.71094000 | -3.40833700 |
| C | -4.95554800 | 1.38039800 | -2.20473400 |
| H | -5.13010100 | -0.58217900 | -1.30466600 |
| H | -4.45626900 | 3.27386500 | -3.12675600 |
| H | -6.01106600 | 1.63019500 | -2.06878800 |
| C | 0.56894300 | -0.10162000 | 0.70086900 |
| N | -0.14089100 | -0.32058900 | 1.84876800 |
| N | 1.80421500 | 0.27188700 | 1.14811800 |
| C | -1.50510500 | -0.77341200 | 1.86417200 |
| C | 0.64056000 | -0.10719200 | 2.98150300 |
| C | 1.87066800 | 0.26303700 | 2.53982400 |
| C | 2.90224500 | 0.55025200 | 0.26492300 |
| C | -2.53573900 | 0.18516300 | 1.94836400 |
| C | -1.75419800 | -2.15951600 | 1.78147600 |
| H | 0.24584900 | -0.23012200 | 3.98546000 |
| H | 2.78191300 | 0.50739300 | 3.07679500 |
| C | 3.73819100 | -0.51613000 | -0.11927600 |
| C | 3.07577900 | 1.86931600 | -0.20956000 |
| C | -3.85736900 | -0.28134300 | 1.91398400 |
| C | -2.22445800 | 1.67591100 | 2.02238200 |
| C | -3.09326600 | -2.57376300 | 1.75566100 |
| C | -0.61581500 | -3.17265600 | 1.77723900 |
| C | 4.77934300 | -0.23275900 | -1.01698500 |
| C | 3.51438600 | -1.94047100 | 0.37614600 |
| C | 4.13568100 | 2.10024900 | -1.09634200 |
| C | 2.15322900 | 2.99604200 | 0.24361500 |
| C | -4.13339200 | -1.64500600 | 1.81342500 |
| H | -4.68313400 | 0.43015300 | 1.95884000 |
| C | -3.21295300 | 2.46257500 | 2.89348100 |
| C | -2.13450100 | 2.26930200 | 0.60698800 |
| H | -1.23062700 | 1.78219000 | 2.48540000 |
| H | -3.32750900 | -3.63779300 | 1.69013400 |
| C | -0.85013600 | -4.34277600 | 0.81392200 |
| C | -0.34223200 | -3.67336200 | 3.20725900 |
| H | 0.28423900 | -2.65128100 | 1.42366800 |
| C | 4.97694400 | 1.05981400 | -1.49871700 |
| H | 5.43905700 | -1.03805700 | -1.34719800 |
| C | 4.78896000 | -2.55301100 | 0.97741900 |
| C | 2.92956400 | -2.81992700 | -0.74205000 |
| H | 2.76447900 | -1.90533300 | 1.17984200 |
| H | 4.30558200 | 3.10379200 | -1.48880800 |
| C | 1.99315100 | 4.11518200 | -0.79434100 |
| C | 2.62581400 | 3.58858400 | 1.58529100 |
| H | 1.15924000 | 2.55010100 | 0.40103700 |
| H | -5.17087700 | -1.98821100 | 1.78369400 |
| H | -3.32374700 | 2.01344500 | 3.89330800 |
| H | -2.85997900 | 3.49852100 | 3.01915000 |
| H | -4.21216600 | 2.51654400 | 2.43217400 |
| H | -1.39819100 | 1.72354400 | 0.00549100 |
| H | -3.10229600 | 2.19686300 | 0.08632900 |
| H | -1.83768000 | 3.33057500 | 0.64540800 |
| H | -1.06418500 | -3.97299700 | -0.19991100 |
| H | 0.05242500 | -4.97302400 | 0.76365300 |
| H | -1.68198500 | -4.98984200 | 1.13679800 |
| H | -0.10294200 | -2.84057200 | 3.88674800 |
| H | -1.22234400 | -4.19813600 | 3.61461800 |
| H | 0.50795300 | -4.37505300 | 3.21673800 |
| H | 5.79249000 | 1.26131500 | -2.19810500 |
| H | 5.19830300 | -1.92105400 | 1.78179300 |
| H | 4.56948000 | -3.54649100 | 1.40050400 |
| H | 5.57711200 | -2.68649500 | 0.21882400 |
| H | 1.97465600 | -2.40208500 | -1.09247000 |
| H | 3.62274900 | -2.89164000 | -1.59644300 |
| H | 2.73938400 | -3.84015100 | -0.36956200 |
| H | 1.73944700 | 3.71942300 | -1.78789900 |
| H | 1.18788000 | 4.79930000 | -0.48358600 |
| H | 2.91100500 | 4.71764300 | -0.89116900 |

| | | | |
|---|---|---|---|
| H | 2.67721700 | 2.82774100 | 2.37660200 |
| H | 3.62820600 | 4.03524100 | 1.47872900 |
| H | 1.93502900 | 4.37854900 | 1.92258100 |
| H | -1.13346800 | -1.57017000 | -3.28544500 |
| C | 1.00097800 | -1.19751600 | -3.64317900 |
| H | 1.26034200 | -2.25246900 | -3.46930700 |
| H | 0.97273800 | -1.03716500 | -4.73781900 |
| H | 1.83011900 | -0.59480700 | -3.24372100 |

**(*Z*)-TS-E'-F'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.757415 (Hartree/Particle)
Thermal correction to Energy= 0.798536
Thermal correction to Enthalpy= 0.799480
Thermal correction to Gibbs Free Energy= 0.684333
Sum of electronic and zero-point Energies= -3054.782861
Sum of electronic and thermal Energies= -3054.741740
Sum of electronic and thermal Enthalpies= -3054.740796
Sum of electronic and thermal Free Energies= -3054.855944

| | | | |
|---|---|---|---|
| Ni | 0.26037300 | -0.32003500 | -1.08092000 |
| C | -0.67049000 | 0.21201700 | -2.74277500 |
| C | 0.27681200 | 1.22622800 | -2.47522900 |
| H | 1.30432600 | 1.15058000 | -2.85286500 |
| H | -0.07887100 | 2.24414600 | -2.29926200 |
| C | -0.21637700 | -1.17309600 | -2.85878600 |
| H | 0.11207300 | -1.78400300 | -1.45439800 |
| H | 0.77519300 | -1.26265800 | -3.32967800 |
| C | -2.12579500 | 0.54303000 | -2.62303100 |
| C | -2.95593100 | -0.06910000 | -1.66565300 |
| C | -2.68298300 | 1.52827500 | -3.45622700 |
| C | -4.30193300 | 0.28555000 | -1.55488200 |
| H | -2.53205000 | -0.80312000 | -0.97610100 |
| C | -4.03053300 | 1.88551200 | -3.34594000 |
| H | -2.04457300 | 2.01703100 | -4.19645400 |
| C | -4.84697900 | 1.26197000 | -2.39636800 |
| H | -4.92080400 | -0.19483200 | -0.79363700 |
| H | -4.44424700 | 2.65405900 | -4.00456400 |
| H | -5.90077800 | 1.53935700 | -2.30859300 |
| C | -1.15752400 | -2.26485200 | -3.34181000 |
| H | -0.67380500 | -3.25149800 | -3.27369300 |
| H | -2.08431100 | -2.30730800 | -2.75461400 |
| H | -1.43922600 | -2.09539300 | -4.39533400 |
| C | 0.91656200 | -0.16237400 | 0.65016700 |
| N | 0.19652900 | -0.40884900 | 1.79144900 |
| N | 2.16597000 | 0.14252100 | 1.12221700 |
| C | -1.19730500 | -0.74717900 | 1.77183300 |
| C | 0.97842500 | -0.27566500 | 2.93630400 |
| C | 2.22161400 | 0.07237900 | 2.51515900 |
| C | 3.27261100 | 0.49452100 | 0.27808600 |
| C | -2.14433300 | 0.28268500 | 1.94867200 |
| C | -1.56353600 | -2.09062900 | 1.54581900 |
| H | 0.57536900 | -0.42863300 | 3.93299000 |
| H | 3.13499700 | 0.27442500 | 3.06662300 |
| C | 4.23846700 | -0.49150900 | -0.01170500 |
| C | 3.34207900 | 1.80840700 | -0.23719800 |
| C | -3.50003900 | -0.07417100 | 1.93074300 |
| C | -1.71104000 | 1.74055800 | 2.05501000 |
| C | -2.93209200 | -2.39430000 | 1.52963500 |
| C | -0.50548400 | -3.16937800 | 1.35166000 |
| C | 5.32560100 | -0.11886900 | -0.81653700 |
| C | 4.05311200 | -1.93237000 | 0.45296600 |
| C | 4.44620000 | 2.12696700 | -1.04032800 |
| C | 2.24845400 | 2.82734500 | 0.06929200 |
| C | -3.88975800 | -1.39822300 | 1.72892700 |
| H | -4.26339400 | 0.69566200 | 2.05466200 |
| C | -2.55646600 | 2.56123500 | 3.03752700 |
| C | -1.69681700 | 2.37960000 | 0.65368500 |
| H | -0.67547700 | 1.75520200 | 2.42755200 |
| H | -3.25600800 | -3.42253500 | 1.35946100 |
| C | -0.90072300 | -4.21821300 | 0.30486100 |
| C | -0.14566200 | -3.82464400 | 2.69672600 |
| H | 0.39286000 | -2.66964100 | 0.96459500 |
| C | 5.43111300 | 1.17756400 | -1.31950500 |
| H | 6.09436800 | -0.85276600 | -1.06400000 |
| C | 5.36920100 | -2.65710100 | 0.76199200 |
| C | 3.21794500 | -2.70680900 | -0.58512700 |
| H | 3.46930900 | -1.91229700 | 1.38584800 |
| H | 4.54089800 | 3.12982900 | -1.45871900 |
| C | 2.12549700 | 3.93232900 | -0.98668500 |
| C | 2.42570100 | 3.44519300 | 1.46831200 |
| H | 1.30024400 | 2.26995800 | 0.05448500 |
| H | -4.95213100 | -1.65539900 | 1.71332100 |
| H | -2.59919800 | 2.08764600 | 4.03137000 |
| H | -2.12472200 | 3.56787400 | 3.15550000 |
| H | -3.59014800 | 2.69357700 | 2.67944500 |
| H | -1.07475800 | 1.79041800 | -0.03470500 |
| H | -2.71360000 | 2.41912300 | 0.23102200 |
| H | -1.29572100 | 3.40563200 | 0.69884000 |
| H | -1.18193800 | -3.73769900 | -0.64472400 |
| H | -0.04942600 | -4.88891300 | 0.10603800 |
| H | -1.74127100 | -4.84834500 | 0.63837700 |
| H | 0.20130100 | -3.07692200 | 3.42683200 |
| H | -1.01957600 | -4.33960200 | 3.12959700 |
| H | 0.65770000 | -4.56796800 | 2.56467400 |
| H | 6.28491400 | 1.44956900 | -1.94570100 |
| H | 5.99185200 | -2.08600900 | 1.46895100 |
| H | 5.15985900 | -3.64241500 | 1.20778700 |
| H | 5.96499200 | -2.83499800 | -0.14779200 |
| H | 2.25892200 | -2.20231700 | -0.77596400 |
| H | 3.76240500 | -2.77932400 | -1.54158800 |
| H | 3.00709700 | -3.72971000 | -0.23121500 |
| H | 2.05356300 | 3.51692700 | -2.00247800 |
| H | 1.21641000 | 4.52493900 | -0.79803100 |
| H | 2.97974200 | 4.62898000 | -0.96019100 |
| H | 2.44215500 | 2.68052300 | 2.25766400 |
| H | 3.36804400 | 4.01516800 | 1.52654200 |
| H | 1.59567600 | 4.13632400 | 1.68922500 |

**(*Z*)-F'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.758342 (Hartree/Particle)
Thermal correction to Energy= 0.799892
Thermal correction to Enthalpy= 0.800836
Thermal correction to Gibbs Free Energy= 0.684969
Sum of electronic and zero-point Energies= -3054.796577
Sum of electronic and thermal Energies= -3054.755028
Sum of electronic and thermal Enthalpies= -3054.754084
Sum of electronic and thermal Free Energies= -3054.869951

| | | | |
|---|---|---|---|
| Ni | 0.32501600 | -0.56845800 | -1.15281900 |
| C | -0.58142100 | 0.33020100 | -2.70420000 |
| C | 0.25175100 | 1.28383000 | -2.06322000 |
| H | 1.29098900 | 1.41725300 | -2.38810000 |
| H | -0.20980900 | 2.16164600 | -1.60562200 |
| C | 0.01185200 | -0.88985500 | -3.13201300 |
| H | 0.34268100 | -2.03650700 | -0.88824200 |
| H | 1.07040200 | -0.81604700 | -3.42679600 |
| C | -2.06832700 | 0.50501200 | -2.63450900 |
| C | -2.88673900 | -0.35937500 | -1.88775100 |
| C | -2.66516000 | 1.58532600 | -3.30493500 |
| C | -4.26738000 | -0.15579600 | -1.82478000 |
| H | -2.42641000 | -1.17639700 | -1.32747700 |
| C | -4.04679800 | 1.79008300 | -3.24282600 |
| H | -2.03348800 | 2.27125500 | -3.87505000 |
| C | -4.85349700 | 0.91755200 | -2.50386500 |
| H | -4.88251800 | -0.82873900 | -1.22287300 |
| H | -4.49461300 | 2.63685800 | -3.76977500 |
| H | -5.93321900 | 1.07944200 | -2.45015900 |
| C | -0.72091800 | -2.01925300 | -3.81234900 |
| H | -1.73077100 | -2.17173100 | -3.40902700 |
| H | -0.82135200 | -1.83537600 | -4.89852800 |

| | | | |
|---|---|---|---|
| H | -0.16775500 | -2.96263700 | -3.68769100 |
| C | 0.86520700 | -0.26213900 | 0.60681500 |
| N | 0.13355200 | -0.45851000 | 1.74074500 |
| N | 2.10955200 | 0.05791000 | 1.06691800 |
| C | -1.27129200 | -0.75576600 | 1.73501700 |
| C | 0.91508700 | -0.30562200 | 2.88483100 |
| C | 2.16346600 | 0.01856600 | 2.45966000 |
| C | 3.18279900 | 0.46711900 | 0.20485300 |
| C | -2.18467400 | 0.30439600 | 1.53037500 |
| C | -1.68045300 | -2.08904600 | 1.92141300 |
| H | 0.50840500 | -0.43834300 | 3.88266700 |
| H | 3.07859400 | 0.21826800 | 3.00826500 |
| C | 4.05556100 | -0.50832500 | -0.31165200 |
| C | 3.29651600 | 1.84012200 | -0.11267900 |
| C | -3.54899500 | -0.00526300 | 1.57876000 |
| C | -1.68962200 | 1.72072400 | 1.24946900 |
| C | -3.06009500 | -2.34515900 | 1.96344100 |
| C | -0.67611300 | -3.22517000 | 2.06689900 |
| C | 5.08379600 | -0.07396100 | -1.16325300 |
| C | 3.88385100 | -1.99096300 | -0.00724100 |
| C | 4.34204600 | 2.22165100 | -0.96297100 |
| C | 2.33023200 | 2.86863300 | 0.46602400 |
| C | -3.98347200 | -1.31352600 | 1.80506900 |
| H | -4.28753200 | 0.78042100 | 1.41846600 |
| C | -1.26846800 | 2.44497100 | 2.54131600 |
| C | -2.68541200 | 2.57569100 | 0.45680800 |
| H | -0.79823500 | 1.60749300 | 0.61502100 |
| H | -3.41292600 | -3.36756900 | 2.11631100 |
| C | -0.93598000 | -4.35095800 | 1.05389200 |
| C | -0.64683900 | -3.75561300 | 3.51024100 |
| H | 0.31987700 | -2.82013300 | 1.83748600 |
| C | 5.22856000 | 1.27471500 | -1.48228600 |
| H | 5.77440500 | -0.80619100 | -1.58766500 |
| C | 5.15121300 | -2.60086500 | 0.61214600 |
| C | 3.43572600 | -2.75284500 | -1.26632100 |
| H | 3.07494600 | -2.09094100 | 0.73117400 |
| H | 4.46439300 | 3.27204500 | -1.23217800 |
| C | 2.01805800 | 4.02532100 | -0.49430100 |
| C | 2.84914600 | 3.41858000 | 1.80800600 |
| H | 1.38217800 | 2.34707000 | 0.66159000 |
| H | -5.05427600 | -1.53086100 | 1.83933500 |
| H | -0.49951600 | 1.88960600 | 3.09672800 |
| H | -0.85635000 | 3.43999700 | 2.30550700 |
| H | -2.13583300 | 2.58489500 | 3.20760700 |
| H | -3.02645400 | 2.06242900 | -0.45270400 |
| H | -3.57071700 | 2.84185900 | 1.05760300 |
| H | -2.20338300 | 3.51910400 | 0.15480500 |
| H | -0.92921300 | -3.95379200 | 0.02758000 |
| H | -0.14856000 | -5.11845500 | 1.12943900 |
| H | -1.90238500 | -4.85025400 | 1.23096100 |
| H | -0.40216000 | -2.95537900 | 4.22694000 |
| H | -1.62488300 | -4.17547400 | 3.79818500 |
| H | 0.10752400 | -4.55202600 | 3.61738900 |
| H | 6.03488700 | 1.59361100 | -2.14788100 |
| H | 5.45359100 | -2.05954000 | 1.52294200 |
| H | 4.97532100 | -3.65454500 | 0.88245600 |
| H | 5.99964500 | -2.57735900 | -0.09093100 |
| H | 2.47723300 | -2.35026800 | -1.62638200 |
| H | 4.18577700 | -2.67595000 | -2.07080600 |
| H | 3.28994800 | -3.82152000 | -1.03801500 |
| H | 1.71870500 | 3.66085600 | -1.48710900 |
| H | 1.19269800 | 4.63266500 | -0.08999000 |
| H | 2.88225000 | 4.69693700 | -0.62264000 |
| H | 3.02573000 | 2.61692300 | 2.53912500 |
| H | 3.79869300 | 3.95987700 | 1.66288100 |
| H | 2.11926100 | 4.11916000 | 2.24547800 |

**(*Z*)-G'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.759412 (Hartree/Particle)

Thermal correction to Energy= 0.800453

Thermal correction to Enthalpy= 0.801397

Thermal correction to Gibbs Free Energy= 0.687268

Sum of electronic and zero-point Energies= -3054.790267

Sum of electronic and thermal Energies= -3054.749226

Sum of electronic and thermal Enthalpies= -3054.748282

Sum of electronic and thermal Free Energies= -3054.862411

| | | | |
|---|---|---|---|
| Ni | 0.30815100 | 0.69256100 | -0.97591100 |
| N | 0.55931500 | 0.69390700 | 1.97876000 |
| N | -1.44063100 | 0.27231900 | 1.30029900 |
| C | 2.73351100 | -0.25211200 | 2.60138400 |
| C | 4.13233000 | -0.15489000 | 2.56708600 |
| C | 4.76405600 | 0.94034500 | 1.97890100 |
| C | 4.01022000 | 1.97715400 | 1.42987600 |
| C | 2.60843600 | 1.93779700 | 1.44151200 |
| C | 1.99381500 | 0.80196200 | 2.01390600 |
| C | -0.26287700 | 0.72595000 | 3.10521800 |
| C | -1.52062900 | 0.44768700 | 2.67756300 |
| C | -0.16265200 | 0.44131200 | 0.83878000 |
| C | -2.55957900 | -0.00200100 | 0.44267000 |
| C | -2.81867000 | -1.33909000 | 0.08049400 |
| C | -3.88350600 | -1.57908900 | -0.80051300 |
| C | -4.66789100 | -0.52947100 | -1.27819700 |
| C | -4.40608700 | 0.78299800 | -0.88084100 |
| C | -3.34380000 | 1.07756100 | -0.01549600 |
| H | 4.74114000 | -0.94924400 | 2.99963600 |
| H | 5.85571800 | 0.98974600 | 1.95514600 |
| H | 4.52427400 | 2.83132700 | 0.98841000 |
| H | 0.12156900 | 0.94662200 | 4.09623200 |
| H | -2.45759700 | 0.35793300 | 3.21829500 |
| H | -4.10044000 | -2.60077800 | -1.11831700 |
| H | -5.49393700 | -0.73550400 | -1.96389200 |
| H | -5.03504000 | 1.59233400 | -1.25668700 |
| C | 1.25405500 | -0.06934900 | -2.59746700 |
| C | 2.11769700 | -0.29928300 | -1.50284400 |
| C | 0.81220000 | 1.27378600 | -2.81098700 |
| H | -0.71856800 | 1.75370900 | -1.04337700 |
| H | 1.51348300 | 2.09951800 | -2.63741000 |
| H | 0.07913300 | 1.46608900 | -3.59807500 |
| C | 0.57033600 | -1.18011700 | -3.33422900 |
| C | -0.82993000 | -1.19609100 | -3.47591100 |
| C | 1.31244000 | -2.21907100 | -3.91876000 |
| C | -1.46730700 | -2.22291400 | -4.17393500 |
| H | -1.42190100 | -0.40965400 | -3.00227400 |
| C | 0.67524000 | -3.24749100 | -4.62100700 |
| H | 2.40051000 | -2.21706000 | -3.83018700 |
| C | -0.71734000 | -3.25543400 | -4.74927300 |
| H | -2.55742900 | -2.22242700 | -4.25731300 |
| H | 1.27124300 | -4.04633200 | -5.07049300 |
| H | -1.21553600 | -4.06195200 | -5.29362000 |
| C | -3.07606400 | 2.50841900 | 0.43462500 |
| C | -4.03952000 | 2.90617400 | 1.56774300 |
| C | -3.13610600 | 3.51934800 | -0.71911600 |
| H | -2.05203600 | 2.54081500 | 0.83308500 |
| H | -3.96106500 | 2.22159000 | 2.42647000 |
| H | -3.81978000 | 3.92560200 | 1.92492300 |
| H | -5.08497200 | 2.88618800 | 1.21780400 |
| H | -2.45434600 | 3.22231600 | -1.52962500 |
| H | -4.15322900 | 3.61654400 | -1.13215100 |
| H | -2.83226200 | 4.51656700 | -0.36191200 |
| C | -1.95271600 | -2.48471100 | 0.58930700 |
| C | -0.91063000 | -2.87948500 | -0.46853400 |
| C | -2.77348800 | -3.69803800 | 1.04947700 |
| H | -1.40220200 | -2.11766700 | 1.46808900 |
| H | -0.30086000 | -2.01041000 | -0.75047100 |
| H | -0.24270500 | -3.66692100 | -0.08447500 |
| H | -1.39679300 | -3.25193400 | -1.38353900 |
| H | -3.54043200 | -3.41231300 | 1.78693700 |
| H | -3.28115900 | -4.19500200 | 0.20721000 |
| H | -2.11131600 | -4.44537800 | 1.51559000 |

| | | | |
|---|---|---|---|
| C | 2.04432900 | -1.46682400 | 3.22710300 |
| C | 2.89409700 | -2.18556100 | 4.28261900 |
| C | 1.55508400 | -2.46032300 | 2.15864400 |
| H | 1.14822300 | -1.10085900 | 3.74803100 |
| H | 3.27009300 | -1.49024700 | 5.04957100 |
| H | 2.28820000 | -2.95498100 | 4.78648800 |
| H | 3.75994500 | -2.69928500 | 3.83459900 |
| H | 0.98289300 | -1.95794300 | 1.36920800 |
| H | 2.40576000 | -2.96961100 | 1.67993700 |
| H | 0.91225400 | -3.23012300 | 2.61546500 |
| C | 1.77712100 | 3.09650000 | 0.89758900 |
| C | 2.51417000 | 3.96240900 | -0.12854200 |
| C | 1.22839000 | 3.95745700 | 2.05008200 |
| H | 0.91594100 | 2.66276400 | 0.36724800 |
| H | 2.94258200 | 3.35030600 | -0.93748400 |
| H | 1.81037800 | 4.67647800 | -0.58394900 |
| H | 3.32928900 | 4.54971900 | 0.32526400 |
| H | 0.63073000 | 3.35950300 | 2.75425800 |
| H | 2.05133900 | 4.42646600 | 2.61508000 |
| H | 0.58263600 | 4.75950000 | 1.65701200 |
| C | 2.67024700 | -1.63056400 | -1.07161100 |
| H | 3.54363300 | -1.92908400 | -1.68139100 |
| H | 3.01639000 | -1.56797000 | -0.03148200 |
| H | 1.92981000 | -2.43995900 | -1.13941600 |
| H | 2.75152200 | 0.54993300 | -1.21028700 |

**(*Z*)-TS-G'-P'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.757486 (Hartree/Particle)
Thermal correction to Energy= 0.798612
Thermal correction to Enthalpy= 0.799556
Thermal correction to Gibbs Free Energy= 0.684129
Sum of electronic and zero-point Energies= -3054.782475
Sum of electronic and thermal Energies= -3054.741349
Sum of electronic and thermal Enthalpies= -3054.740405
Sum of electronic and thermal Free Energies= -3054.855831

| | | | |
|---|---|---|---|
| Ni | 0.51814300 | 0.19779300 | -0.77698500 |
| N | 0.50842000 | 0.52716600 | 2.14737000 |
| N | -1.45369700 | 0.14521600 | 1.34884400 |
| C | 2.73924000 | -0.28373500 | 2.73014700 |
| C | 4.11532300 | -0.03588500 | 2.84093400 |
| C | 4.65405600 | 1.18824400 | 2.44573900 |
| C | 3.83239900 | 2.18132300 | 1.90964900 |
| C | 2.44945100 | 1.98867600 | 1.78423900 |
| C | 1.92511200 | 0.75369100 | 2.22978700 |
| C | -0.37488500 | 0.55958700 | 3.22657800 |
| C | -1.61351700 | 0.31773700 | 2.72240500 |
| C | -0.14242900 | 0.26039900 | 0.97392000 |
| C | -2.50509200 | -0.10089600 | 0.40143700 |
| C | -2.94476400 | -1.42610000 | 0.21327400 |
| C | -3.98495100 | -1.64223000 | -0.70242100 |
| C | -4.54290000 | -0.58154900 | -1.41379100 |
| C | -4.05425600 | 0.71623600 | -1.24657700 |
| C | -3.01916000 | 0.98733100 | -0.34129200 |
| H | 4.77778700 | -0.81247100 | 3.22574400 |
| H | 5.72880000 | 1.36488500 | 2.53884100 |
| H | 4.28049600 | 3.11896700 | 1.57902400 |
| H | -0.04100400 | 0.75362700 | 4.24165400 |
| H | -2.58346500 | 0.25385800 | 3.20659000 |
| H | -4.34680800 | -2.65653900 | -0.87898200 |
| H | -5.35105200 | -0.76911300 | -2.12547500 |
| H | -4.48074200 | 1.52557200 | -1.83983300 |
| C | 0.96271300 | 0.26277600 | -2.68117300 |
| C | 2.13696000 | 0.24314600 | -1.88462500 |
| C | 0.50168900 | 1.58302600 | -3.27885300 |
| H | -0.59365000 | 1.68725400 | -3.24591200 |
| H | 0.92859000 | 2.43804700 | -2.73322500 |
| H | 0.79933200 | 1.66876100 | -4.34144900 |
| C | 0.28373700 | -0.95779700 | -3.20328700 |
| C | -1.12723300 | -1.04380700 | -3.14443400 |
| C | 0.97591200 | -2.05219900 | -3.76159800 |
| C | -1.80729900 | -2.17280500 | -3.59910300 |
| H | -1.69629200 | -0.22271800 | -2.70254700 |
| C | 0.29468400 | -3.18764900 | -4.21224400 |
| H | 2.06157600 | -2.00582400 | -3.85757800 |
| C | -1.10007800 | -3.25748800 | -4.13261700 |
| H | -2.89653400 | -2.20923400 | -3.51838900 |
| H | 0.85976900 | -4.02074200 | -4.64014400 |
| H | -1.63070800 | -4.14559900 | -4.48573800 |
| C | -2.43500400 | 2.38941100 | -0.18400900 |
| C | -2.97241200 | 3.09687100 | 1.07261200 |
| C | -2.63306400 | 3.27872600 | -1.41737400 |
| H | -1.34773600 | 2.25076600 | -0.06767800 |
| H | -2.77744300 | 2.51956400 | 1.98666300 |
| H | -2.49500500 | 4.08278600 | 1.19224300 |
| H | -4.06113300 | 3.25205400 | 0.99175700 |
| H | -2.29253000 | 2.78029200 | -2.33709200 |
| H | -3.68790600 | 3.56733200 | -1.55474700 |
| H | -2.05298100 | 4.20776900 | -1.30188900 |
| C | -2.22449100 | -2.59431900 | 0.87539500 |
| C | -1.13180100 | -3.11515300 | -0.07834500 |
| C | -3.16249000 | -3.72154200 | 1.32592300 |
| H | -1.71764000 | -2.21281700 | 1.77470900 |
| H | -0.45662400 | -2.29821200 | -0.37651800 |
| H | -0.53568500 | -3.90430600 | 0.40684400 |
| H | -1.57726500 | -3.52562400 | -0.99790500 |
| H | -3.96595800 | -3.34431700 | 1.97865800 |
| H | -3.63217700 | -4.23251300 | 0.47000300 |
| H | -2.59536100 | -4.48287400 | 1.88466700 |
| C | 2.15229500 | -1.66212200 | 3.01775900 |
| C | 2.91697000 | -2.45764200 | 4.08197200 |
| C | 2.04705400 | -2.45384200 | 1.69928300 |
| H | 1.12771700 | -1.52186600 | 3.39509100 |
| H | 3.04097900 | -1.88009800 | 5.01183500 |
| H | 2.37080900 | -3.38314400 | 4.32348000 |
| H | 3.91799700 | -2.75649300 | 3.73139900 |
| H | 1.49121300 | -1.88798700 | 0.93706800 |
| H | 3.05139700 | -2.66102100 | 1.29532700 |
| H | 1.53532700 | -3.41608300 | 1.86219400 |
| C | 1.54566600 | 3.04443000 | 1.15270400 |
| C | 2.28485700 | 4.00855900 | 0.21918400 |
| C | 0.73541200 | 3.81787200 | 2.20664500 |
| H | 0.84211800 | 2.48435000 | 0.51568300 |
| H | 2.87943400 | 3.46392100 | -0.53081100 |
| H | 1.55539200 | 4.63555000 | -0.31771000 |
| H | 2.95968600 | 4.68821500 | 0.76532400 |
| H | 0.13049200 | 3.14694700 | 2.83312100 |
| H | 1.40421400 | 4.39322200 | 2.86846600 |
| H | 0.04807700 | 4.52691000 | 1.71714700 |
| C | 3.01782400 | -0.94180100 | -1.55899700 |
| H | 3.81548800 | -1.08799500 | -2.31378100 |
| H | 3.51277800 | -0.78269700 | -0.58763800 |
| H | 2.45085000 | -1.88027000 | -1.48778300 |
| H | 2.66817300 | 1.20357900 | -1.80014000 |

**(*Z*)-P'**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.762088 (Hartree/Particle)
Thermal correction to Energy= 0.803807
Thermal correction to Enthalpy= 0.804751
Thermal correction to Gibbs Free Energy= 0.688743
Sum of electronic and zero-point Energies= -3054.799656
Sum of electronic and thermal Energies= -3054.757937
Sum of electronic and thermal Enthalpies= -3054.756992
Sum of electronic and thermal Free Energies= -3054.873001

| | | | |
|---|---|---|---|
| Ni | 0.04890300 | 0.28131000 | -1.16451100 |
| N | 0.05952200 | 0.63474400 | 1.76917100 |
| N | -1.86301400 | 0.08309800 | 0.97162800 |
| C | 2.29383300 | -0.04638600 | 2.48811100 |
| C | 3.65770000 | 0.25476600 | 2.61079000 |

| | | | |
|---|---|---|---|
| C | 4.16775400 | 1.46560900 | 2.14102400 |
| C | 3.32627500 | 2.39963400 | 1.53555400 |
| C | 1.95255400 | 2.15249700 | 1.39648700 |
| C | 1.46124800 | 0.92253700 | 1.88687000 |
| C | -0.84529100 | 0.68421300 | 2.83151300 |
| C | -2.05593900 | 0.33432100 | 2.32775700 |
| C | -0.55422900 | 0.26663600 | 0.59755600 |
| C | -2.91140100 | -0.18781300 | 0.03077800 |
| C | -3.25192800 | -1.52622100 | -0.24853100 |
| C | -4.28161600 | -1.75522300 | -1.17219600 |
| C | -4.93952400 | -0.69208300 | -1.79059300 |
| C | -4.57301400 | 0.62494900 | -1.50783600 |
| C | -3.54870400 | 0.90626000 | -0.59304800 |
| H | 4.33469500 | -0.46755600 | 3.06889800 |
| H | 5.23468500 | 1.68114300 | 2.24215200 |
| H | 3.74782600 | 3.33601200 | 1.16766600 |
| H | -0.53943400 | 0.95764900 | 3.83701600 |
| H | -3.02844100 | 0.23685600 | 2.80071000 |
| H | -4.56214100 | -2.77928600 | -1.42464800 |
| H | -5.73920700 | -0.89151400 | -2.50872300 |
| H | -5.09129200 | 1.44572400 | -2.00741000 |
| C | 0.66343300 | -0.32171900 | -2.96413200 |
| C | 1.60587500 | -0.87431800 | -2.06806900 |
| C | 0.41461000 | 1.11513500 | -2.94298100 |
| H | -0.48670400 | 1.57526200 | -1.71814900 |
| H | 1.27956700 | 1.78213800 | -2.82327900 |
| H | -0.28870700 | 1.48419900 | -3.69555300 |
| C | -0.27697500 | -1.17668400 | -3.75700400 |
| C | -1.67102300 | -1.02557300 | -3.63523500 |
| C | 0.21282600 | -2.13726800 | -4.65859100 |
| C | -2.54504300 | -1.81593300 | -4.38483200 |
| H | -2.07410000 | -0.30017700 | -2.92429400 |
| C | -0.66107600 | -2.92795800 | -5.41083100 |
| H | 1.29183700 | -2.26034900 | -4.77313000 |
| C | -2.04499600 | -2.77182500 | -5.27593900 |
| H | -3.62285100 | -1.68889300 | -4.25858700 |
| H | -0.25851600 | -3.66892600 | -6.10692500 |
| H | -2.72915600 | -3.39144100 | -5.86171100 |
| C | -3.15837800 | 2.34273000 | -0.26514100 |
| C | -4.11505100 | 2.94161800 | 0.78087600 |
| C | -3.06642200 | 3.23628500 | -1.50947800 |
| H | -2.15221000 | 2.31499300 | 0.17449900 |
| H | -4.13334600 | 2.33807800 | 1.70141900 |
| H | -3.80354500 | 3.96388200 | 1.05130600 |
| H | -5.14448600 | 2.99050500 | 0.38861200 |
| H | -2.39635800 | 2.79246300 | -2.26114500 |
| H | -4.05069300 | 3.40484900 | -1.97557600 |
| H | -2.66199100 | 4.22359500 | -1.23363700 |
| C | -2.46635800 | -2.68096200 | 0.35845200 |
| C | -1.35805000 | -3.11415700 | -0.61758500 |
| C | -3.34623800 | -3.86641500 | 0.77619800 |
| H | -1.97021300 | -2.30386100 | 1.26601000 |
| H | -0.72100600 | -2.25671600 | -0.87723900 |
| H | -0.72482300 | -3.89647400 | -0.16916600 |
| H | -1.78993300 | -3.50591900 | -1.55276700 |
| H | -4.15861700 | -3.55154600 | 1.45058800 |
| H | -3.80182000 | -4.36651200 | -0.09370700 |
| H | -2.73793800 | -4.62071400 | 1.30045500 |
| C | 1.73144700 | -1.40236300 | 2.90424500 |
| C | 2.52032900 | -2.08940500 | 4.02493500 |
| C | 1.61415300 | -2.31578300 | 1.66987000 |
| H | 0.71175200 | -1.23888200 | 3.28517300 |
| H | 2.64941200 | -1.42980800 | 4.89771100 |
| H | 1.98846600 | -2.99532100 | 4.35586100 |
| H | 3.52020100 | -2.40744100 | 3.68795100 |
| H | 1.07201200 | -1.82144100 | 0.85049400 |
| H | 2.61868500 | -2.57823400 | 1.29913500 |
| H | 1.08937800 | -3.25166000 | 1.92275700 |
| C | 1.01498100 | 3.17081200 | 0.75499000 |
| C | 1.70572800 | 4.09209100 | -0.25628500 |
| C | 0.26325900 | 3.98750300 | 1.82089200 |
| H | 0.27422800 | 2.59364800 | 0.18375100 |
| H | 2.27427500 | 3.51341000 | -1.00128100 |
| H | 0.94972600 | 4.68579800 | -0.79423300 |
| H | 2.39662200 | 4.80283300 | 0.22630600 |
| H | -0.30060300 | 3.33788300 | 2.50660600 |
| H | 0.96484600 | 4.59019200 | 2.42167200 |
| H | -0.45467200 | 4.67419800 | 1.34284400 |
| C | 1.95365300 | -2.33848000 | -1.98481000 |
| H | 2.71590800 | -2.62502400 | -2.73403600 |
| H | 2.37326700 | -2.58019400 | -0.99828000 |
| H | 1.07937900 | -2.98525200 | -2.14557300 |
| H | 2.41334600 | -0.20558700 | -1.73503500 |

## *A1.3.b Coordinates & Energies in the Study of Directing-Group-Free Catalytic Dicarbofunctionalization of Unactivated Alkenes.*

**i-1**

uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.573027 (Hartree/Particle)

Thermal correction to Energy= 0.606083

Thermal correction to Enthalpy= 0.607027

Thermal correction to Gibbs Free Energy= 0.507862

Sum of electronic and zero-point Energies= -3127.088547

Sum of electronic and thermal Energies= -3127.055492

Sum of electronic and thermal Enthalpies= -3127.054547

Sum of electronic and thermal Free Energies= -3127.153712

| | | | |
|---|---|---|---|
| Ni | -1.39145500 | -0.08316600 | 0.04556100 |
| Cl | 0.68966400 | -0.68296200 | 0.12655100 |
| C | -3.26446100 | 0.10541500 | 0.01108300 |
| C | -5.43301100 | -0.06590800 | -0.66429000 |
| C | -5.44219900 | 0.18009300 | 0.67406900 |
| N | -4.11184800 | 0.28463600 | 1.06450700 |
| N | -4.09752700 | -0.10318100 | -1.04868200 |
| H | -6.26081200 | 0.29053600 | 1.37905400 |
| H | -6.24198500 | -0.21505600 | -1.37328400 |
| C | -3.66308500 | 0.47381100 | 2.41771200 |
| C | -3.36400100 | -0.66400200 | 3.19334900 |
| C | -3.52063400 | 1.79073600 | 2.90333600 |
| C | -2.93579300 | -0.45133900 | 4.51251100 |
| C | -3.09259200 | 1.94810800 | 4.22826800 |
| C | -2.80952800 | 0.83813600 | 5.02710100 |
| H | -2.69119400 | -1.30966200 | 5.14225100 |
| H | -2.96517700 | 2.95078400 | 4.64000200 |
| H | -2.47503000 | 0.98217400 | 6.05761200 |
| C | -3.62922500 | -0.40342100 | -2.37502200 |
| C | -3.30260500 | -1.73787400 | -2.68899900 |
| C | -3.49604700 | 0.65483300 | -3.29868600 |
| C | -2.85849000 | -2.00376700 | -3.99321100 |
| C | -3.05041100 | 0.33523200 | -4.58807600 |
| C | -2.74166200 | -0.98200900 | -4.93425100 |
| H | -2.59442900 | -3.02636400 | -4.27190000 |
| H | -2.92948200 | 1.12626200 | -5.33018500 |
| H | -2.39421900 | -1.21049400 | -5.94502600 |
| C | -3.45155200 | -2.07856700 | 2.63333600 |
| C | -4.44157300 | -2.94706000 | 3.42562500 |
| C | -2.05803700 | -2.72753000 | 2.55783400 |
| H | -3.83109700 | -2.01224800 | 1.60393500 |
| H | -5.44439800 | -2.49143300 | 3.44847400 |
| H | -4.52877600 | -3.94464800 | 2.96574100 |
| H | -4.11187900 | -3.08937600 | 4.46756500 |

| | | | |
|---|---|---|---|
| H | -1.36206200 | -2.11601400 | 1.96252300 |
| H | -1.62371300 | -2.85945400 | 3.56229800 |
| H | -2.12476600 | -3.72122500 | 2.08592200 |
| C | -3.71511200 | 2.99122500 | 1.98524200 |
| C | -2.36146000 | 3.37005200 | 1.35443900 |
| C | -4.36962000 | 4.19562800 | 2.67391500 |
| H | -4.38213700 | 2.68302100 | 1.16539400 |
| H | -1.91454800 | 2.50347300 | 0.84369400 |
| H | -2.48363600 | 4.18065600 | 0.61818300 |
| H | -1.65450400 | 3.70879500 | 2.12937800 |
| H | -5.31985200 | 3.91840200 | 3.15719500 |
| H | -3.71423100 | 4.63705000 | 3.44169000 |
| H | -4.57806800 | 4.98497900 | 1.93444700 |
| C | -3.38422800 | -2.86190000 | -1.66328700 |
| C | -1.99352300 | -3.45798300 | -1.38230200 |
| C | -4.39264000 | -3.94267100 | -2.08486500 |
| H | -3.74505600 | -2.43209300 | -0.71831900 |
| H | -1.28269400 | -2.68258000 | -1.05633800 |
| H | -2.05855400 | -4.21549500 | -0.58445500 |
| H | -1.57878300 | -3.94826300 | -2.27812800 |
| H | -5.39414900 | -3.51362600 | -2.24834500 |
| H | -4.08324400 | -4.44180700 | -3.01757100 |
| H | -4.47443800 | -4.71632700 | -1.30437400 |
| C | -3.71868500 | 2.10098000 | -2.87314200 |
| C | -4.37241500 | 2.96942500 | -3.95561400 |
| C | -2.38034600 | 2.70165800 | -2.40190200 |
| H | -4.39737400 | 2.09600200 | -2.00632800 |
| H | -5.31051400 | 2.52256100 | -4.32116300 |
| H | -4.60268900 | 3.96730500 | -3.54997900 |
| H | -3.70724000 | 3.11814700 | -4.82123100 |
| H | -1.93243500 | 2.08239600 | -1.60999600 |
| H | -1.66364100 | 2.75296900 | -3.23783600 |
| H | -2.52408900 | 3.71971700 | -2.00559100 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3128.925525
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3127.401283

**TS-i-ii-1**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.719324 (Hartree/Particle)
Thermal correction to Energy= 0.767749
Thermal correction to Enthalpy= 0.768693
Thermal correction to Gibbs Free Energy= 0.634910
Sum of electronic and zero-point Energies= -4358.578609
Sum of electronic and thermal Energies= -4358.530184
Sum of electronic and thermal Enthalpies= -4358.529240
Sum of electronic and thermal Free Energies= -4358.663023

| | | | |
|---|---|---|---|
| Ni | 8.08764200 | -3.23894400 | -0.49962600 |
| C | 8.36479100 | -1.49781400 | 0.31054600 |
| C | 9.03980900 | 0.63695600 | 0.56742400 |
| C | 8.99837800 | 0.07056300 | 1.80068400 |
| N | 8.57742700 | -1.24237900 | 1.62553400 |
| N | 8.65034500 | -0.34274700 | -0.33782300 |
| H | 9.25060700 | 0.46901500 | 2.77686600 |
| H | 9.32389400 | 1.63366300 | 0.24829100 |
| C | 8.52096400 | -2.22862300 | 2.68127600 |
| C | 9.58878300 | -3.15240400 | 2.78386400 |
| C | 7.42127900 | -2.21803700 | 3.56724100 |
| C | 9.51505500 | -4.10371300 | 3.81061700 |
| C | 7.41141200 | -3.18873400 | 4.58117500 |
| C | 8.44025100 | -4.12124600 | 4.69919600 |
| H | 10.31102900 | -4.84034800 | 3.92129500 |
| H | 6.57790200 | -3.22095800 | 5.28325500 |
| H | 8.40430900 | -4.87209200 | 5.49252600 |
| C | 8.63342500 | -0.15979000 | -1.77124300 |
| C | 7.59011100 | 0.60155800 | -2.33650000 |
| C | 9.69027200 | -0.71040500 | -2.53686100 |
| C | 7.60133500 | 0.77321800 | -3.72937200 |
| C | 9.63979100 | -0.51583900 | -3.92390900 |
| C | 8.60621200 | 0.21325600 | -4.51439200 |
| H | 6.80758800 | 1.35349000 | -4.20290600 |
| H | 10.42517000 | -0.93139500 | -4.55525700 |
| H | 8.59138800 | 0.35171600 | -5.59845900 |
| C | 5.27606700 | -5.38129100 | 0.67596800 |
| C | 4.72766700 | -5.74733900 | -0.56140800 |
| C | 4.92484600 | -4.90191500 | -1.67358100 |
| C | 5.65425100 | -3.71840900 | -1.56595400 |
| C | 6.22873500 | -3.45333400 | -0.32490900 |
| C | 6.00224300 | -4.19194200 | 0.82866300 |
| H | 5.11346100 | -6.01231200 | 1.55342200 |
| H | 4.47844500 | -5.16216000 | -2.63736100 |
| H | 5.78080400 | -3.03767400 | -2.40784300 |
| H | 6.38136200 | -3.87848100 | 1.80109700 |
| O | 5.35068100 | -1.30415500 | -0.02379900 |
| S | 3.95138000 | -1.31921300 | 0.53791000 |
| O | 3.57768100 | -2.59007800 | 1.18117800 |
| O | 3.61050400 | -0.07024700 | 1.24348300 |
| C | 2.80731900 | -1.30933700 | -0.98297800 |
| F | 2.41618600 | -0.07284000 | -1.29907600 |
| F | 1.71828400 | -2.03374200 | -0.72641300 |
| F | 3.41611100 | -1.84176400 | -2.05506100 |
| C | 6.28874000 | -1.20187000 | 3.45770800 |
| C | 6.58430700 | 0.05901000 | 4.29344600 |
| C | 4.92569200 | -1.77307400 | 3.87592400 |
| H | 6.20959200 | -0.90384600 | 2.40106100 |
| H | 7.52076600 | 0.55470400 | 4.00465100 |
| H | 5.76780600 | 0.78789900 | 4.17105900 |
| H | 6.65792500 | -0.19703400 | 5.36326100 |
| H | 4.70449700 | -2.71877600 | 3.36533900 |
| H | 4.86876500 | -1.92837100 | 4.96556800 |
| H | 4.13525500 | -1.06649300 | 3.58839100 |
| C | 10.80710600 | -3.08842700 | 1.86462000 |
| C | 11.48993700 | -4.44337700 | 1.64937000 |
| C | 11.81606100 | -2.04235900 | 2.37443000 |
| H | 10.46240900 | -2.76390800 | 0.87354600 |
| H | 10.77027000 | -5.20066700 | 1.30859900 |
| H | 12.26014400 | -4.34605400 | 0.86894800 |
| H | 11.99020400 | -4.80374800 | 2.56258000 |
| H | 11.36365500 | -1.04450500 | 2.46841700 |
| H | 12.20708200 | -2.33238500 | 3.36335400 |
| H | 12.66695000 | -1.96135500 | 1.67918000 |
| C | 6.51278600 | 1.26444000 | -1.48980400 |
| C | 5.11163200 | 1.10733900 | -2.09018100 |
| C | 6.83406600 | 2.75389000 | -1.26592000 |
| H | 6.48653900 | 0.75765800 | -0.51677500 |
| H | 4.91862900 | 0.06475500 | -2.37045600 |
| H | 4.35747300 | 1.39842300 | -1.34653100 |
| H | 4.96794600 | 1.74026500 | -2.98127900 |
| H | 7.81180200 | 2.90520900 | -0.78425900 |
| H | 6.85006300 | 3.29828200 | -2.22462500 |
| H | 6.06619600 | 3.21623300 | -0.62523400 |
| C | 10.88058700 | -1.41363900 | -1.88696800 |
| C | 11.87738000 | -0.38428500 | -1.32114800 |
| C | 11.59646200 | -2.40244600 | -2.81261300 |
| H | 10.49968800 | -2.00769600 | -1.04544000 |
| H | 12.71061400 | -0.89851900 | -0.81573600 |
| H | 12.29716500 | 0.23356800 | -2.13170900 |
| H | 11.40818500 | 0.28917600 | -0.58976500 |
| H | 10.89021100 | -3.12290400 | -3.24770300 |
| H | 12.13591600 | -1.88893800 | -3.62490700 |
| H | 12.33793900 | -2.97496700 | -2.23472300 |
| Cl | 9.50423800 | -4.73688300 | -1.27238700 |
| C | 3.92010200 | -7.01055600 | -0.71433400 |
| H | 2.94010700 | -6.79929900 | -1.17188500 |
| H | 4.43678800 | -7.72720000 | -1.37496400 |
| H | 3.74813300 | -7.50431400 | 0.25264200 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-

CPCM(toluene)
HF = -4361.570451
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4359.153845

**ii-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.719698 (Hartree/Particle)
Thermal correction to Energy= 0.768827
Thermal correction to Enthalpy= 0.769772
Thermal correction to Gibbs Free Energy= 0.634276
Sum of electronic and zero-point Energies= -4358.621671
Sum of electronic and thermal Energies= -4358.572542
Sum of electronic and thermal Enthalpies= -4358.571598
Sum of electronic and thermal Free Energies= -4358.707094

| | | | |
|---|---|---|---|
| Ni | 7.67693500 | -2.94078800 | -1.16590900 |
| C | 8.33115700 | -1.51554500 | 0.15396300 |
| C | 9.06163300 | 0.56220800 | 0.69586000 |
| C | 8.93632600 | -0.14209400 | 1.84914800 |
| N | 8.48667700 | -1.41208600 | 1.49758900 |
| N | 8.69757200 | -0.29848100 | -0.33082100 |
| H | 9.14475200 | 0.12896600 | 2.87824900 |
| H | 9.38298500 | 1.58179800 | 0.51105100 |
| C | 8.39068900 | -2.48966200 | 2.45287200 |
| C | 9.46343300 | -3.41063200 | 2.51454900 |
| C | 7.26881400 | -2.55596300 | 3.30369600 |
| C | 9.39626700 | -4.40814200 | 3.49647600 |
| C | 7.25189600 | -3.58398600 | 4.25970800 |
| C | 8.30369200 | -4.49223200 | 4.36142900 |
| H | 10.20021500 | -5.14042300 | 3.57741700 |
| H | 6.39843300 | -3.67530700 | 4.93282600 |
| H | 8.26873800 | -5.28204800 | 5.11608100 |
| C | 8.82180100 | 0.01285000 | -1.73683900 |
| C | 7.74114200 | 0.63677300 | -2.39309400 |
| C | 10.03603700 | -0.31202100 | -2.38720800 |
| C | 7.89802700 | 0.92695600 | -3.75676300 |
| C | 10.13404300 | -0.00089900 | -3.74999100 |
| C | 9.07785100 | 0.60997900 | -4.42735300 |
| H | 7.08305200 | 1.40674400 | -4.30055800 |
| H | 11.04959800 | -0.23889500 | -4.29263500 |
| H | 9.17749800 | 0.84101700 | -5.49104600 |
| C | 6.55637700 | -6.36895200 | 0.96590500 |
| C | 5.55655500 | -6.90213500 | 0.13940800 |
| C | 5.35182300 | -6.31726100 | -1.12151700 |
| C | 6.10330900 | -5.21648700 | -1.54486700 |
| C | 7.03836800 | -4.69807100 | -0.66018400 |
| C | 7.32634700 | -5.26901400 | 0.56342200 |
| H | 6.75106300 | -6.81288200 | 1.94640400 |
| H | 4.58051200 | -6.71516600 | -1.78732400 |
| H | 5.90830400 | -4.75870400 | -2.51543800 |
| H | 8.09782100 | -4.87010500 | 1.21500000 |
| O | 5.86603200 | -2.19355400 | -1.37110300 |
| S | 4.72347900 | -2.16089300 | -0.35203900 |
| O | 4.71628200 | -3.30137400 | 0.56662800 |
| O | 4.50676200 | -0.82198000 | 0.21413700 |
| C | 3.26166000 | -2.47756600 | -1.48227100 |
| F | 3.12691200 | -1.51349300 | -2.39238700 |
| F | 2.15313100 | -2.53114300 | -0.74607000 |
| F | 3.41707800 | -3.64258300 | -2.11354600 |
| C | 6.12580600 | -1.54965700 | 3.22505300 |
| C | 6.35119900 | -0.37859800 | 4.20133000 |
| C | 4.74874100 | -2.17891900 | 3.48502900 |
| H | 6.10382000 | -1.14672100 | 2.20197500 |
| H | 7.29050200 | 0.15845800 | 4.01049900 |
| H | 5.52748000 | 0.34840400 | 4.11871400 |
| H | 6.37985300 | -0.74365000 | 5.24135300 |
| H | 4.59938900 | -3.07535900 | 2.87175400 |
| H | 4.61059800 | -2.43549700 | 4.54821400 |
| H | 3.96341400 | -1.45751400 | 3.21187100 |
| C | 10.63710800 | -3.33915800 | 1.54040100 |
| C | 11.25242600 | -4.70604600 | 1.21706200 |
| C | 11.71482900 | -2.35533800 | 2.02985600 |
| H | 10.24051300 | -2.96219700 | 0.58837300 |
| H | 10.48714300 | -5.42165100 | 0.88179100 |
| H | 11.98090700 | -4.59453900 | 0.39935200 |
| H | 11.78603100 | -5.13885900 | 2.07864400 |
| H | 11.30724300 | -1.34685200 | 2.19118500 |
| H | 12.15471800 | -2.70094700 | 2.97975200 |
| H | 12.52475200 | -2.27420400 | 1.28704400 |
| C | 6.47310400 | 1.02761700 | -1.65010700 |
| C | 5.20421800 | 0.83721800 | -2.48841600 |
| C | 6.57237200 | 2.47463900 | -1.13302100 |
| H | 6.37406000 | 0.36452800 | -0.78212600 |
| H | 5.17255800 | -0.16833500 | -2.92741600 |
| H | 4.32005600 | 0.94397200 | -1.84453400 |
| H | 5.12714100 | 1.58049800 | -3.29885500 |
| H | 7.44198800 | 2.61842000 | -0.47405100 |
| H | 6.66585000 | 3.18494900 | -1.97134300 |
| H | 5.66822600 | 2.73734600 | -0.56072900 |
| C | 11.21808800 | -0.91898200 | -1.63762100 |
| C | 12.08838100 | 0.18543700 | -1.00703900 |
| C | 12.08715300 | -1.84140600 | -2.50269300 |
| H | 10.81058300 | -1.53564800 | -0.82488500 |
| H | 12.91694800 | -0.26086900 | -0.43390500 |
| H | 12.52178600 | 0.82903600 | -1.78997300 |
| H | 11.51560600 | 0.82652800 | -0.32267400 |
| H | 11.47671700 | -2.58795300 | -3.02838200 |
| H | 12.67232100 | -1.27534700 | -3.24544900 |
| H | 12.80574700 | -2.37816600 | -1.86333900 |
| Cl | 9.40803000 | -4.02881700 | -1.90840600 |
| C | 4.70216500 | -8.05814500 | 0.59837500 |
| H | 3.75340500 | -7.69252300 | 1.02854000 |
| H | 4.44327000 | -8.72733500 | -0.23672900 |
| H | 5.20674100 | -8.65337600 | 1.37429200 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4361.6116044
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4359.1929579

**ii'-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.829900 (Hartree/Particle)
Thermal correction to Energy= 0.885221
Thermal correction to Enthalpy= 0.886166
Thermal correction to Gibbs Free Energy= 0.737324
Sum of electronic and zero-point Energies= -4515.640975
Sum of electronic and thermal Energies= -4515.585654
Sum of electronic and thermal Enthalpies= -4515.584709
Sum of electronic and thermal Free Energies= -4515.733551

| | | | |
|---|---|---|---|
| C | 0.85487700 | 0.69509700 | 0.90975300 |
| C | 2.67498900 | 1.71047500 | -0.00967300 |
| C | 3.00166600 | 1.34617100 | 1.25540900 |
| N | 1.87766000 | 0.73487800 | 1.79990200 |
| N | 1.35552700 | 1.31925400 | -0.19955300 |
| H | 3.91608300 | 1.47194400 | 1.82613800 |
| H | 3.24970100 | 2.20994600 | -0.78229600 |
| C | 1.85513000 | 0.34552600 | 3.19039300 |
| C | 1.26038400 | 1.22953500 | 4.11623500 |
| C | 2.54329800 | -0.81920300 | 3.57413600 |
| C | 1.38461700 | 0.91286000 | 5.47405200 |
| C | 2.67229000 | -1.06528900 | 4.94729100 |
| C | 2.10204200 | -0.21026800 | 5.88604500 |
| H | 0.92003400 | 1.55668800 | 6.22173100 |
| H | 3.20051800 | -1.95977500 | 5.28309600 |
| H | 2.19573800 | -0.43221900 | 6.95207600 |
| C | 0.59833100 | 1.61880500 | -1.38977500 |
| C | -0.11895400 | 2.83871100 | -1.43814400 |

| | | | |
|---|---|---|---|
| C | 0.61576300 | 0.69927600 | -2.45969000 |
| C | -0.89700300 | 3.08189000 | -2.57834800 |
| C | -0.17484700 | 0.99956000 | -3.58032900 |
| C | -0.93545500 | 2.16635200 | -3.63186300 |
| H | -1.47771500 | 4.00246600 | -2.64978200 |
| H | -0.19467500 | 0.30834400 | -4.42420500 |
| H | -1.55330400 | 2.37456800 | -4.50896000 |
| C | -4.28228700 | -2.89515400 | -0.17678600 |
| C | -4.46012700 | -2.57860300 | -1.53461700 |
| C | -3.53114000 | -1.71798000 | -2.13935100 |
| C | -2.46253400 | -1.17835300 | -1.41076800 |
| C | -2.34277900 | -1.48871200 | -0.05904600 |
| C | -3.21815600 | -2.36707200 | 0.56518700 |
| H | -4.98181500 | -3.57793000 | 0.31514000 |
| H | -3.63375500 | -1.46202100 | -3.19816400 |
| H | -1.75432300 | -0.51070400 | -1.90602900 |
| H | -3.07608400 | -2.64230700 | 1.60659400 |
| C | -2.18312100 | 1.55252000 | 1.17607200 |
| H | -1.63417400 | 1.68262500 | 2.10785200 |
| H | -1.78480000 | 2.00558400 | 0.26939400 |
| C | -3.46310900 | 1.08831200 | 1.19320500 |
| Ni | -0.89207500 | -0.48476200 | 0.81828800 |
| C | 1.52440400 | -0.52420800 | -2.44772600 |
| C | 2.86451200 | -0.17982800 | -3.12636800 |
| C | 0.89818800 | -1.76876100 | -3.08971000 |
| H | 1.72676000 | -0.77878300 | -1.39894800 |
| H | 3.36194200 | 0.67416000 | -2.64250300 |
| H | 3.54999800 | -1.04120400 | -3.08070900 |
| H | 2.71071600 | 0.07885700 | -4.18711500 |
| H | -0.05849700 | -2.02563100 | -2.61565000 |
| H | 0.73928300 | -1.64194900 | -4.17294200 |
| H | 1.57195200 | -2.62907800 | -2.95591900 |
| C | 0.00436900 | 3.88992000 | -0.33554900 |
| C | -1.25996000 | 4.73783100 | -0.13001700 |
| C | 1.20480400 | 4.81720300 | -0.61303100 |
| H | 0.20663300 | 3.36307200 | 0.60946000 |
| H | -2.16138300 | 4.12123000 | -0.00483500 |
| H | -1.14635600 | 5.35717300 | 0.77319600 |
| H | -1.43111400 | 5.42444500 | -0.97432200 |
| H | 2.14622400 | 4.25965100 | -0.70720700 |
| H | 1.04878400 | 5.37810300 | -1.54883300 |
| H | 1.32396700 | 5.54343100 | 0.20691200 |
| C | 3.11579600 | -1.79506500 | 2.55472600 |
| C | 2.62882500 | -3.23019900 | 2.81306500 |
| C | 4.65126300 | -1.72425700 | 2.50791600 |
| H | 2.72864300 | -1.50985300 | 1.56609100 |
| H | 1.53460100 | -3.25579800 | 2.89552800 |
| H | 2.93812600 | -3.88693200 | 1.98401300 |
| H | 3.05553600 | -3.64190800 | 3.74250000 |
| H | 5.00679300 | -0.71239200 | 2.25629000 |
| H | 5.08866600 | -1.99918400 | 3.48205300 |
| H | 5.04841700 | -2.42070200 | 1.75139400 |
| C | 0.57034100 | 2.51310200 | 3.66600300 |
| C | 1.57040900 | 3.68212500 | 3.60014700 |
| C | -0.65503900 | 2.87872000 | 4.51367400 |
| H | 0.20764800 | 2.34498200 | 2.64274700 |
| H | 2.41894200 | 3.45605200 | 2.93686400 |
| H | 1.07704000 | 4.59213200 | 3.21986300 |
| H | 1.97266500 | 3.90419300 | 4.60213300 |
| H | -1.31949000 | 2.01202500 | 4.63476400 |
| H | -0.36575500 | 3.22712600 | 5.51842200 |
| H | -1.21141500 | 3.69931100 | 4.03261900 |
| S | -1.31720400 | -1.32503100 | 4.14087900 |
| O | -0.09862500 | -2.09755700 | 4.39384800 |
| O | -1.67293100 | -0.24527200 | 5.07648700 |
| O | -1.54146500 | -0.93443700 | 2.70217800 |
| C | -2.68163500 | -2.58376100 | 4.40524300 |
| F | -3.88768900 | -2.06997400 | 4.13212200 |
| F | -2.49761900 | -3.65084200 | 3.61686700 |
| F | -2.67458500 | -2.99078700 | 5.67356300 |
| Cl | 0.27472200 | -2.31984800 | 0.31179900 |
| C | -5.62792700 | -3.13911400 | -2.30988800 |
| H | -5.82905500 | -4.18616000 | -2.03410400 |
| H | -6.54959100 | -2.56776300 | -2.10228800 |
| H | -5.45245900 | -3.09757900 | -3.39540500 |
| C | -4.11556800 | 0.58580500 | 2.44049400 |
| H | -3.46183600 | 0.63946700 | 3.31768600 |
| H | -5.04439600 | 1.15231100 | 2.62641700 |
| H | -4.40821000 | -0.46683400 | 2.29836500 |
| C | -4.31287300 | 1.08710700 | -0.04031400 |
| H | -5.16732300 | 1.77031200 | 0.10940200 |
| H | -3.75871300 | 1.40140500 | -0.93442100 |
| H | -4.73196800 | 0.08401000 | -0.21692100 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4518.8765897
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4516.2861609

**TS-A-branched-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.830791 (Hartree/Particle)
Thermal correction to Energy= 0.884619
Thermal correction to Enthalpy= 0.885563
Thermal correction to Gibbs Free Energy= 0.743413
Sum of electronic and zero-point Energies= -4515.634411
Sum of electronic and thermal Energies= -4515.580583
Sum of electronic and thermal Enthalpies= -4515.579639
Sum of electronic and thermal Free Energies= -4515.721789

| | | | |
|---|---|---|---|
| C | 0.66674100 | 0.53464800 | 0.84878100 |
| C | 2.34099800 | 1.60985700 | -0.24721200 |
| C | 2.79238900 | 1.29436100 | 0.99184800 |
| N | 1.74727300 | 0.65446200 | 1.65495700 |
| N | 1.02880200 | 1.15672500 | -0.31401600 |
| H | 3.74652900 | 1.47169500 | 1.47801700 |
| H | 2.82044900 | 2.11683200 | -1.07788400 |
| C | 1.87240100 | 0.37584500 | 3.07057400 |
| C | 1.40355000 | 1.35178000 | 3.97779000 |
| C | 2.61118400 | -0.74882000 | 3.47382200 |
| C | 1.76000600 | 1.19967700 | 5.32287400 |
| C | 2.95922800 | -0.83920800 | 4.82840700 |
| C | 2.55423400 | 0.13112800 | 5.73965100 |
| H | 1.41645600 | 1.93050100 | 6.05670500 |
| H | 3.53415400 | -1.70048600 | 5.17536800 |
| H | 2.83026100 | 0.03892600 | 6.79311700 |
| C | 0.13477200 | 1.45236000 | -1.40935800 |
| C | -0.64279200 | 2.63397800 | -1.32813900 |
| C | 0.09275600 | 0.59155900 | -2.52648500 |
| C | -1.55490800 | 2.88060100 | -2.36277300 |
| C | -0.84009500 | 0.88847900 | -3.53342500 |
| C | -1.66835400 | 2.00530600 | -3.44422700 |
| H | -2.18211900 | 3.77244100 | -2.32854700 |
| H | -0.91105400 | 0.23638800 | -4.40522400 |
| H | -2.39372900 | 2.21031200 | -4.23548600 |
| C | -3.63664600 | -3.84579000 | 0.11872800 |
| C | -3.76035700 | -3.78394000 | -1.28022200 |
| C | -3.27129300 | -2.64222200 | -1.93546000 |
| C | -2.68958400 | -1.59513500 | -1.21617100 |
| C | -2.57560900 | -1.67617700 | 0.17384300 |
| C | -3.05054200 | -2.80493300 | 0.84221300 |
| H | -3.99342000 | -4.73110200 | 0.65356300 |
| H | -3.33730200 | -2.57063300 | -3.02513000 |
| H | -2.30254400 | -0.72960600 | -1.75765300 |
| H | -2.94138200 | -2.88818600 | 1.92048400 |
| C | -2.10549800 | 0.93828400 | 1.50187700 |
| H | -1.87714500 | 0.94690300 | 2.56966000 |
| H | -1.76577800 | 1.79516300 | 0.92620400 |
| C | -3.30410100 | 0.31828900 | 1.08111400 |
| Ni | -0.96561500 | -0.65325300 | 0.89541800 |

| | | | |
|---|---|---|---|
| C | 1.09033900 | -0.54389400 | -2.70787800 |
| C | 2.27640400 | -0.05024800 | -3.55931900 |
| C | 0.47594400 | -1.81238900 | -3.31329300 |
| H | 1.46702600 | -0.81910000 | -1.71461400 |
| H | 2.76481000 | 0.82954400 | -3.11268200 |
| H | 3.03357600 | -0.84467400 | -3.65727900 |
| H | 1.94390400 | 0.23129900 | -4.57232000 |
| H | -0.37670100 | -2.16140600 | -2.71595900 |
| H | 0.15088400 | -1.66019500 | -4.35567100 |
| H | 1.22664300 | -2.61783600 | -3.31872400 |
| C | -0.43524100 | 3.66318100 | -0.21903800 |
| C | -1.71655700 | 4.39697500 | 0.20517000 |
| C | 0.63866300 | 4.68510800 | -0.64204200 |
| H | -0.04764100 | 3.13801500 | 0.66547700 |
| H | -2.54116500 | 3.70349800 | 0.42788300 |
| H | -1.52141400 | 4.99209200 | 1.11069800 |
| H | -2.06488700 | 5.09323700 | -0.57366400 |
| H | 1.59095100 | 4.19731400 | -0.89288200 |
| H | 0.30475200 | 5.25181700 | -1.52619400 |
| H | 0.82930300 | 5.39998400 | 0.17415900 |
| C | 2.97392600 | -1.86404100 | 2.50634700 |
| C | 2.28960800 | -3.17520200 | 2.93179700 |
| C | 4.49303200 | -2.03130800 | 2.35381100 |
| H | 2.55964100 | -1.60856800 | 1.52174700 |
| H | 1.21012600 | -3.02180100 | 3.06081800 |
| H | 2.44058300 | -3.94683500 | 2.16039100 |
| H | 2.70172200 | -3.55266400 | 3.88246200 |
| H | 4.96770600 | -1.10079600 | 2.00139400 |
| H | 4.96818100 | -2.30875900 | 3.30934600 |
| H | 4.72094500 | -2.82603300 | 1.62491900 |
| C | 0.57601900 | 2.54851100 | 3.51945000 |
| C | 1.46602300 | 3.76430500 | 3.20488000 |
| C | -0.53786500 | 2.91987300 | 4.50892400 |
| H | 0.07841700 | 2.25834700 | 2.58411900 |
| H | 2.21934400 | 3.53208300 | 2.43745800 |
| H | 0.85599700 | 4.60522200 | 2.83538300 |
| H | 1.99597100 | 4.10005500 | 4.11111000 |
| H | -1.12597900 | 2.03453900 | 4.79005600 |
| H | -0.13245000 | 3.37497500 | 5.42701300 |
| H | -1.21205300 | 3.66155900 | 4.05028200 |
| S | -1.14322100 | -1.32006500 | 4.27862400 |
| O | 0.06844600 | -1.53144700 | 5.07079100 |
| O | -1.99607000 | -0.16364600 | 4.62705200 |
| O | -0.96917300 | -1.51000800 | 2.79375800 |
| C | -2.17767700 | -2.82221000 | 4.72470200 |
| F | -3.40903100 | -2.75135900 | 4.19077500 |
| F | -1.59579200 | -3.93503400 | 4.27567900 |
| F | -2.30451700 | -2.90415300 | 6.04757700 |
| Cl | 0.33726700 | -2.34335900 | 0.09313900 |
| C | -4.42040700 | -4.90297000 | -2.04620800 |
| H | -4.13368700 | -4.89270200 | -3.10858000 |
| H | -4.15667600 | -5.88644700 | -1.62668500 |
| H | -5.52031100 | -4.81673200 | -1.99983900 |
| C | -4.21382900 | -0.28600500 | 2.11243800 |
| H | -3.65800700 | -0.76042200 | 2.92350300 |
| H | -4.78030800 | 0.55430100 | 2.55420300 |
| H | -4.93013800 | -0.99104700 | 1.67262200 |
| C | -3.97576300 | 0.85953400 | -0.15352300 |
| H | -4.54031100 | 1.75378800 | 0.16894700 |
| H | -3.25661800 | 1.18207000 | -0.91667100 |
| H | -4.68636700 | 0.14694500 | -0.59006400 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4518.8702339
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4516.2810976

**iii-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.834068 (Hartree/Particle)
Thermal correction to Energy= 0.887499
Thermal correction to Enthalpy= 0.888444
Thermal correction to Gibbs Free Energy= 0.748566
Sum of electronic and zero-point Energies= -4515.685142
Sum of electronic and thermal Energies= -4515.631711
Sum of electronic and thermal Enthalpies= -4515.630766
Sum of electronic and thermal Free Energies= -4515.770644

| | | | |
|---|---|---|---|
| C | 1.06776800 | 0.91461700 | -0.47916500 |
| C | 2.70752600 | 2.08696500 | -1.50779700 |
| C | 3.11547900 | 1.83283400 | -0.23934500 |
| N | 2.10134300 | 1.10754000 | 0.37481900 |
| N | 1.44409300 | 1.52280300 | -1.63870900 |
| H | 4.02573800 | 2.09359800 | 0.29044500 |
| H | 3.19204300 | 2.60835500 | -2.32585000 |
| C | 2.24302400 | 0.64816400 | 1.73957600 |
| C | 1.68298100 | 1.42568200 | 2.77103600 |
| C | 3.03336600 | -0.49263500 | 1.97354700 |
| C | 1.95790400 | 1.03565900 | 4.08735500 |
| C | 3.30734900 | -0.81435500 | 3.30900100 |
| C | 2.77915000 | -0.05950500 | 4.35303300 |
| H | 1.52535700 | 1.59805400 | 4.91600200 |
| H | 3.91597500 | -1.69186700 | 3.53366200 |
| H | 2.98689900 | -0.34228800 | 5.38792800 |
| C | 0.66541200 | 1.58408700 | -2.85301100 |
| C | -0.07503200 | 2.75817300 | -3.11842900 |
| C | 0.70622300 | 0.48219100 | -3.73486400 |
| C | -0.86673600 | 2.76856400 | -4.27570700 |
| C | -0.09859000 | 0.55314600 | -4.88127300 |
| C | -0.89022500 | 1.67207900 | -5.13870900 |
| H | -1.46606800 | 3.64917000 | -4.51179200 |
| H | -0.10443900 | -0.27939000 | -5.58564400 |
| H | -1.51975700 | 1.69813400 | -6.03150400 |
| C | -3.18540600 | -2.73951100 | -1.11294000 |
| C | -2.71535300 | -2.76243800 | -2.43256300 |
| C | -2.39864700 | -1.53491100 | -3.03423600 |
| C | -2.50531700 | -0.33904700 | -2.33072300 |
| C | -2.97326000 | -0.31334500 | -0.99621500 |
| C | -3.31858400 | -1.54324100 | -0.40838000 |
| H | -3.42760800 | -3.67859700 | -0.60931200 |
| H | -2.03614900 | -1.51281500 | -4.06402800 |
| H | -2.21486100 | 0.58811900 | -2.82739200 |
| H | -3.67643700 | -1.57774500 | 0.61739500 |
| C | -1.62420000 | 1.54040000 | -0.12936400 |
| H | -1.37005000 | 2.02494200 | 0.81797100 |
| H | -1.30736000 | 2.12491300 | -0.99479700 |
| C | -3.06816100 | 1.03625800 | -0.24655700 |
| Ni | -0.52766500 | -0.16840000 | -0.17557500 |
| C | 1.66565800 | -0.68146500 | -3.51212800 |
| C | 3.03785600 | -0.34626700 | -4.12923500 |
| C | 1.15141300 | -2.02512700 | -4.03904600 |
| H | 1.79477900 | -0.80655900 | -2.42918200 |
| H | 3.45974900 | 0.58285500 | -3.71821800 |
| H | 3.75462400 | -1.15866500 | -3.92884000 |
| H | 2.95569900 | -0.22396100 | -5.22194400 |
| H | 0.17562100 | -2.26954300 | -3.60088200 |
| H | 1.07282500 | -2.04049100 | -5.13844500 |
| H | 1.85143600 | -2.82313100 | -3.74830100 |
| C | 0.04436800 | 4.00750400 | -2.24730600 |
| C | -1.28043100 | 4.75752100 | -2.04547000 |
| C | 1.09916400 | 4.96142300 | -2.84318100 |
| H | 0.40088000 | 3.69622400 | -1.25283400 |
| H | -2.07190800 | 4.10024500 | -1.66199600 |
| H | -1.13880900 | 5.57581900 | -1.32262900 |
| H | -1.64057700 | 5.21059300 | -2.98236600 |
| H | 2.07731400 | 4.47468900 | -2.96414600 |
| H | 0.77865100 | 5.31570000 | -3.83624800 |
| H | 1.23458500 | 5.84054400 | -2.19323000 |
| C | 3.56226800 | -1.36213600 | 0.83931300 |
| C | 3.29643800 | -2.85480100 | 1.08980600 |

| | | | |
|---|---|---|---|
| C | 5.05571400 | -1.09859300 | 0.58084700 |
| H | 3.00263600 | -1.09922200 | -0.07012300 |
| H | 2.23783800 | -3.01984700 | 1.32688000 |
| H | 3.54998000 | -3.43441900 | 0.18762900 |
| H | 3.91166700 | -3.24381500 | 1.91775500 |
| H | 5.25089600 | -0.04474500 | 0.32819200 |
| H | 5.65568300 | -1.34571600 | 1.47235000 |
| H | 5.41912400 | -1.71950500 | -0.25429000 |
| C | 0.85649800 | 2.67144400 | 2.48262600 |
| C | 1.71595300 | 3.93903300 | 2.63311500 |
| C | -0.41924900 | 2.74804700 | 3.33393100 |
| H | 0.53730000 | 2.62131200 | 1.43253200 |
| H | 2.59466400 | 3.91146300 | 1.96904900 |
| H | 1.12923000 | 4.83921800 | 2.38624000 |
| H | 2.07969900 | 4.04232100 | 3.66851000 |
| H | -0.97782600 | 1.80399800 | 3.28582000 |
| H | -0.18983200 | 2.94916600 | 4.39252600 |
| H | -1.06204800 | 3.56919400 | 2.97702200 |
| S | -0.63350600 | -1.24660500 | 2.99165900 |
| O | 0.58061900 | -2.05605200 | 2.88587600 |
| O | -0.91393100 | -0.54755300 | 4.25172100 |
| O | -0.91395800 | -0.33981200 | 1.80058000 |
| C | -2.01156700 | -2.51596400 | 2.88335700 |
| F | -3.21641800 | -1.92351100 | 2.91643300 |
| F | -1.92806700 | -3.23119000 | 1.76130200 |
| F | -1.92625500 | -3.34361300 | 3.92432700 |
| Cl | 0.28849300 | -2.19514900 | -0.68578600 |
| C | -2.48478000 | -4.06294300 | -3.15459600 |
| H | -1.47902000 | -4.44647800 | -2.90964100 |
| H | -3.21182600 | -4.83260100 | -2.85391500 |
| H | -2.53521400 | -3.93933100 | -4.24701400 |
| C | -3.71389100 | 0.90614000 | 1.14066900 |
| H | -3.13446900 | 0.25587100 | 1.80233500 |
| H | -3.76549700 | 1.89999400 | 1.61153500 |
| H | -4.74012300 | 0.51510500 | 1.06133300 |
| C | -3.90487300 | 2.03874000 | -1.07513600 |
| H | -3.95138400 | 3.01352500 | -0.56411400 |
| H | -3.49055200 | 2.20084700 | -2.08020000 |
| H | -4.93384000 | 1.66018900 | -1.18766500 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4518.9195341
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4516.336073

**iv-OTf-1**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.922922 (Hartree/Particle)
Thermal correction to Energy= 0.980432
Thermal correction to Enthalpy= 0.981377
Thermal correction to Gibbs Free Energy= 0.828168
Sum of electronic and zero-point Energies= -4286.960555
Sum of electronic and thermal Energies= -4286.903045
Sum of electronic and thermal Enthalpies= -4286.902101
Sum of electronic and thermal Free Energies= -4287.055309

| | | | |
|---|---|---|---|
| Ni | -1.10810300 | -0.01201800 | -0.03766600 |
| N | 0.92145700 | 1.61494000 | 1.48287900 |
| N | -0.60862800 | 1.07895700 | 2.88927500 |
| C | 2.74293900 | 1.07700700 | -0.05715500 |
| C | 3.45790400 | 1.39570200 | -1.22201500 |
| C | 3.05814000 | 2.44837100 | -2.04112100 |
| C | 1.92901400 | 3.20662600 | -1.72186000 |
| C | 1.18561400 | 2.94665200 | -0.56324300 |
| C | 1.62829300 | 1.87876300 | 0.25623400 |
| C | 1.37121300 | 2.03806900 | 2.72689900 |
| C | 0.40340600 | 1.69988200 | 3.61445900 |
| C | -0.29221200 | 1.00586100 | 1.56688500 |
| C | -1.88433000 | 0.77247000 | 3.49584900 |
| C | -2.10747300 | -0.51249600 | 4.03039100 |
| C | -3.33569900 | -0.73409700 | 4.66877400 |
| C | -4.29233100 | 0.27622100 | 4.76255900 |
| C | -4.04175600 | 1.53800100 | 4.22631700 |
| C | -2.82679600 | 1.81961400 | 3.58673600 |
| H | 4.32796900 | 0.79787600 | -1.49833900 |
| H | 3.62229200 | 2.67552400 | -2.94915500 |
| H | 1.62693600 | 4.01244800 | -2.39074600 |
| H | 2.31654300 | 2.55390700 | 2.85755400 |
| H | 0.33194000 | 1.85219300 | 4.68605900 |
| H | -3.55443400 | -1.71564500 | 5.08990900 |
| H | -5.24663900 | 0.07574100 | 5.25627000 |
| H | -4.80087200 | 2.31774000 | 4.30860000 |
| C | -1.76551600 | -0.83781500 | -1.73747300 |
| H | -2.83628200 | -0.74954500 | -1.95030300 |
| H | -1.53795100 | -1.89870800 | -1.57191200 |
| C | -1.45685300 | -0.96581600 | -4.18609900 |
| C | -2.23061300 | -0.34766400 | -5.17983800 |
| C | -1.15250900 | -2.32951400 | -4.37082000 |
| C | -2.67204700 | -1.05312900 | -6.30649200 |
| H | -2.50502300 | 0.70405500 | -5.09498100 |
| C | -1.59293400 | -3.03025400 | -5.49168400 |
| H | -0.56788700 | -2.86150800 | -3.62063600 |
| C | -2.36377200 | -2.40630500 | -6.48798600 |
| H | -3.27057400 | -0.53182800 | -7.05966800 |
| H | -1.33444400 | -4.08860400 | -5.59582400 |
| C | -0.96910300 | -0.23137200 | -2.92216900 |
| C | -0.04169400 | 3.78589800 | -0.19767200 |
| C | -0.64142400 | 4.56652900 | -1.37501900 |
| C | 0.25839900 | 4.76508900 | 0.95498000 |
| H | -0.81718300 | 3.08360400 | 0.15306700 |
| H | -0.83900700 | 3.92734700 | -2.24645000 |
| H | -1.59526800 | 5.02119300 | -1.06573100 |
| H | 0.02072700 | 5.38626300 | -1.69724200 |
| H | 0.60806600 | 4.25639000 | 1.86196500 |
| H | 1.03175100 | 5.48854600 | 0.64970400 |
| H | -0.64996500 | 5.32894700 | 1.22062000 |
| C | 3.15669000 | -0.10238300 | 0.81440700 |
| C | 4.30681500 | 0.27363200 | 1.76482400 |
| C | 3.52777600 | -1.33424800 | -0.02200700 |
| H | 2.28336800 | -0.39086000 | 1.41546300 |
| H | 4.04219800 | 1.10672300 | 2.43253500 |
| H | 4.57828600 | -0.58929000 | 2.39382800 |
| H | 5.20154200 | 0.57287000 | 1.19399400 |
| H | 2.77625500 | -1.51559500 | -0.79825200 |
| H | 4.51369600 | -1.22546500 | -0.50303000 |
| H | 3.55843700 | -2.22427900 | 0.62334300 |
| C | -1.05466100 | -1.60915100 | 3.92886500 |
| C | -1.63806200 | -3.02616600 | 3.97238100 |
| C | 0.03000200 | -1.46709000 | 5.01345700 |
| H | -0.55865300 | -1.48656000 | 2.95661700 |
| H | -2.47373100 | -3.14512400 | 3.26989500 |
| H | -0.86177500 | -3.74560100 | 3.67818800 |
| H | -1.98557500 | -3.28747600 | 4.98556600 |
| H | 0.54281000 | -0.49679600 | 4.97094900 |
| H | -0.40997500 | -1.57608100 | 6.01855500 |
| H | 0.79172200 | -2.25139800 | 4.88162800 |
| C | -2.52388000 | 3.22875900 | 3.08336800 |
| C | -2.02696900 | 4.12120700 | 4.23691400 |
| C | -3.70911700 | 3.89835100 | 2.37464400 |
| H | -1.71212400 | 3.15478500 | 2.34609800 |
| H | -1.14287100 | 3.69952800 | 4.73564700 |
| H | -1.75831000 | 5.12207500 | 3.86170300 |
| H | -2.81593600 | 4.24196500 | 4.99718100 |
| H | -4.11572300 | 3.25503800 | 1.58469100 |
| H | -4.52431200 | 4.13797400 | 3.07613600 |
| H | -3.38359200 | 4.84761500 | 1.91914500 |
| C | -1.25861700 | 1.27682700 | -2.99567600 |
| H | -0.76675500 | 1.74551900 | -3.86238000 |
| H | -2.33656300 | 1.48831800 | -3.04796500 |
| H | -0.86876000 | 1.77713200 | -2.09823900 |

| | | | |
|---|---|---|---|
| C | 0.55479900 | -0.42775400 | -2.77201600 |
| H | 0.95127900 | 0.13508800 | -1.91576600 |
| H | 0.82061500 | -1.47982200 | -2.60926400 |
| H | 1.07721500 | -0.07112300 | -3.67345200 |
| C | -2.83404100 | -3.17767600 | -7.69654500 |
| H | -3.45874000 | -4.03772600 | -7.40189300 |
| H | -3.42618500 | -2.54761200 | -8.37693900 |
| H | -1.98167400 | -3.58375100 | -8.26700900 |
| C | -2.98310200 | 0.11034100 | 0.24190100 |
| C | -3.58463400 | -0.89523800 | 1.00311400 |
| C | -3.72708500 | 1.21285100 | -0.19149200 |
| C | -4.93028400 | -0.77171300 | 1.36884400 |
| H | -3.00662600 | -1.77236100 | 1.30153800 |
| C | -5.07922500 | 1.31834100 | 0.16118000 |
| H | -3.26439800 | 1.98739500 | -0.80826200 |
| C | -5.68187700 | 0.33040000 | 0.94664900 |
| H | -5.39235800 | -1.54860500 | 1.98373900 |
| H | -5.66080800 | 2.17945400 | -0.18016900 |
| H | -6.73581100 | 0.41597600 | 1.22318900 |
| S | 0.17528700 | -2.89462900 | 0.74409600 |
| O | 0.28983400 | -1.49681200 | 0.16901300 |
| O | 1.17946800 | -3.15882600 | 1.78402600 |
| O | -1.21489500 | -3.30443700 | 0.99292800 |
| C | 0.67396500 | -4.00425600 | -0.69125600 |
| F | -0.29800500 | -4.02190700 | -1.61189400 |
| F | 1.79793100 | -3.59807300 | -1.28486600 |
| F | 0.85257700 | -5.24309700 | -0.24062000 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4290.3437999
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4287.6679443

**TS-iv-H16-1-OTf**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.922579 (Hartree/Particle)
Thermal correction to Energy= 0.979564
Thermal correction to Enthalpy= 0.980508
Thermal correction to Gibbs Free Energy= 0.827991
Sum of electronic and zero-point Energies= -4286.957830
Sum of electronic and thermal Energies= -4286.900844
Sum of electronic and thermal Enthalpies= -4286.899900
Sum of electronic and thermal Free Energies= -4287.052417

| | | | |
|---|---|---|---|
| Ni | -1.39811100 | -0.00772700 | 0.12586300 |
| N | 0.84445300 | 1.60130600 | 1.41003200 |
| N | -0.67007300 | 1.18765300 | 2.87159200 |
| C | 2.56080300 | 0.93228600 | -0.20448100 |
| C | 3.24346800 | 1.20269500 | -1.40069600 |
| C | 2.89645900 | 2.29318500 | -2.19467500 |
| C | 1.84668800 | 3.13514900 | -1.82245200 |
| C | 1.13119300 | 2.91766900 | -0.63773600 |
| C | 1.52440700 | 1.81447700 | 0.15857200 |
| C | 1.33265600 | 2.07071100 | 2.62290200 |
| C | 0.37558800 | 1.80897900 | 3.54686900 |
| C | -0.38877500 | 1.03798900 | 1.54833700 |
| C | -1.93485500 | 0.96087500 | 3.52946100 |
| C | -2.25157200 | -0.32413400 | 4.01978300 |
| C | -3.43062300 | -0.44118600 | 4.76851400 |
| C | -4.25549600 | 0.66040300 | 5.00273100 |
| C | -3.93401600 | 1.90722100 | 4.47316300 |
| C | -2.76423400 | 2.08512800 | 3.72035300 |
| H | 4.05085600 | 0.54227600 | -1.71982800 |
| H | 3.43921900 | 2.48355400 | -3.12402400 |
| H | 1.58046700 | 3.96880900 | -2.47240600 |
| H | 2.29715100 | 2.55977900 | 2.70845000 |
| H | 0.33195400 | 2.00762600 | 4.61281400 |
| H | -3.72140600 | -1.41211800 | 5.16809800 |
| H | -5.16849200 | 0.53733500 | 5.59086300 |
| H | -4.59862300 | 2.75670400 | 4.64498400 |
| C | -2.35098500 | -0.81002000 | -1.53709800 |
| H | -3.41356500 | -0.89162700 | -1.77636300 |
| H | -1.96936800 | -1.83150400 | -1.41945500 |
| C | -2.08502800 | -0.81238600 | -3.98244200 |
| C | -3.02443000 | -0.32439500 | -4.90289300 |
| C | -1.53570700 | -2.08376100 | -4.24135400 |
| C | -3.39321500 | -1.06705600 | -6.03147200 |
| H | -3.48935300 | 0.65100700 | -4.75676800 |
| C | -1.90539200 | -2.82220400 | -5.36368100 |
| H | -0.81253600 | -2.51630400 | -3.55063400 |
| C | -2.84336500 | -2.32894700 | -6.28691200 |
| H | -4.12754700 | -0.64921500 | -6.72663100 |
| H | -1.45709600 | -3.80723900 | -5.52568300 |
| C | -1.67595900 | -0.04208800 | -2.71221000 |
| C | -0.02924200 | 3.82924700 | -0.23486000 |
| C | -0.66296700 | 4.58009200 | -1.41397600 |
| C | 0.38290400 | 4.84209700 | 0.85150200 |
| H | -0.81127800 | 3.17981400 | 0.19311300 |
| H | -0.91087800 | 3.90993600 | -2.24842600 |
| H | -1.59134000 | 5.07149000 | -1.08345400 |
| H | 0.00345600 | 5.36892200 | -1.79834200 |
| H | 0.76805200 | 4.35465600 | 1.75602500 |
| H | 1.16506000 | 5.51733000 | 0.46805200 |
| H | -0.48274600 | 5.45619800 | 1.14759700 |
| C | 2.92802800 | -0.27343700 | 0.65252300 |
| C | 4.05028400 | 0.06331300 | 1.65131100 |
| C | 3.32153600 | -1.49342300 | -0.19025800 |
| H | 2.02975000 | -0.56030000 | 1.21758400 |
| H | 3.77445700 | 0.87869000 | 2.33485500 |
| H | 4.28961100 | -0.82076900 | 2.26370200 |
| H | 4.96678100 | 0.36637000 | 1.11817500 |
| H | 2.60298300 | -1.66055600 | -1.00089800 |
| H | 4.32553400 | -1.38174500 | -0.63187600 |
| H | 3.32101800 | -2.39206500 | 0.44206100 |
| C | -1.37605300 | -1.53254000 | 3.69858300 |
| C | -2.07810000 | -2.87321800 | 3.93613800 |
| C | -0.02156800 | -1.53169700 | 4.43255100 |
| H | -1.16324000 | -1.46302200 | 2.62133600 |
| H | -3.04992800 | -2.92090200 | 3.42464200 |
| H | -1.45855900 | -3.68389600 | 3.53242200 |
| H | -2.23892900 | -3.05843000 | 5.01111900 |
| H | 0.55536400 | -0.61352500 | 4.26238400 |
| H | -0.16705300 | -1.64767200 | 5.51936300 |
| H | 0.58723300 | -2.37224000 | 4.06567300 |
| C | -2.41507500 | 3.46266700 | 3.16287000 |
| C | -2.00760400 | 4.43066100 | 4.28672800 |
| C | -3.54817300 | 4.05319200 | 2.30948200 |
| H | -1.54845100 | 3.35326300 | 2.49705800 |
| H | -1.16107900 | 4.03759800 | 4.87032000 |
| H | -1.70876000 | 5.40550200 | 3.86828000 |
| H | -2.84483700 | 4.60233900 | 4.98277100 |
| H | -3.83158600 | 3.36529500 | 1.50123100 |
| H | -4.44871700 | 4.26065800 | 2.90931000 |
| H | -3.22465000 | 5.00496300 | 1.85752500 |
| C | -2.19018500 | 1.40558900 | -2.72833800 |
| H | -1.79395500 | 1.96192300 | -3.59168600 |
| H | -3.28812600 | 1.45745000 | -2.75378200 |
| H | -1.86011500 | 1.92671800 | -1.81785200 |
| C | -0.13573100 | -0.01821900 | -2.60830900 |
| H | 0.20489600 | 0.64857200 | -1.80427500 |
| H | 0.27997600 | -1.01023600 | -2.39637900 |
| H | 0.30461500 | 0.35768300 | -3.54446600 |
| C | -3.22702700 | -3.13533200 | -7.50308800 |
| H | -3.56171200 | -4.14746900 | -7.22149400 |
| H | -4.03747000 | -2.65507500 | -8.07143200 |
| H | -2.36758900 | -3.26137000 | -8.18357800 |
| C | -3.26858600 | -0.25767500 | 0.28862100 |
| C | -3.70998900 | -1.40172700 | 0.96844000 |
| C | -4.07322200 | 0.89318400 | 0.24889400 |
| C | -4.92527600 | -1.36649500 | 1.65868500 |

| | | | |
|---|---|---|---|
| H | -3.09299400 | -2.30225100 | 0.96913600 |
| C | -5.28582800 | 0.91572700 | 0.94536100 |
| H | -3.75191300 | 1.77227500 | -0.31269200 |
| C | -5.71586600 | -0.21178300 | 1.65339400 |
| H | -5.25374400 | -2.25208600 | 2.20944700 |
| H | -5.89636200 | 1.82270100 | 0.93328800 |
| H | -6.66421300 | -0.19107300 | 2.19558600 |
| S | -0.00130900 | -3.03667800 | 0.63332200 |
| O | -0.06743800 | -1.59309300 | 0.19592300 |
| O | 1.16549400 | -3.33020100 | 1.47605600 |
| O | -1.29779800 | -3.59556700 | 1.05153400 |
| C | 0.31091700 | -3.94787500 | -0.98755200 |
| F | -0.83595100 | -4.04872400 | -1.67125200 |
| F | 1.19377100 | -3.31498700 | -1.77026200 |
| F | 0.76674600 | -5.17160600 | -0.73679500 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4290.3380123
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4287.6669036

**H16-1-OTf**

uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.925453 (Hartree/Particle)
Thermal correction to Energy= 0.982476
Thermal correction to Enthalpy= 0.983420
Thermal correction to Gibbs Free Energy= 0.831349
Sum of electronic and zero-point Energies= -4287.029240
Sum of electronic and thermal Energies= -4286.972217
Sum of electronic and thermal Enthalpies= -4286.971273
Sum of electronic and thermal Free Energies= -4287.123344

| | | | |
|---|---|---|---|
| Ni | -0.61570000 | -0.42669500 | 0.69726300 |
| N | 1.90920000 | 1.03200600 | 1.41906200 |
| N | 0.62463100 | 0.80102000 | 3.12288100 |
| C | 3.18547400 | -0.00202500 | -0.40642900 |
| C | 3.67314400 | 0.09573600 | -1.71730700 |
| C | 3.37767700 | 1.20054600 | -2.51764700 |
| C | 2.58091700 | 2.23436200 | -2.02782200 |
| C | 2.07907200 | 2.19450000 | -0.71889200 |
| C | 2.40026000 | 1.07004800 | 0.06686300 |
| C | 2.59092400 | 1.57506200 | 2.50187900 |
| C | 1.78021800 | 1.42508200 | 3.58134700 |
| C | 0.68668400 | 0.55450600 | 1.78188400 |
| C | -0.52147200 | 0.51370300 | 3.94793800 |
| C | -0.75561300 | -0.81739000 | 4.36237500 |
| C | -1.90638700 | -1.04936400 | 5.13077900 |
| C | -2.76983800 | -0.00910300 | 5.47619400 |
| C | -2.50033900 | 1.29685100 | 5.07028000 |
| C | -1.36624500 | 1.58904200 | 4.29876300 |
| H | 4.28215600 | -0.71145500 | -2.12610400 |
| H | 3.76194500 | 1.24801500 | -3.53976600 |
| H | 2.34086600 | 3.08250500 | -2.67250500 |
| H | 3.57430600 | 2.02301700 | 2.40013500 |
| H | 1.91557100 | 1.69726000 | 4.62371700 |
| H | -2.13653500 | -2.05994500 | 5.46628300 |
| H | -3.66073900 | -0.22017000 | 6.07319100 |
| H | -3.18400700 | 2.09777600 | 5.35483500 |
| C | -2.36437700 | -0.93196000 | -2.86962000 |
| H | -3.19620600 | -0.64244500 | -3.53294300 |
| H | -2.35252700 | -2.03078200 | -2.84456000 |
| C | -0.88048700 | -1.26503900 | -4.85305900 |
| C | -1.03429200 | -0.70330000 | -6.12856100 |
| C | -0.58587000 | -2.64248900 | -4.79572800 |
| C | -0.90117900 | -1.47573300 | -7.29000300 |
| H | -1.26259600 | 0.35664700 | -6.24248100 |
| C | -0.45328200 | -3.41001600 | -5.95124500 |
| H | -0.45590900 | -3.13266800 | -3.83028200 |
| C | -0.60811700 | -2.84253200 | -7.22798000 |
| H | -1.02896400 | -0.99630100 | -8.26524100 |
| H | -0.22268800 | -4.47602800 | -5.86069900 |
| C | -1.03433100 | -0.45238600 | -3.55391800 |
| C | 1.17587600 | 3.30806200 | -0.20072500 |
| C | -0.22106900 | 3.19090300 | -0.82912300 |
| C | 1.77518900 | 4.70593400 | -0.41334600 |
| H | 1.05329600 | 3.17362800 | 0.88348800 |
| H | -0.65407800 | 2.19825100 | -0.63492500 |
| H | -0.90407500 | 3.94858700 | -0.41548100 |
| H | -0.17178200 | 3.33375900 | -1.91961200 |
| H | 2.77644700 | 4.78547700 | 0.03864100 |
| H | 1.86614200 | 4.95493700 | -1.48274500 |
| H | 1.12908100 | 5.47023800 | 0.04777900 |
| C | 3.49160800 | -1.21119500 | 0.46957700 |
| C | 4.73949900 | -0.97491500 | 1.33985600 |
| C | 3.64027400 | -2.50766000 | -0.33497000 |
| H | 2.62592000 | -1.35307000 | 1.13134900 |
| H | 4.63099900 | -0.10024900 | 1.99711200 |
| H | 4.92820400 | -1.85277800 | 1.97873600 |
| H | 5.62974000 | -0.81547600 | 0.70884100 |
| H | 2.82300800 | -2.61803200 | -1.05713700 |
| H | 4.59857600 | -2.54693100 | -0.87920300 |
| H | 3.59420200 | -3.37074200 | 0.34408700 |
| C | 0.19613000 | -1.95419000 | 3.99205000 |
| C | -0.39249900 | -3.35101200 | 4.21705000 |
| C | 1.54668900 | -1.84662700 | 4.72581100 |
| H | 0.39668800 | -1.85288000 | 2.91494100 |
| H | -1.36141600 | -3.47377900 | 3.71552500 |
| H | 0.28509600 | -4.09937400 | 3.78408500 |
| H | -0.51031300 | -3.56962000 | 5.29137600 |
| H | 2.06353200 | -0.89786100 | 4.53118200 |
| H | 1.40380100 | -1.94155300 | 5.81502800 |
| H | 2.21161000 | -2.65992100 | 4.39523300 |
| C | -1.09505200 | 3.01072900 | 3.81177800 |
| C | -1.56073800 | 4.09563100 | 4.79171400 |
| C | -1.70533100 | 3.22973000 | 2.41779200 |
| H | -0.00660200 | 3.12783200 | 3.70610200 |
| H | -1.16654600 | 3.92401900 | 5.80560700 |
| H | -1.21179200 | 5.08293300 | 4.45026300 |
| H | -2.65928300 | 4.14724300 | 4.85840200 |
| H | -1.36304600 | 2.46803300 | 1.70501000 |
| H | -2.80479800 | 3.17349800 | 2.46270800 |
| H | -1.42930300 | 4.22118800 | 2.02461500 |
| C | -1.11225200 | 1.05663900 | -3.83053000 |
| H | -0.20814700 | 1.41009200 | -4.35049900 |
| H | -1.98962100 | 1.32608000 | -4.43839200 |
| H | -1.18257400 | 1.60502100 | -2.88436100 |
| C | 0.18100100 | -0.70746400 | -2.64183900 |
| H | 0.15068600 | -0.06226900 | -1.75077400 |
| H | 0.23318300 | -1.74022100 | -2.27964300 |
| H | 1.11645700 | -0.47875700 | -3.17162600 |
| C | -0.45745100 | -3.68494700 | -8.47086800 |
| H | 0.55659200 | -4.11372700 | -8.54106100 |
| H | -1.16224900 | -4.53329200 | -8.46576000 |
| H | -0.63954800 | -3.09932700 | -9.38436200 |
| C | -2.64997100 | -0.43946600 | -1.46798200 |
| C | -2.40787800 | -1.30118800 | -0.36772100 |
| C | -3.20925500 | 0.81787800 | -1.20878700 |
| C | -2.71117000 | -0.90776600 | 0.95607200 |
| H | -2.10127200 | -2.32831300 | -0.55236700 |
| C | -3.50855200 | 1.22005000 | 0.10513600 |
| H | -3.43375100 | 1.49042400 | -2.03942600 |
| C | -3.26550300 | 0.37269800 | 1.18457400 |
| H | -2.64368000 | -1.64010700 | 1.76455700 |
| H | -3.93855700 | 2.20930300 | 0.27908400 |
| H | -3.50221900 | 0.68257600 | 2.20401500 |
| S | 0.20816800 | -3.55992400 | 0.69620400 |
| O | 0.46161600 | -2.13506800 | 0.26727300 |
| O | 1.33484900 | -4.16290000 | 1.42248500 |
| O | -1.14903500 | -3.78375400 | 1.22673100 |

| | | | |
|---|---|---|---|
| C | 0.15853200 | -4.47288200 | -0.94682400 |
| F | -0.91168700 | -4.07457800 | -1.65790700 |
| F | 1.24462400 | -4.24277300 | -1.68822100 |
| F | 0.05674800 | -5.78152700 | -0.73261800 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4290.4126112
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4287.7458944

**PhMgBr**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.090456 (Hartree/Particle)
Thermal correction to Energy= 0.098446
Thermal correction to Enthalpy= 0.099390
Thermal correction to Gibbs Free Energy= 0.055142
Sum of electronic and zero-point Energies= -3005.394430
Sum of electronic and thermal Energies= -3005.386440
Sum of electronic and thermal Enthalpies= -3005.385495
Sum of electronic and thermal Free Energies= -3005.429743

| | | | |
|---|---|---|---|
| C | 7.61573100 | -1.97326700 | -0.84178900 |
| C | 7.97084900 | -1.39825900 | -2.08348800 |
| C | 8.13358900 | -3.26187800 | -0.57879800 |
| C | 8.79102300 | -2.06092400 | -3.00633100 |
| H | 7.60235300 | -0.40015600 | -2.34931400 |
| C | 8.95485800 | -3.93684200 | -1.49177200 |
| H | 7.89641600 | -3.76435300 | 0.36657700 |
| C | 9.28661900 | -3.33531800 | -2.71060100 |
| H | 9.04536600 | -1.58253300 | -3.95710100 |
| H | 9.33832100 | -4.93340000 | -1.25230400 |
| H | 9.92877700 | -3.85673100 | -3.42603400 |
| Mg | 6.41532900 | -0.94140200 | 0.53776800 |
| Br | 5.06696900 | 0.27937300 | 2.11979400 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3005.9195183
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3005.3781845

**AlkSM**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.107088 (Hartree/Particle)
Thermal correction to Energy= 0.112373
Thermal correction to Enthalpy= 0.113317
Thermal correction to Gibbs Free Energy= 0.079808
Sum of electronic and zero-point Energies= -157.012595
Sum of electronic and thermal Energies= -157.007309
Sum of electronic and thermal Enthalpies= -157.006365
Sum of electronic and thermal Free Energies= -157.039875

| | | | |
|---|---|---|---|
| C | 4.24976200 | -1.34040400 | 2.19282600 |
| H | 5.22688900 | -1.45578000 | 2.69499300 |
| H | 3.58273100 | -0.77517600 | 2.86061600 |
| H | 3.84032700 | -2.35959100 | 2.07500700 |
| C | 4.41511200 | -0.67329600 | 0.85067700 |
| C | 3.80257300 | 0.47898600 | 0.54210000 |
| H | 3.93238000 | 0.95134200 | -0.43659300 |
| H | 3.15035800 | 0.98933200 | 1.25762700 |
| C | 5.31732700 | -1.39232900 | -0.12031400 |
| H | 4.94405500 | -2.41297700 | -0.31833600 |
| H | 5.40267700 | -0.86323300 | -1.08110600 |
| H | 6.33121400 | -1.51029100 | 0.30201100 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -157.259677
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -157.0862617

**ArOTf**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.146341 (Hartree/Particle)
Thermal correction to Energy= 0.159640
Thermal correction to Enthalpy= 0.160584
Thermal correction to Gibbs Free Energy= 0.103860
Sum of electronic and zero-point Energies= -1231.506319
Sum of electronic and thermal Energies= -1231.493020
Sum of electronic and thermal Enthalpies= -1231.492076
Sum of electronic and thermal Free Energies= -1231.548800

| | | | |
|---|---|---|---|
| C | 3.72803800 | -0.83626400 | -0.54489700 |
| C | 5.06973600 | -1.22664600 | -0.51781400 |
| C | 6.00728300 | -0.35763400 | 0.03333800 |
| C | 5.63785900 | 0.88193000 | 0.55499000 |
| C | 4.29313500 | 1.25039200 | 0.52450400 |
| C | 3.31607600 | 0.40128300 | -0.02579400 |
| H | 2.98744000 | -1.51285900 | -0.97890700 |
| H | 5.39203000 | -2.18619100 | -0.92283900 |
| H | 6.40099300 | 1.53717000 | 0.97823600 |
| H | 3.99608400 | 2.21956700 | 0.93433000 |
| C | 1.86606500 | 0.81752600 | -0.04047800 |
| H | 1.46311400 | 0.87627100 | 0.98471700 |
| H | 1.74371900 | 1.81571500 | -0.49126200 |
| H | 1.24434400 | 0.10848800 | -0.60610500 |
| O | 7.35787800 | -0.73786400 | 0.12933800 |
| S | 8.29980600 | -0.80952200 | -1.20935300 |
| O | 9.49352100 | -1.52246600 | -0.80726300 |
| O | 7.51210200 | -1.14861000 | -2.38199500 |
| C | 8.76197800 | 1.01279100 | -1.36317200 |
| F | 9.71434300 | 1.12993500 | -2.27540000 |
| F | 9.19931100 | 1.46053400 | -0.19459300 |
| F | 7.69377000 | 1.70713100 | -1.73476100 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1232.6710681
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1231.7875301

**Prod**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.321655 (Hartree/Particle)
Thermal correction to Energy= 0.337570
Thermal correction to Enthalpy= 0.338514
Thermal correction to Gibbs Free Energy= 0.277015
Sum of electronic and zero-point Energies= -659.112819
Sum of electronic and thermal Energies= -659.096904
Sum of electronic and thermal Enthalpies= -659.095960
Sum of electronic and thermal Free Energies= -659.157459

| | | | |
|---|---|---|---|
| C | 4.02779100 | -1.82182200 | 2.21243500 |
| H | 3.34377800 | -1.38232800 | 2.95564200 |
| H | 4.96576400 | -2.05474400 | 2.74102100 |
| C | 4.33404400 | -0.73806800 | 1.13187000 |
| C | 3.02696700 | -0.34625200 | 0.40805000 |
| H | 2.58232900 | -1.21708900 | -0.09670500 |
| H | 2.28720700 | 0.05381200 | 1.11986600 |
| H | 3.20858800 | 0.42338500 | -0.35645200 |
| C | 4.94271000 | 0.52154100 | 1.78496600 |
| C | 5.29497800 | 1.62274800 | 0.97775300 |
| C | 5.17677300 | 0.65348300 | 3.16174900 |
| C | 5.84717400 | 2.78336000 | 1.51545100 |
| H | 5.13537900 | 1.57772100 | -0.10200200 |
| C | 5.73211600 | 1.82065300 | 3.70338700 |
| H | 4.93028800 | -0.15497900 | 3.84950500 |
| C | 6.07929000 | 2.90891400 | 2.89615600 |
| H | 6.10461100 | 3.61245800 | 0.84906300 |
| H | 5.89632900 | 1.87785400 | 4.78358400 |
| C | 3.42488000 | -3.11629700 | 1.71252800 |
| C | 4.24063500 | -4.19487200 | 1.32978100 |
| C | 2.03179800 | -3.27934200 | 1.62295100 |

| | | | |
|---|---|---|---|
| C | 3.68674700 | -5.38940700 | 0.85946100 |
| H | 5.32686700 | -4.09643300 | 1.40565700 |
| C | 1.47178700 | -4.47134300 | 1.15346400 |
| H | 1.37703500 | -2.45931200 | 1.92983200 |
| C | 2.29830600 | -5.53128800 | 0.76620200 |
| H | 4.34260500 | -6.21449600 | 0.56900800 |
| H | 0.38494400 | -4.57409900 | 1.09431600 |
| H | 1.86282700 | -6.46498300 | 0.40109100 |
| C | 6.67951000 | 4.16994600 | 3.46740900 |
| H | 7.68025700 | 4.36182500 | 3.04483900 |
| H | 6.05894000 | 5.05026600 | 3.22971500 |
| H | 6.78067400 | 4.11321800 | 4.56146000 |
| C | 5.33666300 | -1.30398300 | 0.10214400 |
| H | 6.27845800 | -1.60033400 | 0.59118400 |
| H | 4.92033700 | -2.18692500 | -0.40566100 |
| H | 5.57869500 | -0.56007500 | -0.67103000 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -660.0105098
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -659.320612

**MgBrOTf**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.030224 (Hartree/Particle)
Thermal correction to Energy= 0.040858
Thermal correction to Enthalpy= 0.041802
Thermal correction to Gibbs Free Energy= -0.009084
Sum of electronic and zero-point Energies= -3734.934519
Sum of electronic and thermal Energies= -3734.923886
Sum of electronic and thermal Enthalpies= -3734.922941
Sum of electronic and thermal Free Energies= -3734.973827

| | | | |
|---|---|---|---|
| O | 0.49776200 | -0.65530600 | -1.19108500 |
| S | 1.42905900 | -0.82083500 | 0.00004700 |
| O | 0.49755300 | -0.65510900 | 1.19098000 |
| O | 2.35618800 | -1.93384300 | 0.00020200 |
| C | 2.44808900 | 0.75501200 | 0.00000200 |
| F | 3.20646400 | 0.78981100 | 1.08434600 |
| F | 1.62232600 | 1.80066100 | -0.00017300 |
| F | 3.20666600 | 0.78960300 | -1.08420700 |
| Mg | -1.17048200 | -0.28675100 | -0.00022700 |
| Br | -3.50396700 | 0.21650600 | 0.00004300 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3735.9813843
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3735.0788263

**MgBrCl**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.002080 (Hartree/Particle)
Thermal correction to Energy= 0.006291
Thermal correction to Enthalpy= 0.007235
Thermal correction to Gibbs Free Energy= -0.023616
Sum of electronic and zero-point Energies= -3234.150896
Sum of electronic and thermal Energies= -3234.146685
Sum of electronic and thermal Enthalpies= -3234.145741
Sum of electronic and thermal Free Energies= -3234.176591

| | | | |
|---|---|---|---|
| Br | -3.39592000 | 0.18763500 | 0.00021000 |
| Mg | -1.05491500 | -0.30020400 | -0.00061000 |
| Cl | 1.12374100 | -0.78744300 | -0.00030200 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3234.5271503
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3234.0780116

**iv-Cl**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.894368 (Hartree/Particle)
Thermal correction to Energy= 0.944991
Thermal correction to Enthalpy= 0.945935
Thermal correction to Gibbs Free Energy= 0.809010
Sum of electronic and zero-point Energies= -3786.170273
Sum of electronic and thermal Energies= -3786.119649
Sum of electronic and thermal Enthalpies= -3786.118705
Sum of electronic and thermal Free Energies= -3786.255631

| | | | |
|---|---|---|---|
| Ni | -0.18017600 | -0.43427300 | -0.18709600 |
| N | 1.96729100 | 1.13098500 | 1.19639400 |
| N | 0.54753500 | 0.53593400 | 2.69485400 |
| C | 3.66654600 | 0.72959400 | -0.53087300 |
| C | 4.23397500 | 1.10731200 | -1.75795300 |
| C | 3.69721500 | 2.14967200 | -2.50775100 |
| C | 2.57575700 | 2.84340200 | -2.04863500 |
| C | 1.97559600 | 2.52199300 | -0.82455000 |
| C | 2.54919800 | 1.46069300 | -0.07963200 |
| C | 2.54340800 | 1.43575100 | 2.42557500 |
| C | 1.64810200 | 1.05377300 | 3.37188300 |
| C | 0.74498700 | 0.55359400 | 1.35044500 |
| C | -0.69079300 | 0.20374000 | 3.35708300 |
| C | -0.91234600 | -1.11742200 | 3.78692500 |
| C | -2.12530100 | -1.38829000 | 4.43893300 |
| C | -3.06574900 | -0.38285400 | 4.65486700 |
| C | -2.81039100 | 0.92262300 | 4.23338000 |
| C | -1.61663400 | 1.24791500 | 3.57810400 |
| H | 5.10231400 | 0.56488200 | -2.13590300 |
| H | 4.14857000 | 2.42154900 | -3.46520500 |
| H | 2.16518800 | 3.64778000 | -2.65888200 |
| H | 3.51782600 | 1.90530300 | 2.50886500 |
| H | 1.68372300 | 1.10717900 | 4.45524900 |
| H | -2.33264300 | -2.40260100 | 4.78536400 |
| H | -4.00670500 | -0.61661000 | 5.15959100 |
| H | -3.55549200 | 1.69923400 | 4.41299800 |
| C | -0.92216400 | -1.28386800 | -1.84399800 |
| H | -1.98987800 | -1.09249500 | -2.00993300 |
| H | -0.79257600 | -2.35525200 | -1.63780400 |
| C | -0.71111500 | -1.67235000 | -4.27348100 |
| C | -1.47448100 | -1.11362100 | -5.30898400 |
| C | -0.50478500 | -3.06641400 | -4.31594400 |
| C | -2.00039000 | -1.90474400 | -6.33897100 |
| H | -1.67492000 | -0.04205800 | -5.33166300 |
| C | -1.02704700 | -3.85268200 | -5.34046700 |
| H | 0.07275500 | -3.55094900 | -3.52555000 |
| C | -1.78869700 | -3.28750300 | -6.37868500 |
| H | -2.58916600 | -1.42782900 | -7.12850900 |
| H | -0.84237800 | -4.93150800 | -5.33547100 |
| C | -0.13566900 | -0.84609200 | -3.10733300 |
| C | 0.76560900 | 3.30148000 | -0.30744600 |
| C | -0.00198600 | 4.06237200 | -1.39564800 |
| C | 1.16572700 | 4.27315000 | 0.82001800 |
| H | 0.06643800 | 2.56438400 | 0.11791000 |
| H | -0.26321600 | 3.41816200 | -2.24777100 |
| H | -0.93749600 | 4.46093700 | -0.97411600 |
| H | 0.57440000 | 4.91846300 | -1.78185400 |
| H | 1.64505800 | 3.75935700 | 1.66409400 |
| H | 1.86821200 | 5.03301200 | 0.44056900 |
| H | 0.27623200 | 4.79434900 | 1.20838100 |
| C | 4.26713400 | -0.42132600 | 0.26773800 |
| C | 5.54771800 | 0.02773700 | 0.99466300 |
| C | 4.54333500 | -1.65742400 | -0.60210100 |
| H | 3.52382700 | -0.72866100 | 1.01641300 |
| H | 5.36856800 | 0.88654500 | 1.65931900 |
| H | 5.95332100 | -0.79483600 | 1.60552500 |
| H | 6.32360000 | 0.32622900 | 0.27026600 |
| H | 3.63448400 | -1.97125200 | -1.13222900 |
| H | 5.34453400 | -1.47551200 | -1.33660600 |
| H | 4.86664300 | -2.49517200 | 0.03604400 |

| | | | |
|---|---|---|---|
| C | 0.13749300 | -2.20568900 | 3.61610200 |
| C | -0.44646500 | -3.51705700 | 3.07419500 |
| C | 0.88899700 | -2.42939400 | 4.94075700 |
| H | 0.86371400 | -1.86100900 | 2.86879700 |
| H | -0.96708400 | -3.34860900 | 2.12025600 |
| H | 0.36540500 | -4.23466900 | 2.87950400 |
| H | -1.14623800 | -3.98731500 | 3.78420200 |
| H | 1.36048700 | -1.49942500 | 5.29723500 |
| H | 0.20527300 | -2.78263800 | 5.73077800 |
| H | 1.68124100 | -3.18489200 | 4.81296000 |
| C | -1.31621000 | 2.68734700 | 3.17381400 |
| C | -0.70837600 | 3.46713600 | 4.35511200 |
| C | -2.53267200 | 3.43422600 | 2.61219500 |
| H | -0.56487100 | 2.65617700 | 2.37315400 |
| H | 0.20043600 | 2.98564200 | 4.74372000 |
| H | -0.44273800 | 4.49095400 | 4.04518900 |
| H | -1.43248600 | 3.53794300 | 5.18336600 |
| H | -3.01100700 | 2.86681700 | 1.80410200 |
| H | -3.28744800 | 3.63411600 | 3.38982100 |
| H | -2.21677000 | 4.41033100 | 2.20942900 |
| C | -0.32400200 | 0.66399300 | -3.32854600 |
| H | 0.16277300 | 1.00267300 | -4.25687500 |
| H | -1.38547500 | 0.94866200 | -3.36513300 |
| H | 0.14222400 | 1.21833500 | -2.50116900 |
| C | 1.37841000 | -1.11952200 | -2.98726500 |
| H | 1.82486300 | -0.50204700 | -2.19570900 |
| H | 1.58875100 | -2.16417000 | -2.72411900 |
| H | 1.88778100 | -0.88075500 | -3.93477100 |
| C | -2.34779800 | -4.15029200 | -7.48345300 |
| H | -1.54155400 | -4.65305300 | -8.04422300 |
| H | -2.99793600 | -4.94464800 | -7.07966400 |
| H | -2.93960200 | -3.56131700 | -8.20009000 |
| Cl | 1.17152100 | -2.24151200 | 0.24042900 |
| C | -1.97892400 | 0.17971800 | 0.02801100 |
| C | -2.80531800 | -0.59937600 | 0.84771400 |
| C | -2.49999400 | 1.33977000 | -0.55979500 |
| C | -4.12928000 | -0.21678200 | 1.09073200 |
| H | -2.41690800 | -1.50981700 | 1.31028600 |
| C | -3.83020000 | 1.71541900 | -0.32749800 |
| H | -1.88140700 | 1.95296800 | -1.21564100 |
| C | -4.64995300 | 0.93936000 | 0.49853800 |
| H | -4.75501600 | -0.82927700 | 1.74562400 |
| H | -4.22335000 | 2.62320000 | -0.79452200 |
| H | -5.68690800 | 1.23366100 | 0.68000600 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3788.8950928
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3786.6697759

**TS-iv-H16-1-Cl**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.893440 (Hartree/Particle)
Thermal correction to Energy= 0.943812
Thermal correction to Enthalpy= 0.944757
Thermal correction to Gibbs Free Energy= 0.807387
Sum of electronic and zero-point Energies= -3786.161209
Sum of electronic and thermal Energies= -3786.110837
Sum of electronic and thermal Enthalpies= -3786.109892
Sum of electronic and thermal Free Energies= -3786.247262

| | | | |
|---|---|---|---|
| Ni | -1.42212600 | 0.18123200 | 0.09427900 |
| N | 0.84904100 | 1.63606900 | 1.41178600 |
| N | -0.60074700 | 1.09054400 | 2.89754700 |
| C | 2.50013100 | 1.09535200 | -0.31378900 |
| C | 3.10510100 | 1.42818800 | -1.53593200 |
| C | 2.66510600 | 2.51921900 | -2.27997100 |
| C | 1.60050300 | 3.30137300 | -1.82557000 |
| C | 0.96959100 | 3.02751400 | -0.60538200 |
| C | 1.45739600 | 1.92579600 | 0.14092700 |
| C | 1.42847100 | 1.91619100 | 2.64513900 |
| C | 0.51025300 | 1.57018200 | 3.58402800 |
| C | -0.39708300 | 1.10770400 | 1.55118800 |
| C | -1.85943800 | 0.79416600 | 3.53597900 |
| C | -2.10631800 | -0.50839100 | 4.01006200 |
| C | -3.33836400 | -0.74053800 | 4.63943000 |
| C | -4.27539900 | 0.28073300 | 4.78572700 |
| C | -3.99698300 | 1.56588000 | 4.31990300 |
| C | -2.77918400 | 1.85495400 | 3.69112900 |
| H | 3.92164100 | 0.81166200 | -1.91597600 |
| H | 3.14328000 | 2.75697600 | -3.23353700 |
| H | 1.25918100 | 4.13588800 | -2.43812800 |
| H | 2.42013300 | 2.34697800 | 2.73654500 |
| H | 0.53728100 | 1.63150500 | 4.66715200 |
| H | -3.56810800 | -1.73809200 | 5.01796800 |
| H | -5.23388200 | 0.07442800 | 5.26898700 |
| H | -4.73884300 | 2.35585700 | 4.44831700 |
| C | -2.44948100 | -0.57618200 | -1.59580900 |
| H | -3.49683000 | -0.57605300 | -1.90753800 |
| H | -2.18814200 | -1.61079300 | -1.34310100 |
| C | -2.01251600 | -0.93198800 | -3.98756400 |
| C | -2.73570100 | -0.47780100 | -5.09909100 |
| C | -1.64789400 | -2.29367000 | -3.97192400 |
| C | -3.07567900 | -1.34075300 | -6.14942200 |
| H | -3.04758900 | 0.56485400 | -5.16860100 |
| C | -1.98720800 | -3.15070800 | -5.01635200 |
| H | -1.09060400 | -2.69412500 | -3.12178200 |
| C | -2.71039600 | -2.69164500 | -6.13169200 |
| H | -3.63868900 | -0.94677300 | -7.00092400 |
| H | -1.68547200 | -4.20151500 | -4.96671100 |
| C | -1.62750900 | -0.02831000 | -2.80111000 |
| C | -0.20051400 | 3.87646100 | -0.10516200 |
| C | -0.88525000 | 4.70510200 | -1.19918000 |
| C | 0.22089000 | 4.80176500 | 1.05296400 |
| H | -0.95635800 | 3.17325700 | 0.28261800 |
| H | -1.17021000 | 4.09316100 | -2.06686200 |
| H | -1.80026300 | 5.16443500 | -0.79391400 |
| H | -0.23981100 | 5.52346000 | -1.55721800 |
| H | 0.64149900 | 4.24723000 | 1.90200300 |
| H | 0.97871400 | 5.52447600 | 0.70891800 |
| H | -0.64758200 | 5.36936200 | 1.42355800 |
| C | 2.96549600 | -0.12376100 | 0.47390200 |
| C | 4.27256000 | 0.17664400 | 1.22886000 |
| C | 3.11911000 | -1.36934400 | -0.41150200 |
| H | 2.18070000 | -0.36390300 | 1.20526800 |
| H | 4.16894400 | 1.03613900 | 1.90859600 |
| H | 4.58096300 | -0.69461200 | 1.82890800 |
| H | 5.08745600 | 0.40758900 | 0.52267200 |
| H | 2.17987900 | -1.58902700 | -0.93627200 |
| H | 3.93101100 | -1.25848600 | -1.14848100 |
| H | 3.35970000 | -2.24201500 | 0.21614900 |
| C | -1.05397200 | -1.60382300 | 3.91270000 |
| C | -1.63661400 | -2.97412100 | 3.54632200 |
| C | -0.24593300 | -1.68054100 | 5.22142400 |
| H | -0.36859200 | -1.33469600 | 3.09814200 |
| H | -2.21435900 | -2.91679500 | 2.61345800 |
| H | -0.81880700 | -3.69216600 | 3.37995400 |
| H | -2.28057000 | -3.38166200 | 4.34294800 |
| H | 0.23259500 | -0.71822500 | 5.46127100 |
| H | -0.89542300 | -1.95188200 | 6.07058700 |
| H | 0.54710700 | -2.44187300 | 5.14179800 |
| C | -2.43321700 | 3.28033900 | 3.27072000 |
| C | -1.85964500 | 4.06527800 | 4.46572000 |
| C | -3.60394700 | 4.04360900 | 2.63932200 |
| H | -1.64549500 | 3.22109900 | 2.50775000 |
| H | -0.98150000 | 3.56517500 | 4.89979000 |
| H | -1.55352200 | 5.07692700 | 4.15301700 |
| H | -2.61675600 | 4.16693600 | 5.26059100 |
| H | -4.04505600 | 3.47574200 | 1.81022300 |
| H | -4.39957300 | 4.25810100 | 3.37094900 |

| | | | |
|---|---|---|---|
| H | -3.25150600 | 5.01235300 | 2.24957100 |
| C | -1.99486100 | 1.44185800 | -3.04458400 |
| H | -1.46645200 | 1.84976100 | -3.92022100 |
| H | -3.07563300 | 1.58590000 | -3.18881000 |
| H | -1.69396500 | 2.03526800 | -2.17003700 |
| C | -0.10083600 | -0.11481400 | -2.59501000 |
| H | 0.24483500 | 0.61845700 | -1.85376000 |
| H | 0.20869600 | -1.10296200 | -2.23508300 |
| H | 0.42229200 | 0.10689100 | -3.53838100 |
| C | -3.07162700 | -3.63114400 | -7.25599600 |
| H | -2.16972900 | -4.07514900 | -7.71013400 |
| H | -3.69038700 | -4.46876600 | -6.89219000 |
| H | -3.63244600 | -3.11789800 | -8.05136500 |
| Cl | -0.32148700 | -1.84620100 | 0.47901200 |
| C | -3.31665300 | 0.28951000 | 0.03878400 |
| C | -3.92891000 | -0.67904400 | 0.85759000 |
| C | -3.99987600 | 1.49408000 | -0.21834200 |
| C | -5.17574300 | -0.43275200 | 1.43430400 |
| H | -3.41264900 | -1.62352400 | 1.04071800 |
| C | -5.25806800 | 1.72355500 | 0.34842800 |
| H | -3.55490300 | 2.25149200 | -0.86476800 |
| C | -5.85238500 | 0.76620300 | 1.17779300 |
| H | -5.62142900 | -1.18462700 | 2.09067000 |
| H | -5.77706500 | 2.66315800 | 0.13858100 |
| H | -6.83459900 | 0.95178300 | 1.61916900 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3788.8860042
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3786.6646274

**H16-1-Cl**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.895606 (Hartree/Particle)
Thermal correction to Energy= 0.946404
Thermal correction to Enthalpy= 0.947348
Thermal correction to Gibbs Free Energy= 0.808089
Sum of electronic and zero-point Energies= -3786.226765
Sum of electronic and thermal Energies= -3786.175967
Sum of electronic and thermal Enthalpies= -3786.175023
Sum of electronic and thermal Free Energies= -3786.314282

| | | | |
|---|---|---|---|
| Ni | -0.77250500 | -0.42282500 | 0.55655400 |
| N | 1.85825700 | 0.91680000 | 1.15016300 |
| N | 0.69805500 | 0.55131300 | 2.91933400 |
| C | 3.07035600 | 0.29185900 | -0.89405300 |
| C | 3.51450900 | 0.66478600 | -2.17229000 |
| C | 3.10838300 | 1.86464700 | -2.75319300 |
| C | 2.21688000 | 2.70483200 | -2.08345900 |
| C | 1.74697000 | 2.38335200 | -0.80398400 |
| C | 2.22432200 | 1.18975300 | -0.21567200 |
| C | 2.67842500 | 1.22057400 | 2.23373800 |
| C | 1.94567900 | 0.98390300 | 3.35382800 |
| C | 0.62919300 | 0.49074000 | 1.55754600 |
| C | -0.45815900 | 0.39119900 | 3.76017300 |
| C | -0.86219100 | -0.90686600 | 4.13647000 |
| C | -2.02760900 | -1.01902800 | 4.90678700 |
| C | -2.75347600 | 0.11328900 | 5.28486200 |
| C | -2.32641200 | 1.38385900 | 4.90188000 |
| C | -1.16901100 | 1.55169400 | 4.12600900 |
| H | 4.17961500 | -0.00141000 | -2.72460000 |
| H | 3.46791800 | 2.13672700 | -3.74886300 |
| H | 1.87737500 | 3.62075100 | -2.56964900 |
| H | 3.69158300 | 1.58831800 | 2.10619700 |
| H | 2.18504900 | 1.10070600 | 4.40647200 |
| H | -2.37801100 | -2.00551000 | 5.21374000 |
| H | -3.66180400 | 0.00148700 | 5.88250600 |
| H | -2.90604900 | 2.26048500 | 5.20035200 |
| C | -2.58058000 | -0.79638800 | -2.74427000 |
| H | -3.44683200 | -0.64639700 | -3.41037700 |
| H | -2.47373300 | -1.88230500 | -2.62378700 |
| C | -0.84410000 | -1.36138500 | -4.46556100 |
| C | -0.91116200 | -1.24522600 | -5.85966900 |
| C | -0.31899400 | -2.56379500 | -3.94481900 |
| C | -0.47233100 | -2.27822300 | -6.70026700 |
| H | -1.30882200 | -0.34071600 | -6.32136300 |
| C | 0.11766300 | -3.58779500 | -4.78190000 |
| H | -0.24788800 | -2.70461400 | -2.86206300 |
| C | 0.05183000 | -3.46708600 | -6.18198500 |
| H | -0.54184500 | -2.14803600 | -7.78453000 |
| H | 0.52164000 | -4.50355000 | -4.33915500 |
| C | -1.30485300 | -0.25700100 | -3.49796100 |
| C | 0.76160700 | 3.29107800 | -0.07328000 |
| C | -0.25971300 | 3.95500000 | -1.00628500 |
| C | 1.50033500 | 4.33828200 | 0.77873400 |
| H | 0.18250700 | 2.65260400 | 0.60925000 |
| H | -0.76610400 | 3.20923000 | -1.63798700 |
| H | -1.02790000 | 4.47130900 | -0.40935700 |
| H | 0.20278100 | 4.70659400 | -1.66585600 |
| H | 2.18268400 | 3.86301900 | 1.49924000 |
| H | 2.09619600 | 5.00992100 | 0.13897200 |
| H | 0.78360200 | 4.95345500 | 1.34615300 |
| C | 3.48625700 | -1.03767500 | -0.27759000 |
| C | 4.89535700 | -0.95279900 | 0.33448200 |
| C | 3.39303700 | -2.19588900 | -1.28212800 |
| H | 2.76581000 | -1.26491800 | 0.52143700 |
| H | 4.96166600 | -0.17274400 | 1.10805600 |
| H | 5.17272000 | -1.91289100 | 0.79918400 |
| H | 5.64563500 | -0.72142900 | -0.44008900 |
| H | 2.39398300 | -2.23809200 | -1.73722300 |
| H | 4.15032100 | -2.11533300 | -2.07918700 |
| H | 3.55971000 | -3.15208200 | -0.76172600 |
| C | -0.03942100 | -2.12488400 | 3.74063400 |
| C | -0.87553200 | -3.39158800 | 3.53240000 |
| C | 1.08761100 | -2.36428500 | 4.76178600 |
| H | 0.42275000 | -1.90841100 | 2.76828400 |
| H | -1.70166600 | -3.20958900 | 2.82893300 |
| H | -0.24477500 | -4.17955200 | 3.09469200 |
| H | -1.29463200 | -3.77972800 | 4.47545900 |
| H | 1.73806700 | -1.48142500 | 4.86054200 |
| H | 0.67428700 | -2.59277000 | 5.75852200 |
| H | 1.71625700 | -3.21348900 | 4.44860500 |
| C | -0.73092500 | 2.95021300 | 3.69954800 |
| C | -0.41896100 | 3.83558900 | 4.91729800 |
| C | -1.75926700 | 3.61239600 | 2.76866800 |
| H | 0.20000300 | 2.85952000 | 3.12393100 |
| H | 0.34080000 | 3.36991200 | 5.56478000 |
| H | -0.03639100 | 4.81610400 | 4.59076400 |
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| H | -1.90580700 | 3.01674300 | 1.85701900 |
| H | -2.73894800 | 3.72656700 | 3.26041100 |
| H | -1.41527000 | 4.61585000 | 2.47084400 |
| C | -1.65110600 | 1.05051100 | -4.23047000 |
| H | -0.78854900 | 1.42091200 | -4.80633100 |
| H | -2.50210700 | 0.93281600 | -4.91921200 |
| H | -1.91559000 | 1.83247700 | -3.50407600 |
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| H | 0.12636400 | -0.82344800 | -1.91761700 |
| H | 0.74171000 | 0.36776200 | -3.07992300 |
| C | 0.53358900 | -4.58416800 | -7.07509300 |
| H | 1.60581900 | -4.78842900 | -6.91461000 |
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| C | -2.87667400 | -0.22296700 | -1.37760200 |
| C | -2.69673800 | -1.05756200 | -0.23945900 |
| C | -3.33261700 | 1.08382800 | -1.17488800 |
| C | -2.92569200 | -0.56245200 | 1.06722200 |
| H | -2.49184800 | -2.11878900 | -0.38880100 |

| | | | |
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| H | -3.51018600 | 1.73495900 | -2.03300500 |
| C | -3.38944000 | 0.76248300 | 1.23675200 |
| H | -2.89715700 | -1.23470100 | 1.92786000 |
| H | -3.95801000 | 2.59151600 | 0.24943000 |
| H | -3.58520500 | 1.13652600 | 2.24286400 |

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PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3786.736757

**TS-A'-linear-1**
uB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.831132 (Hartree/Particle)
Thermal correction to Energy= 0.885216
Thermal correction to Enthalpy= 0.886160
Thermal correction to Gibbs Free Energy= 0.743095
Sum of electronic and zero-point Energies= -4515.617876
Sum of electronic and thermal Energies= -4515.563792
Sum of electronic and thermal Enthalpies= -4515.562848
Sum of electronic and thermal Free Energies= -4515.705913

| | | | |
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| C | 0.52962400 | 0.50309200 | 0.86648500 |
| C | 2.19880700 | 1.24935000 | -0.49369200 |
| C | 2.70366600 | 1.18731200 | 0.76167100 |
| N | 1.67001000 | 0.76015800 | 1.58518400 |
| N | 0.86899800 | 0.85134800 | -0.41378700 |
| H | 3.68974800 | 1.42202500 | 1.14722800 |
| H | 2.64871100 | 1.55488700 | -1.43287600 |
| C | 1.77314100 | 0.83789400 | 3.02906700 |
| C | 1.57326300 | 2.10532300 | 3.63107300 |
| C | 2.11318200 | -0.31010300 | 3.77860200 |
| C | 1.65331000 | 2.18066600 | 5.02867700 |
| C | 2.16915700 | -0.17517200 | 5.17456100 |
| C | 1.93315000 | 1.05007000 | 5.79445400 |
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| H | 1.97729300 | 1.12674100 | 6.88369200 |
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| C | -1.55424900 | 2.42676900 | -2.76666500 |
| C | -0.72839300 | 0.39071500 | -3.76215500 |
| C | -1.53152900 | 1.52359200 | -3.83063200 |
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| C | -3.31466500 | -0.94360900 | -1.78953700 |
| C | -2.75140700 | -0.45766300 | -0.60638500 |
| C | -2.49311800 | -1.34723700 | 0.43275800 |
| C | -2.89208400 | -2.68148900 | 0.36630000 |
| H | -3.72596500 | -4.20630400 | -0.89752600 |
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| H | -2.74825200 | -3.34974100 | 1.21203100 |
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| C | -3.08930700 | -0.47363600 | 2.37945000 |
| Ni | -0.81912400 | -1.01071000 | 1.54481600 |
| C | 0.94990800 | -1.11299900 | -2.62646000 |
| C | 2.13944100 | -0.92739400 | -3.58461400 |
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| H | 2.74112400 | -0.04247700 | -3.32201000 |
| H | 2.80046500 | -1.80828200 | -3.54771700 |
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| H | 0.80057200 | -3.27252400 | -2.81705500 |
| C | -0.74794000 | 3.26369400 | -0.51482100 |
| C | -2.07613600 | 4.01241000 | -0.33601800 |
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| H | -2.26043700 | 4.72249100 | -1.15764000 |
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| H | 0.43607800 | 4.99967400 | 0.08285200 |
| C | 2.46597800 | -1.62933500 | 3.11141600 |
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| H | 1.21133100 | -2.84808700 | 4.43098000 |
| H | 2.30297800 | -3.76537000 | 3.38188000 |
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| H | 4.16154700 | -2.56040600 | 2.11112000 |
| C | 1.34915500 | 3.37988900 | 2.82042900 |
| C | 2.68320600 | 4.11686500 | 2.58833600 |
| C | 0.33671600 | 4.34809700 | 3.45516500 |
| H | 0.95889600 | 3.09161800 | 1.83459600 |
| H | 3.42498500 | 3.48285300 | 2.08429400 |
| H | 2.52419100 | 5.01203000 | 1.96573500 |
| H | 3.11479300 | 4.44007700 | 3.54940000 |
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| H | 0.07700800 | 5.14135400 | 2.73634100 |
| S | -1.65754600 | -3.43625700 | 3.92413100 |
| O | -1.22053700 | -3.40715800 | 5.32720600 |
| O | -3.11296000 | -3.45943000 | 3.66932300 |
| O | -0.91592900 | -2.44979200 | 3.06514600 |
| C | -1.07644600 | -5.09461200 | 3.27036000 |
| F | -1.43655200 | -5.24251500 | 1.99282300 |
| F | 0.24724400 | -5.21220500 | 3.35697700 |
| F | -1.63927700 | -6.06982200 | 3.98589700 |
| Cl | 0.46383400 | -2.55758800 | 0.39259700 |
| C | -4.19704300 | -2.82985700 | -3.22741600 |
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| H | -3.36779500 | -3.13885000 | -3.88824800 |
| H | -3.86640100 | -0.06861100 | 1.73382000 |
| H | -3.30218000 | -1.42745000 | 2.86509600 |
| C | -2.16771500 | 1.84569800 | 2.46800200 |
| H | -2.75985200 | 2.49244000 | 3.13974000 |
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| H | -2.57907400 | 1.93438600 | 1.45706500 |
| C | -1.56656900 | 0.20346100 | 4.31235400 |
| H | -1.98163900 | 0.94488500 | 5.01807700 |
| H | -1.72766300 | -0.80028700 | 4.71178800 |
| H | -0.48469700 | 0.39077200 | 4.27337400 |

uM06-L/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4290.3380123
PBE0-D3/def2-TZVPP-CPCM(toluene)//uB3LYP-D3/def2-SVP-CPCM(toluene)
HF = -4287.6669036

# Appendix 2: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 2 (Mechanistic Studies of Photoactivation for Synthesis of Difluoro-Substituted Products)

## A2.1 Computational Methods

### *A2.1.a Computational Methods in the study of Trifunctionalization of Cinnamyl Alcohols Provides Access to Brominated α,α-Difluoro-γ-lactones via a Photoinduced Radical–Polar–Radical Mechanism*

All optimizations of intermediates and transition states were calculated using unrestricted UB3LYP-D3/def2-SVP,[226,227] level of theory, with the "guess=mix," "nosymm," and "empiricaldispersion=gd3"[228] keywords as implemented in Gaussian16 Revision C.01.[230] These optimizations were performed using the CPCM implicit solvation model[229] with acetonitrile as the solvent by using the "SCRF=(CPCM,solvent=acetonitrile)" keyword. Frequency calculations (at the same level of theory) were used to obtain thermal corrections (at 298K) and to characterize all optimized structures as either transition states (containing only one imaginary frequency) or intermediates (containing no imaginary frequencies). To refine energetics and for method comparison, single point energy calculations were performed in implicit solvent (CPCM(acetonitrile), as above) using UωB97XD/def2-SVP[233] and UB3LYP-D3/def2-TZVPP[226,227] levels of theory. All 3-D structures were generated using CYLview20.[234] Exhaustive conformational searches were performed for all structures to elucidate the lowest energy profiles for each potential reaction pathway.

### *A2.1.b Computational Methods in the study of Transition Metal-Free Photochemical C–F Activation for the Preparation of Difluorinated-Oxindole Derivatives*

All optimizations of intermediates and transition states were calculated using unrestricted UB3LYP-D3/def2-SVP[226,227] level of theory, with the "guess=mix," "nosymm," and "empiricaldispersion=gd3"[228] keywords as implemented in Gaussian16 Revision C.01.[230] These optimizations were performed using the CPCM implicit solvation model[229] with dimethyl

sulfoxide (DMSO) as the solvent by using the "SCRF=(CPCM,solvent=DMSO)" keyword. Frequency calculations (at the same level of theory) were used to obtain thermal corrections (at 298K) and to characterize all optimized structures as either transition states (containing only one imaginary frequency) or intermediates (containing no imaginary frequencies). In order to determine the excitation energy for the thiolate anion, Time-Dependent DFT (TD-DFT)[235] computations were employed. To this end, single point energies of the singlet state structure were calculated using the "td=(nstates=6)" keyword. To refine energetics and for method comparison, single point energy calculations were performed in implicit solvent (CPCM(DMSO), as above) using UωB97XD/def2-SVP[233] and UB3LYP-D3/def2-TZVPP[226,227] levels of theory. All 3-D structures were generated using CYLview20.[234] Exhaustive conformational searches were performed for all structures to elucidate the lowest energy profiles for each potential reaction pathway.

Minimum energy crossing point (MECP) calculations[236] were performed using the ORCA software.[237] Optimizations were performed in the gas phase with a triplet spin state at the UB3LYP-D3/def2-SVP level of theory using the "SurfCrossOpt," "SlowConv," "UNO," "UCO," and "D3" keywords to obtain the geometries of the MECPs. In the "%mecp" block, the keyword "Mult 1" was used to identify the crossing point between the triplet and singlet states. Frequency calculations were then performed using these optimized geometries at the UB3LYP-D3/def2-SVP level of theory with implicit solvent (CPCM(DMSO)) in order to obtain thermal corrections (at 298K). Energetics of the MECPs were then confirmed using single-point calculations using UωB97XD/def2-SVP[233] and UB3LYP-D3/def2-TZVPP[226,227] levels of theory with implicit solvent (CPCM(DMSO)) in Gaussian16.[230]

A2.2 Supplementary Figures

*A2.2.a Supplementary Figures in the study of Trifunctionalization of Cinnamyl Alcohols Provides Access to Brominated α,α-Difluoro-γ-lactones via a Photoinduced Radical–Polar–Radical Mechanism*

Preliminary experimental evidence suggested the formation of the ethyl difluoroacetate radical **I•** was key to the initiation of the reaction. As such, we proposed that this radical is formed by single electron transfer (SET) with the iridium photocatalyst, and this radical can then undergo ring closure before X-atom transfer (XAT) with the bromodifluoroester yields the product **C-2** and reforms the radical intermediate **II•**. The energetics of this proposed pathways are shown in **Figure A2.2.a1** below.

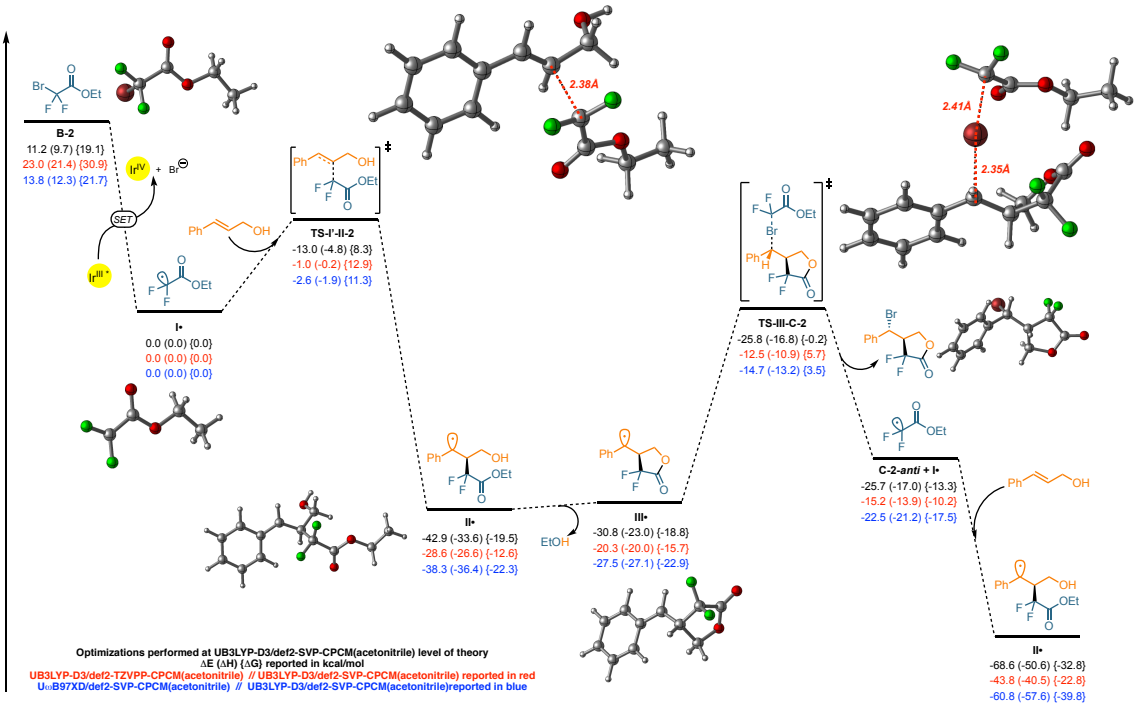



**Figure A2.2.a1.** Potential energy surface for photoinduced cinnamyl alcohol functionalization. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory, ΔE (ΔH in parenthesis) {ΔG in brackets} reported in kcal/mol. Single point energies are also shown.

SET between the excited iridium photocatalyst and the ester starting material **B-2** is highly energetically favorable (ΔG = -30.9 kcal/mol at UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory). Following SET, the radical ethyl

difluoroacetate **I•** can undergo Giese addition with the cinnamyl alcohol to form the linear radical species **II•**. This process is highly energetically favorable (ΔG = -21.4 kcal/mol) with a relatively low energy barrier for the transition state **TS-I'-II-2** ($\Delta G^{\ddagger}$ = +12.9 kcal/mol). This Giese addition should be irreversible. In order to explain the regioselectivity of the Giese addition, we performed calculations on both addition to the benzylic position and the β-position of the benzene ring. These results are summarized in **Figure A2.2.a2** below. Formation of the benzylic radical (via addition to the β-position) is energetically favorable compared to formation of the aliphatic radical ($\Delta\Delta G^{\ddagger}$ = -2.3 kcal/mol), and the benzylic radical product is more favorable in energy by 10.7 kcal/mol. This can be readily explained by the stability provided by resonance with the benzene ring, which likely is the source of the regioselectivity for this step.

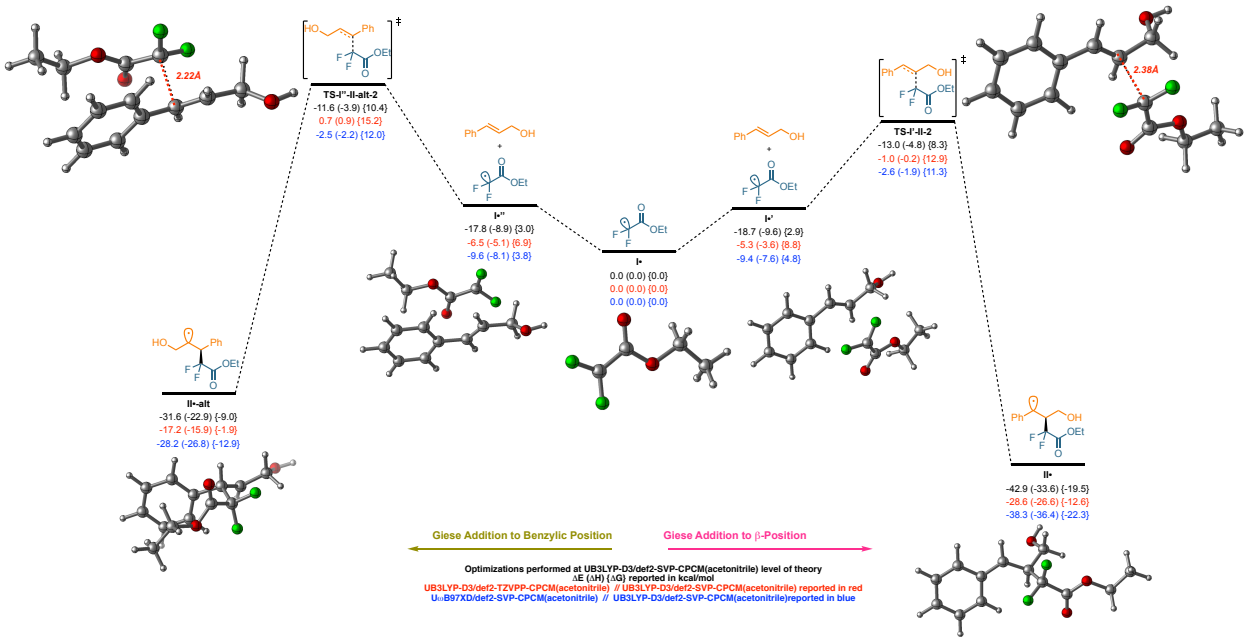



**Figure A2.2.a2** Regioselectivity of Giese addition. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory, ΔE (ΔH in parenthesis) {ΔG in brackets} reported in kcal/mol. Single point energies are also shown.

Following Giese addition to form the linear radical species **II•**, there are two competing mechanistic pathways for the following reaction steps: an "early closure" wherein **II•** undergoes

lactonization and then proceeds through XAT to form the product **C-2**, and a "late closure" mechanism wherein **II•** undergoes XAT to form the linear species **IV**, followed by lactonization to form the product **C-2**. In order to determine which pathway is more feasible, we explored both mechanistic pathways. The results of these computations are summarized in **Figure A2.2.a3** below. These computations suggest that the "early closure" XAT process is significantly lower in energy than the corresponding "late closure" XAT process ($\Delta\Delta G^{\ddagger}$ = 4.2 kcal/mol). Additionally, XAT with the linear radical **III•** is further uphill in energy than XAT for **III•**. Experimental evidence from TEMPO experiments also suggests that the "late closure" pathway is not the major mechanistic pathway. When TEMPO was added to the reaction after 1 hour, a TEMPO adduct with **III•** was detected, while no linear TEMPO adduct with **II•** was isolated. This suggests that **II•** very quickly undergoes lactonization to form the more stable radical **III•** which can be a more long-lived radical intermediate that will then undergo XAT to form the product.

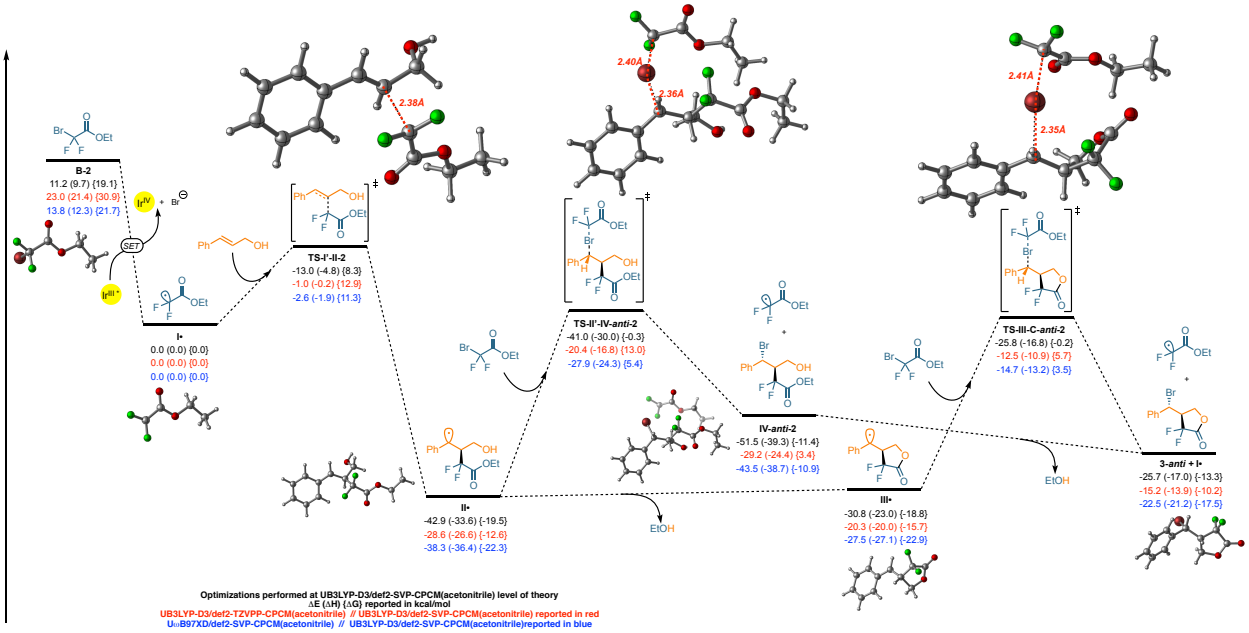



**Figure A2.2.a3.** Comparison of energetics for "early closure" and "late closure" mechanistic pathways. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory, ΔE (ΔH in parenthesis) {ΔG in brackets} reported in kcal/mol. Single point energies are also shown.

As seen in the energetics of the diastereoselective XAT transition states (see **Figure A2.2.a4** below), **TS-III-C-*anti*-2** is slightly preferred over **TS-III-C-*syn*-2** ($\Delta\Delta G^{\ddagger}$ = 1.2 kcal/mol). This predicted selectivity aligns with the experimental observations of the preference for the *anti*-product, which provides further support for the "early closure" pathway. This difference in energy between the diastereoselective transition states may be due to non-covalent interactions between the bromodifluoroester (**B-2**) and the lactone ring which could help stabilize the *anti*-transition state more since the bromodifluoroester is slightly closer to the lactone ring in the *anti*-transition state than in the *syn*-transition state.

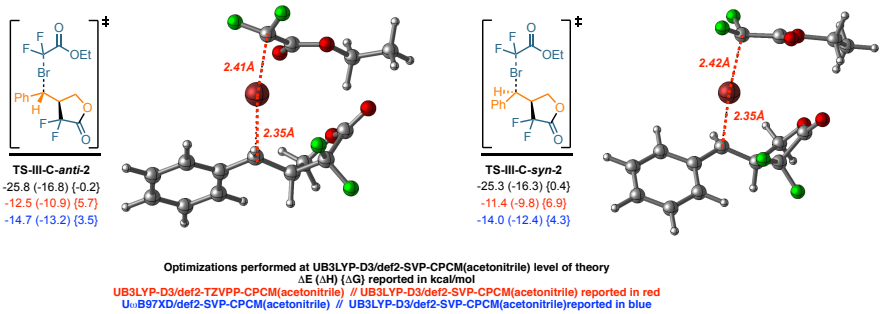



**Figure A2.2.a4.** Energetics of diastereoselective XAT for "early closure" mechanistic pathway. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) level of theory, ΔE (ΔH in parenthesis) {ΔG in brackets} reported in kcal/mol. Single point energies are also shown.

Interestingly, the product (**C-2**) is uphill in energy from the lactone radical intermediate **III•**. This would usually suggest that the radical chain mechanism described herein is not possible, as the long-lived lactone radical intermediate **III•** would be stable enough not to react to form the product. However, when **III•** undergoes XAT with the bromodifluoroester (**B-2**), not only is the product (**C-2**) formed, but the difluoroester radical **I•** is reformed as well. This is of note because Giese addition of the cinnamyl alcohol (**A1-2**) to **I•** is significantly exergonic and proceeds with a relatively low energy barrier. The energy released by performing this Giese addition enough to overcome the energy requirements for the XAT process itself. As such, Giese

addition of the concurrently formed radical **I•** acts as a driving force for the reaction, allowing for turnover of the long-lived radical intermediate **III•**.

*A2.2.b Supplementary Figures in the study of Transition Metal-Free Photochemical C–F Activation for the Preparation of Difluorinated-Oxindole Derivatives*

We proposed that the mechanism for the benzenethiol promoted C-F activation discussed in the manuscript would initiate from defluorination of ethyl 2,2,2-trifluoroacetate (**K-2**). In order to accomplish this defluorination, we proposed the catalytic cycle shown in **Figure A2.2.b1** below. In this reaction, the thiophenol (**i-2**) is deprotonated by the base ($KHCO_3$) to form a thiophenolate anion (**ii-2**). This anion can then be excited (by purple-light irradiation) to an excited singlet state (**ii-2***) before relaxation to the triplet anion **iii-2**. The triplet state anion III can then undergo single-electron transfer (SET) with ethyl 2,2,2-trifluoroacetate (**K-2**) to concurrently form **a•$^-$** and the thiolate radical (**iv-2**). This SET process is exergonic ($\Delta G$ = -5.6 kcal/mol at UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO) level of theory) and will result in the formation of the radical anion species **a•$^-$** which can undergo a spin-center shift to allow for defluorination (see **Figure A2.2.b2** below). The thiolate radical **iv-2** is then able to undergo hydrogen atom transfer (HAT) with the sodium formate to reform **i-2**, which can then proceed through the catalytic cycle again, while a $CO_2$•$^-$ radical anion is also formed. The thiolate radical is also prone to undergo dimerization to form **v-2**, as this process is highly exergonic. From this dimer, SET with the $CO_2$•$^-$ radical anion species formed during the HAT process is highly exergonic and creates both **ii-2**, which can continue the catalytic cycle, and **iv-2**, which can undergo HAT again and form **i-2**.

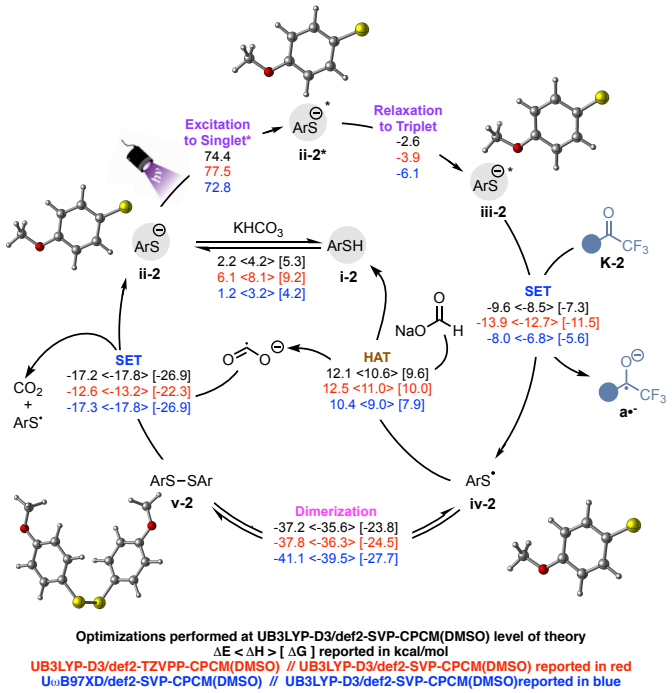



**Figure A2.2.b1.** Energetics of thiolate catalytic cycle. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(DMSO) level of theory, ΔE <ΔH in angle brackets> [ΔG in square brackets] for each relevant step reported in kcal/mol. Single point energies are also shown.

The thiophenol-based catalytic cycle described herein can be exploited to form **a**•$^-$ via SET between **K-2** and **iii-2** as described above. Once **a**•$^-$ is formed, it can undergo the mechanistic pathway outlined in **Figure A2.2.b2** below. **a**•$^-$ can undergo a spin-center shift (SCS) to form the carbon centered radical **b**•$^-$. Scans of the C-F bond suggest that this spin-center shift proceeds via a 1,2-F migration pathway where the fluorine is transferred to the carbonyl carbon to form **b**•$^-$ before being released as a fluoride anion. This migration pathway via **TS-a-b-2** is energetically feasible and reversible ($\Delta G^{\ddagger}$ = 13.3 kcal/mol). Even though the process to form the carbon-centered radical **c**• is endergonic ($\Delta G$ = 6.1 kcal/mol), following Giese addition step (**TS-c-d-2**) is highly exergonic ($\Delta G$ = -23.0 kcal/mol) with a relatively low energy barrier ($\Delta G^{\ddagger}$ = 10.5 kcal/mol), so the SCS process is reasonable. Following radical addition of **c**• to the alkene (*N*-arylmethacrylamide, **J-2**) to form **d**•, ring closure can proceed via **TS-d-e-2** to form the closed ring radical species **e**•.

Subsequently, numerous radical species in solution, including intermediates **a•⁻**, **c•**, and the radical anion $CO_2$•⁻, can be used to perform HAT with **e•** to yield the oxindole product **L-2**. A comparison of the energetics for these pathways can be seen in **Figure A2.2.b3** below. This HAT will proceed through a MECP (**MECP-e-L-2**) to form the product **L-2** irreversibly. This process is extremely exergonic (ΔG = -67.9 kcal/mol) with a very low energy barrier ($\Delta G^{\ddagger}$ = 5.6 kcal/mol).

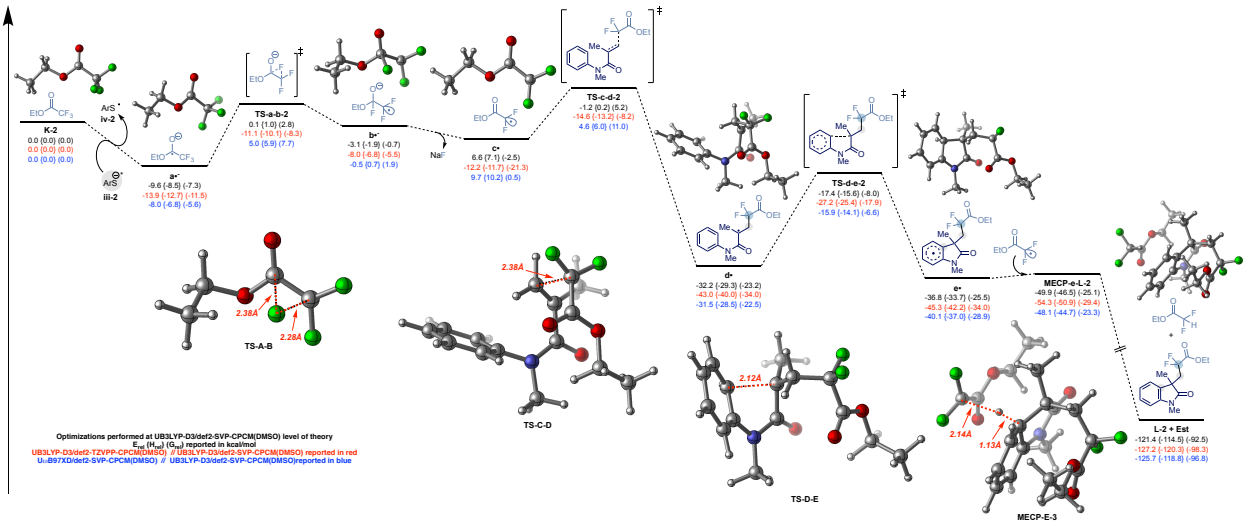



**Figure A2.2.b2.** Potential energy surface for C-F activation to form difluorinated-oxindole derivatives. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(DMSO) level of theory, $E_{rel}$ {$H_{rel}$ in braces} ($G_{rel}$ in parenthesis) for each relevant step reported in kcal/mol. Single point energies are also shown.

Each of these potential HAT pathways can proceed either in the triplet state (via **TS-e-L-2***) before relaxation to the singlet, or via a MECP to cross between the triplet and singlet states during the HAT process. These MECPs are significantly lower in energy than the corresponding triplet state transition states, suggesting that the pathways through the MECPs are more feasible. We propose that HAT with intermediate **c•** is the most likely pathway. The products of this MECP (**L-2** + **Est**) are significantly lower in energy than the alternatives for intermediate **a•⁻** and $CO_2$•⁻. Experimental evidence also suggests that ethyl 2,2-difluoroacetate, which is formed concurrently with product **L-2,** is observed over the course of the reaction, further supporting HAT with intermediate **c•** as a major pathway for HAT.

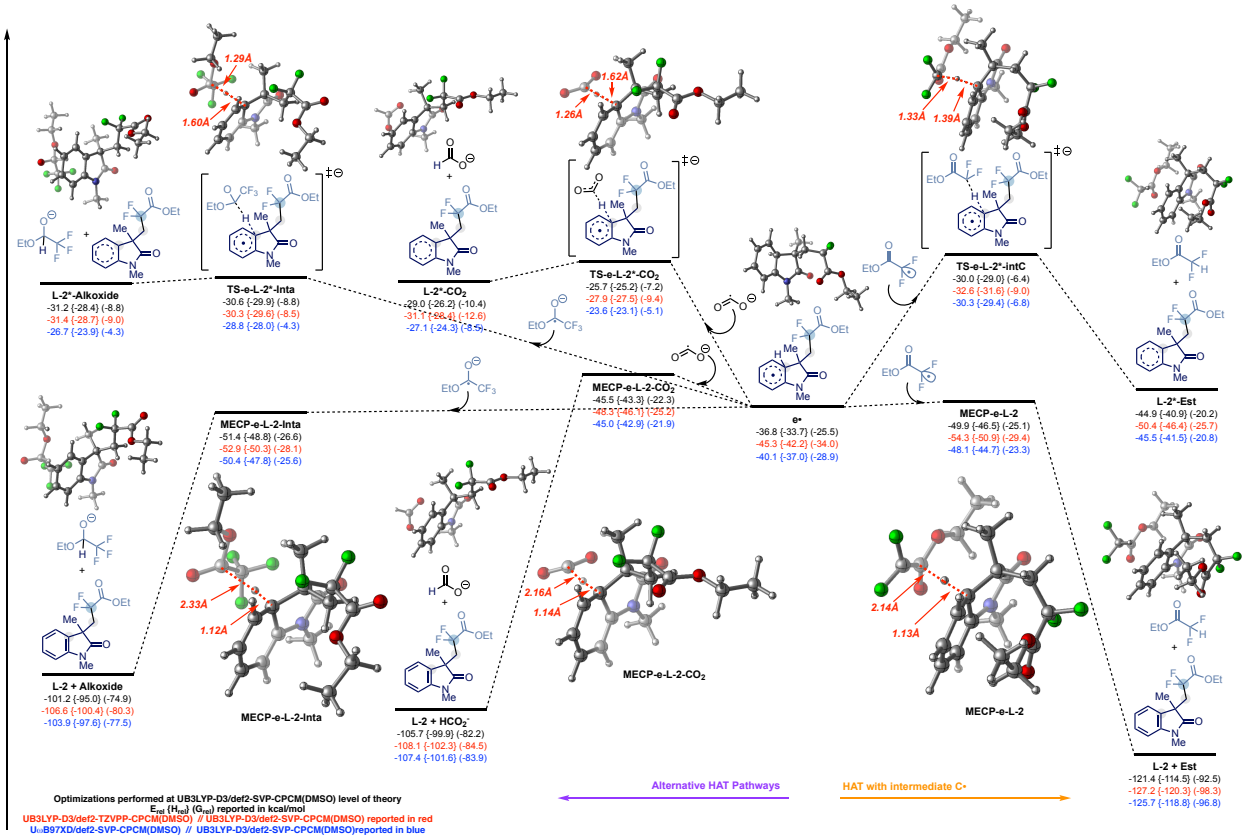



**Figure A2.2.b3.** Comparison of energetics for potential radical HAT pathways. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(DMSO) level of theory, $E_{rel}$ {$H_{rel}$ in braces} ($G_{rel}$ in parenthesis) for each relevant step reported in kcal/mol. Single point energies are also shown.

It is also possible that the HAT could proceed via a carbocation pathway. In this case, the thiol radical **iv-2** could undergo SET to form the thiolate anion **ii-2** and the carbocation **F**. From here, deprotonation with base can rapidly yield the desired product. The energetics of such pathways are shown in **Figure A2.2.b4** below. While this pathway is slightly less energetically favorable than the radical HAT pathways described above, the reaction is still energetically feasible and the rearomatization process is irreversible.

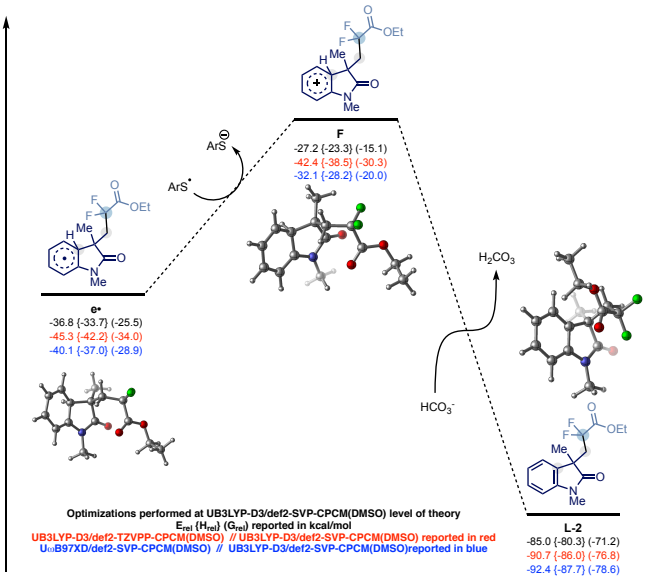



**Figure A2.2.b4.** Energetics for polar HAT pathway. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(DMSO) level of theory, $E_{rel}$ {$H_{rel}$ in braces} ($G_{rel}$ in parenthesis) for each relevant step reported in kcal/mol. Single point energies are also shown.

## A2.3 Coordinates & Energies

### *A2.3.a Coordinates & Energies in the study of Trifunctionalization of Cinnamyl Alcohols Provides Access to Brominated α,α-Difluoro-γ-lactones via a Photoinduced Radical–Polar–Radical Mechanism*

**A1-2**

Zero-point correction= 0.166322 (Hartree/Particle)
Thermal correction to Energy= 0.175677
Thermal correction to Enthalpy= 0.176621
Thermal correction to Gibbs Free Energy= 0.130819
Sum of electronic and zero-point Energies= -423.722192
Sum of electronic and thermal Energies= -423.712837
Sum of electronic and thermal Enthalpies= -423.711892
Sum of electronic and thermal Free Energies= -423.757695

| | | | |
|---|---|---|---|
| C | -3.50003900 | -0.48576100 | -0.17687600 |
| C | -2.10363100 | -0.43334300 | 0.00816900 |
| C | -1.50656800 | 0.83536100 | 0.16952500 |
| C | -2.27582600 | 1.99856500 | 0.13988500 |
| C | -3.66303900 | 1.92797300 | -0.04804700 |
| C | -4.27189900 | 0.67913800 | -0.20556900 |
| H | -3.98494200 | -1.45822000 | -0.30141200 |
| H | -0.42829200 | 0.91480300 | 0.32384200 |
| H | -1.79090100 | 2.96999500 | 0.26721500 |
| H | -4.26293500 | 2.84125100 | -0.06890800 |
| H | -5.35306700 | 0.61015300 | -0.35113200 |
| C | -1.33834400 | -1.69185600 | 0.02139200 |
| H | -1.94712300 | -2.60048100 | -0.06647300 |
| C | -0.00676500 | -1.83752100 | 0.12771200 |
| H | 0.65377800 | -0.96548500 | 0.19695700 |
| C | 0.69646100 | -3.15861500 | 0.17930800 |
| H | -0.02577300 | -3.98192300 | 0.00656500 |
| H | 1.10665200 | -3.30232600 | 1.20170800 |
| O | 1.74253100 | -3.15884500 | -0.78282500 |
| H | 2.29548300 | -3.93512500 | -0.62052100 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -424.3662876
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -423.7342235

**B-2**

Zero-point correction= 0.092485 (Hartree/Particle)
Thermal correction to Energy= 0.102339
Thermal correction to Enthalpy= 0.103283
Thermal correction to Gibbs Free Energy= 0.054778
Sum of electronic and zero-point Energies= -3078.977723
Sum of electronic and thermal Energies= -3078.967870
Sum of electronic and thermal Enthalpies= -3078.966925
Sum of electronic and thermal Free Energies= -3079.015430

| | | | |
|---|---|---|---|
| O | 1.88419600 | -3.10493800 | -0.01335500 |
| C | 0.65267400 | -3.30373900 | -0.43716000 |
| C | 2.81659700 | -4.21481300 | -0.13249700 |
| H | 2.38686200 | -5.08038600 | 0.39519500 |
| H | 2.90300800 | -4.47603300 | -1.19856700 |
| C | 4.13298100 | -3.77149100 | 0.46198700 |
| H | 4.01337000 | -3.50727900 | 1.52361400 |
| H | 4.86346600 | -4.59108200 | 0.38713900 |
| H | 4.53241500 | -2.89887200 | -0.07663500 |
| O | 0.20136100 | -4.30089000 | -0.93515000 |
| C | -0.21011800 | -2.04215300 | -0.19273300 |
| Br | -0.70257300 | -1.96384000 | 1.72158700 |
| F | 0.45096700 | -0.92608000 | -0.51734600 |
| F | -1.32294800 | -2.10517800 | -0.92221600 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3079.9843331

UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3078.944186

**I•**

Zero-point correction= 0.089752 (Hartree/Particle)
Thermal correction to Energy= 0.098557
Thermal correction to Enthalpy= 0.099501
Thermal correction to Gibbs Free Energy= 0.054440
Sum of electronic and zero-point Energies= -505.056088
Sum of electronic and thermal Energies= -505.047284
Sum of electronic and thermal Enthalpies= -505.046340
Sum of electronic and thermal Free Energies= -505.091401

| | | | |
|---|---|---|---|
| O | 2.05558600 | -3.01267500 | 0.04632900 |
| C | 0.73439700 | -3.13903300 | -0.12691300 |
| C | 2.83921300 | -4.22296700 | -0.04907100 |
| H | 2.46999900 | -4.94184400 | 0.70035300 |
| H | 2.67938200 | -4.67004100 | -1.04349300 |
| C | 4.28726900 | -3.85224300 | 0.18200700 |
| H | 4.42288500 | -3.40558200 | 1.17888000 |
| H | 4.91540600 | -4.75352100 | 0.11625200 |
| H | 4.63239700 | -3.13171900 | -0.57523000 |
| O | 0.13895100 | -4.17417600 | -0.36408900 |
| C | 0.05701800 | -1.86664100 | 0.05602900 |
| F | 0.68409200 | -0.72016100 | 0.14679100 |
| F | -1.21978300 | -1.75058500 | -0.20520800 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -505.7471047
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -504.9872513

**I•'**

Zero-point correction= 0.258518 (Hartree/Particle)
Thermal correction to Energy= 0.277907
Thermal correction to Enthalpy= 0.278851
Thermal correction to Gibbs Free Energy= 0.207778
Sum of electronic and zero-point Energies= -928.793814
Sum of electronic and thermal Energies= -928.774425
Sum of electronic and thermal Enthalpies= -928.773481
Sum of electronic and thermal Free Energies= -928.844554

| | | | |
|---|---|---|---|
| O | 0.87052600 | -2.67390600 | 0.44635700 |
| C | -0.14098000 | -2.17214000 | 1.16237000 |
| C | 1.31714500 | -4.01227200 | 0.76937700 |
| H | 0.43589100 | -4.63910500 | 0.97437400 |
| H | 1.91502600 | -3.96029700 | 1.69409700 |
| C | 2.11630500 | -4.52645500 | -0.40784200 |
| H | 1.47839000 | -4.58513300 | -1.30219000 |
| H | 2.50001000 | -5.53288000 | -0.18096700 |
| H | 2.97301300 | -3.86821600 | -0.61896100 |
| O | -0.70376900 | -2.72069300 | 2.09278400 |
| F | -0.04548200 | -0.32185300 | -0.41238000 |
| F | -1.58678400 | -0.26395800 | 1.14512400 |
| C | -0.49449900 | -0.83633600 | 0.70764300 |
| C | -1.74812700 | -2.87286000 | -1.51285900 |
| H | -1.66144000 | -3.67067400 | -0.76655500 |
| C | -0.62880900 | -2.81232500 | -2.50522200 |
| H | 0.25165800 | -2.35864400 | -2.00917400 |
| H | -0.90470800 | -2.15447700 | -3.35227400 |
| C | -3.85976400 | -1.94975500 | -0.48367500 |
| C | -4.99625400 | -1.16222200 | -0.75666700 |
| C | -3.81346300 | -2.64557200 | 0.74301700 |
| C | -6.05809100 | -1.08642000 | 0.14843200 |
| H | -5.04620800 | -0.60551400 | -1.69676000 |
| C | -4.87328000 | -2.56896300 | 1.64681800 |
| H | -2.92885600 | -3.22556600 | 1.00992600 |
| C | -6.00272200 | -1.79278500 | 1.35430200 |
| H | -6.93039000 | -0.47164400 | -0.08813600 |
| H | -4.81404800 | -3.11136300 | 2.59411500 |
| H | -6.82930600 | -1.73318500 | 2.06683000 |
| O | -0.32776100 | -4.13442000 | -2.94006600 |
| H | 0.45853000 | -4.09265300 | -3.50128700 |
| C | -2.77683200 | -2.00782000 | -1.47888200 |
| H | -2.83796100 | -1.25368700 | -2.27332800 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -930.1218611
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -928.7363832

**TS-I'-II-2**

Zero-point correction= 0.257704 (Hartree/Particle)
Thermal correction to Energy= 0.276375
Thermal correction to Enthalpy= 0.277319
Thermal correction to Gibbs Free Energy= 0.207414
Sum of electronic and zero-point Energies= -928.785553
Sum of electronic and thermal Energies= -928.766882
Sum of electronic and thermal Enthalpies= -928.765938
Sum of electronic and thermal Free Energies= -928.835843

| | | | |
|---|---|---|---|
| O | 1.13886100 | -2.92411200 | 0.33662200 |
| C | 0.02415200 | -2.46155300 | 0.90949200 |
| C | 1.68252800 | -4.15755600 | 0.86233900 |
| H | 0.88028000 | -4.91201700 | 0.88574700 |
| H | 2.00585100 | -3.98240000 | 1.90092200 |
| C | 2.83084800 | -4.56946400 | -0.03117400 |
| H | 2.48157900 | -4.74580900 | -1.06018600 |
| H | 3.27962600 | -5.50005100 | 0.34805600 |
| H | 3.60940700 | -3.79169200 | -0.05247200 |
| O | -0.55181000 | -2.97150300 | 1.85203100 |
| F | 0.25513600 | -0.61728800 | -0.63751500 |
| F | -1.42042500 | -0.57427800 | 0.77065800 |
| C | -0.53121900 | -1.32950400 | 0.15513300 |
| C | -1.83920500 | -2.59670500 | -1.37354700 |
| H | -1.81965200 | -3.44710100 | -0.68451000 |
| C | -0.83809200 | -2.66670100 | -2.49469900 |
| H | 0.17939800 | -2.76248700 | -2.07493700 |
| H | -0.86691800 | -1.72408800 | -3.07641200 |
| C | -4.05019300 | -1.79974900 | -0.46129200 |
| C | -5.23684000 | -1.09676600 | -0.76821100 |
| C | -3.97221600 | -2.46250000 | 0.78698200 |
| C | -6.31338800 | -1.07762600 | 0.11967200 |
| H | -5.31059000 | -0.56744500 | -1.72228900 |
| C | -5.04763200 | -2.43727900 | 1.67293600 |
| H | -3.04910200 | -2.96568100 | 1.08154900 |
| C | -6.22548100 | -1.75119000 | 1.34363100 |
| H | -7.22399100 | -0.53276700 | -0.14209500 |
| H | -4.96597100 | -2.94900700 | 2.63539900 |
| H | -7.06526800 | -1.73422900 | 2.04276700 |
| O | -1.16005200 | -3.79566400 | -3.29760200 |
| H | -0.41250600 | -3.96006100 | -3.88887400 |
| C | -2.95858800 | -1.81185400 | -1.42731400 |
| H | -3.03826600 | -1.09086500 | -2.24956400 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -930.1149836
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -928.7256634

**II•**

Zero-point correction= 0.260119 (Hartree/Particle)
Thermal correction to Energy= 0.278283
Thermal correction to Enthalpy= 0.279227
Thermal correction to Gibbs Free Energy= 0.210752
Sum of electronic and zero-point Energies= -928.830815
Sum of electronic and thermal Energies= -928.812651
Sum of electronic and thermal Enthalpies= -928.811707
Sum of electronic and thermal Free Energies= -928.880181

| | | | |
|---|---|---|---|
| O | 1.37044500 | -3.11982700 | 0.22463700 |
| C | 0.16250700 | -3.27163300 | 0.74069500 |
| C | 2.36137700 | -4.12982300 | 0.55232300 |
| H | 1.96120500 | -5.11221800 | 0.25617900 |
| H | 2.49702700 | -4.13723000 | 1.64491300 |
| C | 3.63379800 | -3.77964500 | -0.18434600 |
| H | 3.46737100 | -3.77334500 | -1.27231300 |
| H | 4.40906600 | -4.52639100 | 0.04458700 |
| H | 4.00391500 | -2.78919100 | 0.12117900 |
| O | -0.19569200 | -4.16406100 | 1.46968900 |
| F | -0.16299700 | -1.12005000 | -0.26049100 |
| F | -1.50026900 | -1.74943400 | 1.35462100 |
| C | -0.82678100 | -2.19160200 | 0.25374800 |
| C | -1.82364900 | -2.74740800 | -0.77978500 |
| H | -2.25563300 | -3.64743900 | -0.31321300 |
| C | -1.08248100 | -3.19338100 | -2.04617000 |
| H | -0.25602400 | -3.88096500 | -1.78126400 |
| H | -0.62314400 | -2.30455700 | -2.52044500 |
| C | -4.11902400 | -1.60462300 | -0.38788200 |
| C | -5.07720300 | -0.63825700 | -0.82692400 |
| C | -4.46057900 | -2.38626000 | 0.75914200 |
| C | -6.29044700 | -0.47360700 | -0.17098700 |
| H | -4.84157000 | -0.02339000 | -1.69997100 |
| C | -5.67830900 | -2.21220500 | 1.40670200 |
| H | -3.74951300 | -3.11659600 | 1.14754000 |
| C | -6.60452700 | -1.25976100 | 0.95062800 |
| H | -7.00417400 | 0.27218700 | -0.53084300 |
| H | -5.91353600 | -2.82197100 | 2.28310100 |
| H | -7.55922000 | -1.12909800 | 1.46565600 |
| O | -2.02574500 | -3.82007100 | -2.88770300 |
| H | -1.59148700 | -4.03246600 | -3.72472100 |
| C | -2.89921500 | -1.75105300 | -1.09275300 |
| H | -2.71722800 | -1.08362600 | -1.94028600 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -930.1589546
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -928.7825373

**III•**

Zero-point correction= 0.178807 (Hartree/Particle)
Thermal correction to Energy= 0.191068
Thermal correction to Enthalpy= 0.192012
Thermal correction to Gibbs Free Energy= 0.138481
Sum of electronic and zero-point Energies= -773.961775
Sum of electronic and thermal Energies= -773.949513
Sum of electronic and thermal Enthalpies= -773.948569
Sum of electronic and thermal Free Energies= -774.002100

| | | | |
|---|---|---|---|
| C | -1.16588900 | -2.09141400 | 0.89566800 |
| C | 0.01415100 | -2.56008000 | 1.52411500 |
| C | 1.02363500 | -3.29848600 | 0.83410000 |
| C | 0.22748500 | -2.29732600 | 2.91252600 |
| C | 2.16153600 | -3.74381000 | 1.49722900 |
| H | 0.91403400 | -3.50702500 | -0.23142400 |
| C | 1.36874800 | -2.74748000 | 3.56356000 |
| H | -0.52859200 | -1.73177400 | 3.46382300 |
| C | 2.34543100 | -3.47573700 | 2.86340500 |
| H | 2.92076900 | -4.30523200 | 0.94662800 |
| H | 1.50657400 | -2.53317400 | 4.62649600 |
| H | 3.24266100 | -3.82875700 | 3.37720100 |
| C | -1.51419200 | -2.32591000 | -0.54405000 |
| C | -0.83574800 | -1.32776500 | -1.49214700 |
| C | -2.98671100 | -2.00526300 | -0.86198400 |
| H | -1.25384600 | -3.34583200 | -0.86652100 |
| H | -3.34338700 | -2.54806700 | -1.74893000 |
| H | -3.66498400 | -2.18777900 | -0.02034800 |
| F | 0.40436100 | -0.93953100 | -1.13956100 |
| F | -0.76036000 | -1.84099100 | -2.75663400 |
| C | -1.81713100 | -0.13120100 | -1.52294900 |
| O | -3.02166400 | -0.58217400 | -1.15451200 |
| O | -1.57101200 | 1.00111100 | -1.82746500 |
| H | -1.86348700 | -1.49469000 | 1.49058700 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -775.0252363
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -773.8845381

**III•'**

Zero-point correction= 0.272785 (Hartree/Particle)
Thermal correction to Energy= 0.296719
Thermal correction to Enthalpy= 0.297663
Thermal correction to Gibbs Free Energy= 0.214215
Sum of electronic and zero-point Energies= -3852.955288
Sum of electronic and thermal Energies= -3852.931354
Sum of electronic and thermal Enthalpies= -3852.930410
Sum of electronic and thermal Free Energies= -3853.013858

| | | | |
|---|---|---|---|
| C | -0.69595400 | -1.79988000 | 0.82314400 |
| C | -2.06572900 | -1.61652800 | 0.51253200 |
| C | -2.70501300 | -2.25452600 | -0.59334900 |
| C | -2.86375000 | -0.75261900 | 1.32303100 |
| C | -4.05192000 | -2.03627300 | -0.86367300 |
| H | -2.13829400 | -2.93013600 | -1.23736800 |
| C | -4.20710500 | -0.54199600 | 1.04248800 |
| H | -2.39432200 | -0.24077500 | 2.16628600 |
| C | -4.81388900 | -1.18056500 | -0.05265600 |
| H | -4.51895300 | -2.53769700 | -1.71527700 |
| H | -4.79432400 | 0.12777300 | 1.67604500 |
| H | -5.87094800 | -1.01227900 | -0.27165100 |
| C | 0.24403100 | -2.61792600 | -0.01092800 |
| C | 1.63902700 | -2.70348100 | 0.59915700 |
| C | 0.59897200 | -1.96290800 | -1.37264400 |
| H | -0.13983700 | -3.63862200 | -0.17365100 |
| H | 0.89956700 | -2.70880100 | -2.12239500 |
| H | -0.19494900 | -1.32004200 | -1.76492300 |
| F | 1.68900100 | -2.70248600 | 1.94616100 |
| F | 2.28504400 | -3.82514300 | 0.16392900 |
| C | 2.38318600 | -1.47801300 | 0.01121400 |
| O | 1.74197000 | -1.10858300 | -1.10177700 |
| O | 3.36616500 | -0.94618200 | 0.44463900 |
| Br | 0.94943500 | 1.41640700 | 2.02135700 |
| H | -0.29743400 | -1.29483500 | 1.70406100 |
| O | 1.40487700 | 2.21770800 | -1.09296400 |
| C | 0.21874600 | 1.76101800 | -0.76023500 |
| C | 2.01146800 | 1.80320200 | -2.35165600 |
| H | 1.54655300 | 0.86217700 | -2.66969600 |
| H | 1.77777900 | 2.58678000 | -3.08866600 |
| C | 3.49742000 | 1.65321200 | -2.11535300 |
| H | 3.68449700 | 0.87728500 | -1.35836700 |
| H | 3.98868100 | 1.35780400 | -3.05532600 |
| H | 3.94081400 | 2.60170700 | -1.77573300 |
| O | -0.51118300 | 1.03882600 | -1.38803400 |
| C | -0.16983800 | 2.29275700 | 0.64339200 |
| F | 0.01258500 | 3.61575700 | 0.72078700 |
| F | -1.45016500 | 2.02542100 | 0.89514400 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3855.0186673
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3852.8416147

**TS-III-C-2-*anti***

Zero-point correction= 0.272715 (Hartree/Particle)
Thermal correction to Energy= 0.296240
Thermal correction to Enthalpy= 0.297184
Thermal correction to Gibbs Free Energy= 0.214866
Sum of electronic and zero-point Energies= -3852.930117

Sum of electronic and thermal Energies= -3852.906592
Sum of electronic and thermal Enthalpies= -3852.905648
Sum of electronic and thermal Free Energies= -3852.987966

| | | | |
|---|---|---|---|
| C | -2.60990800 | -1.33242100 | 0.35216000 |
| C | -4.03811600 | -1.51779200 | 0.11283100 |
| C | -4.55290900 | -2.16221500 | -1.03452400 |
| C | -4.95415600 | -1.03165700 | 1.07675400 |
| C | -5.92918700 | -2.31204500 | -1.20802300 |
| H | -3.88440300 | -2.57202200 | -1.79249500 |
| C | -6.32589200 | -1.18002300 | 0.89836800 |
| H | -4.57090600 | -0.52644600 | 1.96693600 |
| C | -6.82047900 | -1.81952600 | -0.24772800 |
| H | -6.30841100 | -2.82038900 | -2.09752800 |
| H | -7.01675300 | -0.79929100 | 1.65422900 |
| H | -7.89756000 | -1.93705300 | -0.38841700 |
| C | -1.58625900 | -2.10949800 | -0.44746800 |
| C | -0.15837000 | -1.98369700 | 0.08906900 |
| C | -1.38741400 | -1.70382000 | -1.93290800 |
| H | -1.86542300 | -3.17420200 | -0.38596900 |
| H | -1.28662300 | -2.58071400 | -2.58641200 |
| H | -2.18131600 | -1.04744200 | -2.30648000 |
| F | -0.05601500 | -1.56269000 | 1.36589100 |
| F | 0.48565100 | -3.18372500 | 0.00159400 |
| C | 0.55598900 | -1.01184900 | -0.87595700 |
| O | -0.15101500 | -0.95339300 | -2.00583900 |
| O | 1.59204700 | -0.44335000 | -0.67791100 |
| Br | -2.17065600 | 0.93210100 | -0.10430000 |
| H | -2.34341500 | -1.22679200 | 1.40639700 |
| O | 0.31078000 | 2.41407000 | -2.22448400 |
| C | -0.97203300 | 2.73205500 | -2.27952400 |
| C | 0.91683100 | 1.90296700 | -3.44178100 |
| H | 0.44227100 | 0.93546400 | -3.66573300 |
| H | 0.69107400 | 2.60072300 | -4.26254700 |
| C | 2.40001500 | 1.76083200 | -3.18905400 |
| H | 2.57475500 | 1.06262800 | -2.35841000 |
| H | 2.88971500 | 1.36821500 | -4.09346200 |
| H | 2.85149200 | 2.73495700 | -2.94531400 |
| O | -1.69191100 | 2.68387500 | -3.24853500 |
| C | -1.49232000 | 3.09991700 | -0.91313400 |
| F | -0.61898400 | 3.57426200 | -0.04335300 |
| F | -2.59327300 | 3.82783600 | -0.92591500 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3854.9970812
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3852.8083284

**C-2-*anti***

Zero-point correction= 0.182554 (Hartree/Particle)
Thermal correction to Energy= 0.196358
Thermal correction to Enthalpy= 0.197303
Thermal correction to Gibbs Free Energy= 0.139521
Sum of electronic and zero-point Energies= -3347.874381
Sum of electronic and thermal Energies= -3347.860576
Sum of electronic and thermal Enthalpies= -3347.859632
Sum of electronic and thermal Free Energies= -3347.917414

| | | | |
|---|---|---|---|
| C | -2.72757600 | -1.11142100 | 0.15624700 |
| C | -4.20174800 | -1.43774000 | 0.17032600 |
| C | -4.94449000 | -1.56914400 | -1.01528600 |
| C | -4.83766000 | -1.66317200 | 1.40021900 |
| C | -6.29209700 | -1.93020900 | -0.96994000 |
| H | -4.47478700 | -1.36027600 | -1.97890100 |
| C | -6.18859300 | -2.02499700 | 1.44570800 |
| H | -4.27237700 | -1.55785400 | 2.33004200 |
| C | -6.91800400 | -2.16178400 | 0.26148100 |
| H | -6.85825100 | -2.02617500 | -1.89957000 |
| H | -6.67058800 | -2.19652600 | 2.41126600 |
| H | -7.97370400 | -2.44177200 | 0.29573700 |
| C | -1.86779700 | -2.24255500 | -0.41833900 |
| C | -0.37980100 | -2.22133700 | -0.09989400 |
| C | -1.85844600 | -2.49193000 | -1.93389800 |
| H | -2.23138600 | -3.16186700 | 0.07133900 |
| H | -2.70582400 | -3.09329500 | -2.28180800 |
| H | -1.80718300 | -1.55495000 | -2.50642200 |
| F | 0.18940200 | -0.99159800 | -0.23211000 |
| F | -0.09284700 | -2.65899100 | 1.14562200 |
| C | 0.22859000 | -3.14865200 | -1.18002600 |
| O | -0.64877500 | -3.24968400 | -2.18509800 |
| O | 1.30078600 | -3.68142700 | -1.15070300 |
| Br | -2.42455500 | 0.64535100 | -0.76904300 |
| H | -2.38367500 | -0.91837000 | 1.17953300 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3349.2543964
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3347.8335905

**I•’’**

Zero-point correction= 0.257803 (Hartree/Particle)
Thermal correction to Energy= 0.277519
Thermal correction to Enthalpy= 0.278464
Thermal correction to Gibbs Free Energy= 0.206648
Sum of electronic and zero-point Energies= -928.793138
Sum of electronic and thermal Energies= -928.773422
Sum of electronic and thermal Enthalpies= -928.772478
Sum of electronic and thermal Free Energies= -928.844293

| | | | |
|---|---|---|---|
| O | 1.43837800 | -2.63098600 | 0.12159700 |
| C | 0.63248400 | -2.84005200 | 1.16401300 |
| C | 2.08343300 | -3.79658700 | -0.44493300 |
| H | 1.30489100 | -4.50059900 | -0.77230400 |
| H | 2.67469900 | -4.28660400 | 0.34531600 |
| C | 2.94306400 | -3.32891100 | -1.59685700 |
| H | 2.32532900 | -2.84249000 | -2.36623900 |
| H | 3.44684300 | -4.19354600 | -2.05503300 |
| H | 3.71070500 | -2.61795500 | -1.25466400 |
| O | 0.39109600 | -3.91240100 | 1.68392700 |
| F | 0.14754600 | -0.46176800 | 0.99097200 |
| F | -0.88568400 | -1.60665600 | 2.54731200 |
| C | 0.09132700 | -1.58325600 | 1.67186800 |
| C | -2.23042300 | -2.81089200 | -0.27709800 |
| H | -2.58083300 | -3.29095800 | 0.64442800 |
| C | -1.53270700 | -3.70600000 | -1.21549100 |
| C | -1.50604200 | -5.08873700 | -0.94680300 |
| C | -0.87568500 | -3.24411200 | -2.37496800 |
| C | -0.86282400 | -5.98075000 | -1.80903100 |
| H | -1.99279500 | -5.46515100 | -0.04336500 |
| C | -0.23426500 | -4.13347400 | -3.23677800 |
| H | -0.85116000 | -2.17572300 | -2.59830000 |
| C | -0.22544200 | -5.50727400 | -2.96038200 |
| H | -0.85533600 | -7.04890600 | -1.57786100 |
| H | 0.27253300 | -3.75233700 | -4.12683900 |
| H | 0.28326200 | -6.20080600 | -3.63435100 |
| C | -2.46956300 | -1.49751500 | -0.43395900 |
| H | -2.15634900 | -0.97226700 | -1.34325800 |
| C | -3.14851400 | -0.63262500 | 0.58236000 |
| H | -2.39685800 | 0.06593400 | 1.00433100 |
| H | -3.51803400 | -1.25074900 | 1.42468300 |
| O | -4.19683600 | 0.08295300 | -0.05522500 |
| H | -4.49939000 | 0.77131300 | 0.55240200 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -930.1238115
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -928.7367682

**TS-I’-II-alt-2**

Zero-point correction= 0.257154 (Hartree/Particle)

Thermal correction to Energy= 0.275646
Thermal correction to Enthalpy= 0.276590
Thermal correction to Gibbs Free Energy= 0.208451
Sum of electronic and zero-point Energies= -928.783878
Sum of electronic and thermal Energies= -928.765386
Sum of electronic and thermal Enthalpies= -928.764441
Sum of electronic and thermal Free Energies= -928.832581

| | | | |
|---|---|---|---|
| O | 1.52188300 | -2.97503200 | -0.03500300 |
| C | 0.67976000 | -2.82915500 | 0.98609500 |
| C | 2.31039000 | -4.18744300 | -0.06732000 |
| H | 1.62537100 | -5.04631800 | 0.00489400 |
| H | 2.96770800 | -4.20205200 | 0.81664000 |
| C | 3.08837500 | -4.19176800 | -1.36358200 |
| H | 2.40133700 | -4.18208000 | -2.22272200 |
| H | 3.70704800 | -5.10025400 | -1.42097600 |
| H | 3.75079100 | -3.31486100 | -1.42739300 |
| O | 0.55213400 | -3.59515300 | 1.92000500 |
| F | 0.14571500 | -0.72895000 | -0.07582800 |
| F | -0.71758700 | -1.13269200 | 1.89516100 |
| C | -0.21895900 | -1.66980300 | 0.78539600 |
| C | -2.02876800 | -2.58578400 | -0.11004100 |
| H | -2.17512000 | -3.11103000 | 0.84116700 |
| C | -1.41159300 | -3.39443400 | -1.18811300 |
| C | -1.18005700 | -4.76544800 | -0.97520400 |
| C | -1.00580100 | -2.82787900 | -2.41094500 |
| C | -0.57825300 | -5.55300100 | -1.96065100 |
| H | -1.47004200 | -5.21668200 | -0.02269700 |
| C | -0.40768000 | -3.61446100 | -3.39641600 |
| H | -1.13660500 | -1.75758800 | -2.58365500 |
| C | -0.19222900 | -4.98110000 | -3.17706400 |
| H | -0.40760000 | -6.61644100 | -1.77537400 |
| H | -0.09590600 | -3.15650900 | -4.33855200 |
| H | 0.28225100 | -5.59369700 | -3.94751100 |
| C | -2.79294400 | -1.46085900 | -0.33316800 |
| H | -2.83781200 | -1.00773600 | -1.32896000 |
| C | -3.48473900 | -0.69565300 | 0.74590800 |
| H | -2.81786500 | 0.13605000 | 1.06415800 |
| H | -3.62607700 | -1.33561500 | 1.64044800 |
| O | -4.71190100 | -0.19866500 | 0.24039300 |
| H | -5.06507500 | 0.43330500 | 0.88078000 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -930.1123479
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -928.725507

**II•-alt**

Zero-point correction= 0.258784 (Hartree/Particle)
Thermal correction to Energy= 0.277282
Thermal correction to Enthalpy= 0.278226
Thermal correction to Gibbs Free Energy= 0.209598
Sum of electronic and zero-point Energies= -928.814179
Sum of electronic and thermal Energies= -928.795681
Sum of electronic and thermal Enthalpies= -928.794737
Sum of electronic and thermal Free Energies= -928.863365

| | | | |
|---|---|---|---|
| O | 1.55495000 | -2.94568000 | 0.02684400 |
| C | 0.62972200 | -2.88487500 | 0.96789600 |
| C | 2.48821600 | -4.05585800 | 0.06415200 |
| H | 1.93833600 | -4.95974500 | 0.36699100 |
| H | 3.24372500 | -3.84168000 | 0.83649900 |
| C | 3.09151900 | -4.18901300 | -1.31604700 |
| H | 2.30710700 | -4.40300100 | -2.05794600 |
| H | 3.81780100 | -5.01593900 | -1.32343300 |
| H | 3.61340000 | -3.26519500 | -1.60872600 |
| O | 0.53057400 | -3.61100800 | 1.92716400 |
| F | 0.05222300 | -0.85744100 | -0.16789600 |
| F | -0.79146900 | -1.21322700 | 1.81914500 |
| C | -0.44151800 | -1.82455600 | 0.65022100 |
| C | -1.69949700 | -2.48649400 | 0.02016500 |
| H | -2.06981700 | -3.13590700 | 0.83335300 |
| C | -1.28427500 | -3.35938600 | -1.15536800 |
| C | -1.25616300 | -4.75502700 | -1.01991600 |
| C | -0.85220800 | -2.78722600 | -2.36265700 |
| C | -0.80670800 | -5.56541000 | -2.06837600 |
| H | -1.58023500 | -5.21325500 | -0.08170600 |
| C | -0.40559500 | -3.59442200 | -3.41144400 |
| H | -0.84392300 | -1.70121600 | -2.47461100 |
| C | -0.37949600 | -4.98679800 | -3.26729800 |
| H | -0.79050400 | -6.65120600 | -1.94576000 |
| H | -0.06883200 | -3.13411400 | -4.34370300 |
| H | -0.02625600 | -5.61745000 | -4.08689400 |
| C | -2.74147800 | -1.46500600 | -0.30807900 |
| H | -2.86155500 | -1.12465800 | -1.33971800 |
| C | -3.48153500 | -0.72159700 | 0.74526600 |
| H | -2.84417300 | 0.10744600 | 1.13151700 |
| H | -3.65844100 | -1.38486300 | 1.62022100 |
| O | -4.68915500 | -0.22264500 | 0.19828500 |
| H | -5.07589100 | 0.39056300 | 0.83733300 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -930.1407841
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -928.7663374

**II•'**

Zero-point correction= 0.355229 (Hartree/Particle)
Thermal correction to Energy= 0.384530
Thermal correction to Enthalpy= 0.385474
Thermal correction to Gibbs Free Energy= 0.289868
Sum of electronic and zero-point Energies= -4007.828715
Sum of electronic and thermal Energies= -4007.799415
Sum of electronic and thermal Enthalpies= -4007.798470
Sum of electronic and thermal Free Energies= -4007.894076

| | | | |
|---|---|---|---|
| O | 0.38411100 | -1.86172500 | -1.55644800 |
| C | -0.35017200 | -2.58613000 | -0.72951600 |
| C | 1.20572800 | -2.57981800 | -2.51574700 |
| H | 1.71541300 | -3.39904800 | -1.98740200 |
| H | 1.95241400 | -1.84074600 | -2.83432300 |
| C | 0.39052500 | -3.10138800 | -3.68511800 |
| H | -0.38213700 | -3.80169000 | -3.34026000 |
| H | 1.06008400 | -3.62964400 | -4.38167700 |
| H | -0.09624000 | -2.27928600 | -4.22774700 |
| O | -0.37916100 | -3.79025600 | -0.66001100 |
| F | -0.85136200 | -0.40939200 | 0.16516300 |
| F | -0.85448000 | -2.14368500 | 1.49813900 |
| C | -1.19584500 | -1.73098500 | 0.24007000 |
| C | -2.70624800 | -1.88367800 | 0.04865000 |
| H | -2.90035600 | -2.96966200 | 0.06442000 |
| C | -3.14941700 | -1.35826300 | -1.32863200 |
| H | -2.84504100 | -0.30230000 | -1.43100200 |
| H | -4.25156700 | -1.39434900 | -1.37384700 |
| C | -4.76778600 | -1.44302400 | 1.54328200 |
| C | -5.55987500 | -2.48011600 | 0.96135800 |
| C | -5.38902400 | -0.62606300 | 2.53902200 |
| C | -6.88003700 | -2.67638000 | 1.35188500 |
| H | -5.12612800 | -3.13464900 | 0.20269100 |
| C | -6.70952000 | -0.83069700 | 2.91807100 |
| H | -4.80645800 | 0.17607500 | 3.00003400 |
| C | -7.46801300 | -1.85650400 | 2.32877600 |
| H | -7.46385500 | -3.47818900 | 0.89229000 |
| H | -7.16001000 | -0.18855800 | 3.67942000 |
| H | -8.50649000 | -2.01564200 | 2.62850700 |
| O | -2.55864900 | -2.17484000 | -2.32556600 |
| H | -2.82561500 | -1.85467100 | -3.19745600 |
| C | -3.42620500 | -1.19083300 | 1.16838600 |
| H | -2.89874900 | -0.37873600 | 1.67222700 |
| O | -1.57231900 | 1.97423500 | -1.94574000 |
| C | -1.59012300 | 2.70113200 | -0.84667700 |

| | | | |
|---|---|---|---|
| C | -0.28975200 | 1.41415600 | -2.35839800 |
| H | 0.10470100 | 0.80431500 | -1.53621300 |
| H | 0.39560000 | 2.25678400 | -2.53845900 |
| C | -0.53504200 | 0.59245100 | -3.60052100 |
| H | -1.17567400 | -0.26904500 | -3.36994500 |
| H | 0.42509400 | 0.21061600 | -3.97799600 |
| H | -1.00428000 | 1.19776300 | -4.39052300 |
| O | -0.68033200 | 2.90339500 | -0.08760700 |
| C | -2.99163600 | 3.33089800 | -0.63438400 |
| Br | -4.22740300 | 1.99512400 | 0.13539300 |
| F | -3.50000500 | 3.77627000 | -1.78891400 |
| F | -2.89445900 | 4.35789800 | 0.21037800 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4010.155442
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4007.7449897

**TS-II'-IV-*anti*-2**

Zero-point correction= 0.355465 (Hartree/Particle)
Thermal correction to Energy= 0.384066
Thermal correction to Enthalpy= 0.385010
Thermal correction to Gibbs Free Energy= 0.293125
Sum of electronic and zero-point Energies= -4007.802585
Sum of electronic and thermal Energies= -4007.773984
Sum of electronic and thermal Enthalpies= -4007.773040
Sum of electronic and thermal Free Energies= -4007.864925

| | | | |
|---|---|---|---|
| O | 0.31382100 | -1.82231600 | -1.53836100 |
| C | -0.37254300 | -2.45750000 | -0.60391300 |
| C | 1.08365400 | -2.63183600 | -2.46762100 |
| H | 1.59500500 | -3.42058100 | -1.89670300 |
| H | 1.83297700 | -1.93822600 | -2.87072800 |
| C | 0.20863600 | -3.21848500 | -3.55992000 |
| H | -0.56981400 | -3.86388500 | -3.13092400 |
| H | 0.83390800 | -3.82062300 | -4.23729100 |
| H | -0.27413000 | -2.42564000 | -4.14886700 |
| O | -0.39745400 | -3.64699800 | -0.40821900 |
| F | -0.75910500 | -0.20835400 | 0.12730400 |
| F | -0.87115300 | -1.83111100 | 1.58809000 |
| C | -1.17868300 | -1.49345000 | 0.29939300 |
| C | -2.69419400 | -1.60998700 | 0.08864000 |
| H | -2.90376500 | -2.69024200 | 0.18479400 |
| C | -3.07670400 | -1.20981500 | -1.34584700 |
| H | -2.59248100 | -0.25324900 | -1.59861500 |
| H | -4.16522900 | -1.04364300 | -1.40186400 |
| C | -4.83789000 | -1.29568200 | 1.51483100 |
| C | -5.61827100 | -2.14173100 | 0.69373300 |
| C | -5.41522500 | -0.81054300 | 2.71367600 |
| C | -6.92185100 | -2.48108100 | 1.05850300 |
| H | -5.20579000 | -2.55939900 | -0.22540400 |
| C | -6.71658000 | -1.14845000 | 3.07146500 |
| H | -4.82631500 | -0.15278600 | 3.35814500 |
| C | -7.47896500 | -1.98440400 | 2.24252600 |
| H | -7.50604000 | -3.14270400 | 0.41446800 |
| H | -7.14203900 | -0.76297400 | 4.00110900 |
| H | -8.50094900 | -2.25102300 | 2.52233000 |
| O | -2.65506300 | -2.25640300 | -2.20206600 |
| H | -2.77360400 | -1.98047400 | -3.12070900 |
| C | -3.46364900 | -0.91115600 | 1.19556100 |
| H | -2.86069500 | -0.67587100 | 2.07492900 |
| O | -1.49674000 | 2.06429800 | -2.12350700 |
| C | -1.50535200 | 2.91413900 | -1.10457500 |
| C | -0.20795200 | 1.53047200 | -2.52877000 |
| H | 0.23513200 | 1.01021200 | -1.66797600 |
| H | 0.44380900 | 2.37432700 | -2.80303800 |
| C | -0.44855800 | 0.59023500 | -3.68694600 |
| H | -1.06464700 | -0.26259000 | -3.37197000 |
| H | 0.51448100 | 0.19686400 | -4.04525500 |
| H | -0.94671300 | 1.10746100 | -4.52068500 |
| O | -0.54432200 | 3.30674400 | -0.48788600 |
| C | -2.91821300 | 3.28662000 | -0.72964400 |
| Br | -3.54755600 | 1.35620600 | 0.55204600 |
| F | -3.79281400 | 3.35330800 | -1.72216000 |
| F | -3.00756800 | 4.35144600 | 0.04905400 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4010.1301607
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4007.7100691

**IV-*anti***

Zero-point correction= 0.356685 (Hartree/Particle)
Thermal correction to Energy= 0.386121
Thermal correction to Enthalpy= 0.387065
Thermal correction to Gibbs Free Energy= 0.292053
Sum of electronic and zero-point Energies= -4007.818120
Sum of electronic and thermal Energies= -4007.788684
Sum of electronic and thermal Enthalpies= -4007.787740
Sum of electronic and thermal Free Energies= -4007.882752

| | | | |
|---|---|---|---|
| O | 0.28405700 | -1.70923500 | -1.51156000 |
| C | -0.51729900 | -2.24259400 | -0.60852600 |
| C | 1.02538400 | -2.62654200 | -2.36313400 |
| H | 1.46902200 | -3.40348900 | -1.72311800 |
| H | 1.82845500 | -2.00772400 | -2.78367600 |
| C | 0.15351700 | -3.23624400 | -3.44576900 |
| H | -0.67263300 | -3.81065900 | -3.00541000 |
| H | 0.76688900 | -3.91648500 | -4.05695000 |
| H | -0.26433600 | -2.46216200 | -4.10386800 |
| O | -0.68473100 | -3.41948200 | -0.40041100 |
| F | -0.81111700 | 0.06816500 | -0.00709500 |
| F | -0.86583000 | -1.46347200 | 1.55187700 |
| C | -1.24648100 | -1.19245600 | 0.26527500 |
| C | -2.77412900 | -1.29923800 | 0.12910200 |
| H | -2.96666800 | -2.38413900 | 0.14911200 |
| C | -3.22428700 | -0.77275600 | -1.23795500 |
| H | -2.79736500 | 0.22711100 | -1.41199900 |
| H | -4.32183900 | -0.66410500 | -1.24693000 |
| C | -4.90632200 | -1.27926200 | 1.60255600 |
| C | -5.59313300 | -2.11493300 | 0.70717000 |
| C | -5.51682900 | -0.97265700 | 2.83388900 |
| C | -6.85925500 | -2.61833400 | 1.03031800 |
| H | -5.15166800 | -2.40233600 | -0.24726800 |
| C | -6.77766600 | -1.47258000 | 3.15556800 |
| H | -4.99467300 | -0.32364800 | 3.54166900 |
| C | -7.45778400 | -2.29745400 | 2.25015300 |
| H | -7.37485000 | -3.26817600 | 0.31909500 |
| H | -7.23129500 | -1.22137200 | 4.11745300 |
| H | -8.44645600 | -2.69062800 | 2.49911400 |
| O | -2.77688600 | -1.70426700 | -2.21006500 |
| H | -2.95489500 | -1.34875400 | -3.09099900 |
| C | -3.52202100 | -0.73030100 | 1.33743400 |
| H | -2.91281300 | -0.87203600 | 2.23536800 |
| O | -1.28919500 | 2.00311100 | -2.39315000 |
| C | -1.31165300 | 2.88277400 | -1.38693000 |
| C | -0.00638900 | 1.43418800 | -2.74673200 |
| H | 0.40288500 | 0.91723100 | -1.86820000 |
| H | 0.67516700 | 2.25562600 | -3.02040000 |
| C | -0.25039700 | 0.47794400 | -3.89062200 |
| H | -0.93530000 | -0.31815000 | -3.56889400 |
| H | 0.69837100 | 0.01347900 | -4.19786700 |
| H | -0.68305400 | 0.99860200 | -4.75830700 |
| O | -0.35905100 | 3.23789900 | -0.72074700 |
| C | -2.64870900 | 3.43896200 | -1.22096700 |
| Br | -3.61136900 | 1.29709400 | 1.25261000 |
| F | -3.70758400 | 2.91947100 | -1.79510100 |
| F | -2.92977700 | 4.16913200 | -0.16978300 |

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

HF = -4010.1442802
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4007.7349738

**II•’’**

Zero-point correction= 0.354371 (Hartree/Particle)
Thermal correction to Energy= 0.384130
Thermal correction to Enthalpy= 0.385074
Thermal correction to Gibbs Free Energy= 0.286729
Sum of electronic and zero-point Energies= -4007.826900
Sum of electronic and thermal Energies= -4007.797141
Sum of electronic and thermal Enthalpies= -4007.796197
Sum of electronic and thermal Free Energies= -4007.894542

| | | | |
|---|---|---|---|
| O | -1.58529600 | -3.76755500 | -2.71713700 |
| C | -1.58228700 | -2.61285900 | -2.07469400 |
| C | -0.47968900 | -4.02030800 | -3.62570600 |
| H | 0.45878100 | -3.89791600 | -3.06308400 |
| H | -0.50377100 | -3.25501400 | -4.41678600 |
| C | -0.64904600 | -5.41845400 | -4.17345200 |
| H | -0.62557500 | -6.16278400 | -3.36284600 |
| H | 0.17050800 | -5.64107500 | -4.87324800 |
| H | -1.60331400 | -5.51472700 | -4.71322000 |
| O | -0.76900300 | -1.72912300 | -2.20060900 |
| F | -3.64405600 | -3.50368800 | -1.23137700 |
| F | -3.46771900 | -1.34829300 | -1.56571800 |
| C | -2.78699700 | -2.44990900 | -1.12137700 |
| C | -2.36529300 | -2.25663200 | 0.33686700 |
| H | -1.55632000 | -1.51125000 | 0.30739900 |
| C | -1.78264800 | -3.57529000 | 0.90577100 |
| H | -2.59580400 | -4.31179300 | 1.01440100 |
| H | -1.39294000 | -3.35974700 | 1.91280200 |
| C | -3.41239900 | -0.86437700 | 2.24398500 |
| C | -2.16995200 | -0.30557900 | 2.67933700 |
| C | -4.59039000 | -0.46002000 | 2.94641500 |
| C | -2.12204100 | 0.60184800 | 3.73264800 |
| H | -1.24024600 | -0.59285200 | 2.18470700 |
| C | -4.52847400 | 0.44535900 | 3.99717500 |
| H | -5.55418300 | -0.87335900 | 2.63726800 |
| C | -3.29527600 | 0.98743600 | 4.39945000 |
| H | -1.15893200 | 1.01592500 | 4.04189000 |
| H | -5.44627500 | 0.73965200 | 4.51284100 |
| H | -3.25011200 | 1.70145500 | 5.22502300 |
| O | -0.72013900 | -4.08089700 | 0.11629300 |
| H | -1.06633500 | -4.76048300 | -0.47747500 |
| C | -3.51556600 | -1.77031000 | 1.16103900 |
| H | -4.50263900 | -2.17486600 | 0.92055500 |
| O | -2.49974200 | 0.94424700 | -3.48536300 |
| C | -1.58064900 | 1.68543700 | -2.90399700 |
| C | -2.05824400 | 0.05172400 | -4.54701800 |
| H | -1.17892600 | -0.49679700 | -4.18393200 |
| H | -1.75262500 | 0.67364500 | -5.40309900 |
| C | -3.21071500 | -0.86552800 | -4.88493600 |
| H | -3.51763900 | -1.44043500 | -3.99986700 |
| H | -2.90078500 | -1.56785800 | -5.67354800 |
| H | -4.07881900 | -0.29451400 | -5.24782300 |
| O | -0.40311300 | 1.72109900 | -3.14851200 |
| C | -2.20824900 | 2.56940300 | -1.79871900 |
| Br | -2.31500400 | 1.54476500 | -0.11149400 |
| F | -3.43645100 | 2.98176700 | -2.13285500 |
| F | -1.44164700 | 3.64440500 | -1.59892500 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4010.1551184
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4007.7424728

**TS-II’-IV-*syn*-2**

Zero-point correction= 0.354539 (Hartree/Particle)
Thermal correction to Energy= 0.383591
Thermal correction to Enthalpy= 0.384535
Thermal correction to Gibbs Free Energy= 0.289686
Sum of electronic and zero-point Energies= -4007.799355
Sum of electronic and thermal Energies= -4007.770303
Sum of electronic and thermal Enthalpies= -4007.769358
Sum of electronic and thermal Free Energies= -4007.864208

| | | | |
|---|---|---|---|
| O | -1.69627800 | -4.02869100 | -2.66044800 |
| C | -1.55684800 | -2.80316500 | -2.19143000 |
| C | -0.63684500 | -4.52844300 | -3.51937100 |
| H | 0.30750600 | -4.48460800 | -2.95472500 |
| H | -0.54696600 | -3.85126000 | -4.38280500 |
| C | -1.00238100 | -5.93714000 | -3.92585200 |
| H | -1.09264000 | -6.58901200 | -3.04360400 |
| H | -0.21848400 | -6.34585900 | -4.58117100 |
| H | -1.95654300 | -5.95143400 | -4.47416300 |
| O | -0.64982700 | -2.04442200 | -2.43600600 |
| F | -3.61516200 | -3.39702500 | -1.10314000 |
| F | -3.43713000 | -1.45007500 | -2.06419200 |
| C | -2.75132400 | -2.36024300 | -1.31318500 |
| C | -2.29613300 | -1.78755800 | 0.03777400 |
| H | -1.39804500 | -1.18499100 | -0.16267400 |
| C | -1.88904300 | -2.98993400 | 0.94270700 |
| H | -2.79806000 | -3.48379300 | 1.32336800 |
| H | -1.33473200 | -2.60519600 | 1.80867300 |
| C | -3.19231500 | -0.51865700 | 2.10216700 |
| C | -1.92960700 | -0.15734400 | 2.62736100 |
| C | -4.32300300 | -0.42518600 | 2.94388700 |
| C | -1.80480600 | 0.25926300 | 3.95035000 |
| H | -1.04576600 | -0.18460700 | 1.98639300 |
| C | -4.19336400 | -0.01072400 | 4.26900800 |
| H | -5.30702100 | -0.68889800 | 2.54782900 |
| C | -2.93449500 | 0.33143000 | 4.77820100 |
| H | -0.82240800 | 0.53503800 | 4.34099100 |
| H | -5.07727900 | 0.04622900 | 4.90873800 |
| H | -2.83282400 | 0.65843500 | 5.81577900 |
| O | -1.04723500 | -3.89780600 | 0.25848700 |
| H | -1.58978300 | -4.59076900 | -0.14314700 |
| C | -3.36372700 | -0.94836800 | 0.71341300 |
| H | -4.38590200 | -1.25426000 | 0.46705600 |
| O | -2.60750800 | 1.22932700 | -3.77558200 |
| C | -2.09756900 | 2.15392200 | -2.97625200 |
| C | -1.66504000 | 0.38026300 | -4.48014000 |
| H | -0.96916900 | -0.04348900 | -3.74171200 |
| H | -1.09017100 | 1.00487300 | -5.18197600 |
| C | -2.45484400 | -0.69944400 | -5.18374700 |
| H | -3.02714900 | -1.28913200 | -4.45361600 |
| H | -1.76395700 | -1.37271600 | -5.71377900 |
| H | -3.15304300 | -0.26843400 | -5.91758100 |
| O | -0.92812400 | 2.42859400 | -2.84280700 |
| C | -3.17463100 | 2.77900500 | -2.12932500 |
| Br | -3.35862500 | 1.09607000 | -0.41870700 |
| F | -4.37786300 | 2.88179100 | -2.67105600 |
| F | -2.82317400 | 3.91111700 | -1.54443900 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4010.1282613
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4007.7066836

**IV-*syn***

Zero-point correction= 0.355415 (Hartree/Particle)
Thermal correction to Energy= 0.385394
Thermal correction to Enthalpy= 0.386338
Thermal correction to Gibbs Free Energy= 0.287395
Sum of electronic and zero-point Energies= -4007.814515
Sum of electronic and thermal Energies= -4007.784537
Sum of electronic and thermal Enthalpies= -4007.783593
Sum of electronic and thermal Free Energies= -4007.882535

| | | | |
|---|---|---|---|
| O | -1.72309700 | -3.53512100 | -2.61986600 |
| C | -1.37146900 | -2.39905900 | -2.04486500 |
| C | -0.71492600 | -4.21467400 | -3.41406500 |
| H | 0.09592600 | -4.52223700 | -2.73513500 |
| H | -0.29826200 | -3.49570300 | -4.13517300 |
| C | -1.38086900 | -5.39010900 | -4.09062100 |
| H | -1.80491300 | -6.08258000 | -3.34770900 |
| H | -0.63912700 | -5.93675100 | -4.69222500 |
| H | -2.18777700 | -5.05028900 | -4.75761100 |
| O | -0.30908600 | -1.83760700 | -2.15998600 |
| F | -3.60799000 | -2.58825700 | -1.18636000 |
| F | -2.92844900 | -0.68135200 | -1.99439900 |
| C | -2.52896800 | -1.75464700 | -1.24661200 |
| C | -2.11149600 | -1.35340600 | 0.17248400 |
| H | -1.12141200 | -0.88243600 | 0.09058800 |
| C | -1.98138500 | -2.65496400 | 1.01202800 |
| H | -2.98307900 | -2.99268000 | 1.32431300 |
| H | -1.41244200 | -2.42999900 | 1.92328700 |
| C | -3.06032500 | -0.32970400 | 2.32837100 |
| C | -1.87463500 | 0.00649800 | 3.00531700 |
| C | -4.20466500 | -0.64438500 | 3.07457800 |
| C | -1.83546700 | 0.01924700 | 4.39945200 |
| H | -0.98179900 | 0.26969500 | 2.43258000 |
| C | -4.16601200 | -0.63172500 | 4.47382500 |
| H | -5.13262700 | -0.90428000 | 2.55828600 |
| C | -2.98243000 | -0.30142200 | 5.13870300 |
| H | -0.90781600 | 0.28173600 | 4.91384400 |
| H | -5.06523900 | -0.88017900 | 5.04275000 |
| H | -2.95094500 | -0.28991100 | 6.23095800 |
| O | -1.28687000 | -3.66884800 | 0.30759100 |
| H | -1.92782800 | -4.23994000 | -0.13785700 |
| C | -3.11517700 | -0.38205600 | 0.82347900 |
| H | -4.13189800 | -0.63439900 | 0.49852100 |
| O | -2.62557000 | 0.83541900 | -4.35454100 |
| C | -2.18957500 | 1.83270500 | -3.57958500 |
| C | -1.63616900 | -0.09838100 | -4.83994500 |
| H | -0.92939900 | -0.32158600 | -4.02836800 |
| H | -1.07344600 | 0.38614500 | -5.65518000 |
| C | -2.36559000 | -1.33676500 | -5.31428200 |
| H | -2.90042500 | -1.81521400 | -4.48080300 |
| H | -1.64365400 | -2.05809500 | -5.72643800 |
| H | -3.09367900 | -1.08933100 | -6.10165300 |
| O | -1.03193800 | 2.06379400 | -3.28560200 |
| C | -3.29298000 | 2.68183800 | -3.15421400 |
| Br | -2.85281500 | 1.49754600 | 0.13324300 |
| F | -4.55022600 | 2.32286000 | -3.24944700 |
| F | -3.08591700 | 3.63888400 | -2.28310500 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4010.1422813
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -4007.7314709

**III•''**

Zero-point correction= 0.272444 (Hartree/Particle)
Thermal correction to Energy= 0.296557
Thermal correction to Enthalpy= 0.297501
Thermal correction to Gibbs Free Energy= 0.212423
Sum of electronic and zero-point Energies= -3852.953631
Sum of electronic and thermal Energies= -3852.929518
Sum of electronic and thermal Enthalpies= -3852.928574
Sum of electronic and thermal Free Energies= -3853.013652

| | | | |
|---|---|---|---|
| C | -1.19225800 | -2.14335400 | 0.88622800 |
| C | -0.00481300 | -2.58977100 | 1.51639400 |
| C | 1.02056400 | -3.30886300 | 0.83069400 |
| C | 0.20465300 | -2.30676200 | 2.90191800 |
| C | 2.17413100 | -3.71094300 | 1.49356900 |
| H | 0.91061600 | -3.53406800 | -0.23117500 |
| C | 1.36354400 | -2.71148400 | 3.55177900 |
| H | -0.56563700 | -1.75838600 | 3.45076100 |
| C | 2.35809200 | -3.41720300 | 2.85476500 |
| H | 2.94678900 | -4.25741600 | 0.94677100 |
| H | 1.50048100 | -2.47847600 | 4.61074500 |
| H | 3.26937200 | -3.73428700 | 3.36712200 |
| C | -1.53656800 | -2.36298200 | -0.55803500 |
| C | -0.83043200 | -1.37357900 | -1.49400500 |
| C | -2.99465000 | -1.98151700 | -0.87154800 |
| H | -1.30884500 | -3.38849200 | -0.88832400 |
| H | -3.36282400 | -2.46935200 | -1.78504600 |
| H | -3.68630400 | -2.17407500 | -0.04351100 |
| F | 0.44312600 | -1.07374400 | -1.18082100 |
| F | -0.82953500 | -1.84228300 | -2.77894400 |
| C | -1.74988100 | -0.12956100 | -1.44823200 |
| O | -2.97120000 | -0.54382800 | -1.09871500 |
| O | -1.45410500 | 1.00715100 | -1.68823100 |
| Br | 0.57915200 | 0.90397200 | 1.50730900 |
| H | -1.90193200 | -1.56511300 | 1.48465400 |
| O | 1.43400400 | 2.29132100 | -1.32392500 |
| C | 0.74612500 | 3.02494200 | -0.47581200 |
| C | 1.14669300 | 2.44064600 | -2.74218900 |
| H | 0.05966900 | 2.52787700 | -2.86231100 |
| H | 1.61954500 | 3.37660700 | -3.07992600 |
| C | 1.70122100 | 1.22556900 | -3.44910200 |
| H | 1.20559100 | 0.31567200 | -3.08366300 |
| H | 1.52186400 | 1.31659900 | -4.53123600 |
| H | 2.78535700 | 1.13086800 | -3.28346100 |
| O | -0.09211000 | 3.85117500 | -0.72228700 |
| C | 1.18047100 | 2.70901200 | 0.97830300 |
| F | 2.51572300 | 2.76546300 | 1.09153300 |
| F | 0.64964200 | 3.60461900 | 1.81159000 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3855.0178152
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3852.8399588

**TS-III''-C-2-*syn***

Zero-point correction= 0.272678 (Hartree/Particle)
Thermal correction to Energy= 0.296239
Thermal correction to Enthalpy= 0.297184
Thermal correction to Gibbs Free Energy= 0.215088
Sum of electronic and zero-point Energies= -3852.929334
Sum of electronic and thermal Energies= -3852.905772
Sum of electronic and thermal Enthalpies= -3852.904828
Sum of electronic and thermal Free Energies= -3852.986923

| | | | |
|---|---|---|---|
| C | -2.72855000 | -0.16387300 | 1.84506700 |
| C | -1.80052200 | -1.10205600 | 2.47513500 |
| C | -1.20597100 | -2.18804100 | 1.79445500 |
| C | -1.50801000 | -0.93199500 | 3.85040700 |
| C | -0.35375200 | -3.06520500 | 2.46595700 |
| H | -1.41376800 | -2.36291400 | 0.73991100 |
| C | -0.65108100 | -1.80405500 | 4.51386100 |
| H | -1.95622600 | -0.09345900 | 4.38939700 |
| C | -0.06782000 | -2.87613900 | 3.82282900 |
| H | 0.08932200 | -3.90467700 | 1.92506200 |
| H | -0.43630200 | -1.65371800 | 5.57446100 |
| H | 0.60393300 | -3.56339200 | 4.34270700 |
| C | -3.32887800 | -0.42474500 | 0.47968800 |
| C | -2.41008500 | -0.30237900 | -0.74592600 |
| C | -4.46236500 | 0.55923300 | 0.09897400 |
| H | -3.72353900 | -1.45385600 | 0.48910400 |
| H | -5.32226200 | 0.04142000 | -0.34645200 |
| H | -4.79998600 | 1.16775200 | 0.94686400 |
| F | -1.08703700 | -0.39904500 | -0.51623300 |
| F | -2.73176900 | -1.26161900 | -1.66288200 |
| C | -2.75217100 | 1.07023400 | -1.37099800 |
| O | -3.93128900 | 1.46750400 | -0.89596700 |
| O | -2.09490800 | 1.66555100 | -2.17772400 |

| | | | |
|---|---|---|---|
| Br | -1.65349200 | 1.91840800 | 1.68203100 |
| H | -3.46182400 | 0.24701500 | 2.54399600 |
| O | -2.24063100 | 4.71185400 | -0.34761800 |
| C | -0.98079200 | 4.42541300 | -0.06346700 |
| C | -2.58752000 | 4.89675300 | -1.74660300 |
| H | -2.13603400 | 5.84238700 | -2.08698400 |
| H | -2.14930500 | 4.06779200 | -2.31881800 |
| C | -4.09630700 | 4.90854900 | -1.83955700 |
| H | -4.52563700 | 5.71443900 | -1.22467400 |
| H | -4.39867000 | 5.07138400 | -2.88543900 |
| H | -4.50327700 | 3.94346000 | -1.50327200 |
| O | -0.06385600 | 4.31357100 | -0.84134400 |
| C | -0.81942400 | 4.17592900 | 1.41548800 |
| F | 0.43273500 | 4.15304200 | 1.82994700 |
| F | -1.57327400 | 4.90197800 | 2.22299800 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3854.9953036
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3852.8071821

**3-*syn***

Zero-point correction= 0.182545 (Hartree/Particle)
Thermal correction to Energy= 0.196402
Thermal correction to Enthalpy= 0.197346
Thermal correction to Gibbs Free Energy= 0.139416
Sum of electronic and zero-point Energies= -3347.878904
Sum of electronic and thermal Energies= -3347.865047
Sum of electronic and thermal Enthalpies= -3347.864103
Sum of electronic and thermal Free Energies= -3347.922034

| | | | |
|---|---|---|---|
| C | -2.71885200 | -1.01986700 | 0.07212000 |
| H | -2.50046500 | -0.31747600 | -0.73995700 |
| C | -4.17592300 | -1.39155800 | 0.06714000 |
| C | -5.05043600 | -0.74376300 | -0.81880300 |
| C | -4.68142300 | -2.38759000 | 0.92067100 |
| C | -6.40542400 | -1.08799200 | -0.85710800 |
| H | -4.66644600 | 0.03336400 | -1.48482100 |
| C | -6.03367200 | -2.73068200 | 0.88253700 |
| H | -4.01813200 | -2.88984900 | 1.62889200 |
| C | -6.89949600 | -2.08213600 | -0.00744900 |
| H | -7.07494000 | -0.57778900 | -1.55376100 |
| H | -6.41500800 | -3.50661100 | 1.55064500 |
| H | -7.95794500 | -2.35221500 | -0.03621900 |
| Br | -2.28608400 | 0.04741700 | 1.72389800 |
| C | -1.77232400 | -2.21133800 | -0.02124300 |
| C | -0.30302200 | -1.88838900 | -0.25865900 |
| C | -2.07769500 | -3.11317200 | -1.23561500 |
| H | -1.80974700 | -2.81847300 | 0.89538100 |
| H | -2.81505000 | -3.89284800 | -1.01438700 |
| H | -2.41425500 | -2.53111500 | -2.10705400 |
| F | -0.14712000 | -0.78329000 | -1.04731500 |
| F | 0.42201500 | -1.69531200 | 0.86030400 |
| C | 0.22256000 | -3.11399100 | -1.04678700 |
| O | -0.82734200 | -3.75723800 | -1.57028900 |
| O | 1.36568600 | -3.44217300 | -1.18392900 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3349.2592166
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -3347.8382664

**$Ir^{III}(ppy)_3$-singlet**

Zero-point correction= 0.481078 (Hartree/Particle)
Thermal correction to Energy= 0.509794
Thermal correction to Enthalpy= 0.510738
Thermal correction to Gibbs Free Energy= 0.420788
Sum of electronic and zero-point Energies= -1539.314328
Sum of electronic and thermal Energies= -1539.285612
Sum of electronic and thermal Enthalpies= -1539.284668
Sum of electronic and thermal Free Energies= -1539.374618

| | | | |
|---|---|---|---|
| Ir | 1.76744600 | -3.15876000 | -1.72001100 |
| C | 3.15989900 | -3.05775000 | 0.93776000 |
| C | 0.84089400 | -3.09282200 | 1.29252900 |
| C | 3.37303300 | -3.01295600 | 2.32756900 |
| C | 4.21524600 | -3.06517400 | -0.08831300 |
| C | 0.98974700 | -3.05128800 | 2.67533800 |
| H | -0.14695700 | -3.12287500 | 0.82812000 |
| C | 2.28745700 | -3.01055100 | 3.19870000 |
| H | 4.38823300 | -2.97903800 | 2.72208700 |
| C | 3.77770500 | -3.10404200 | -1.44808700 |
| C | 5.58630500 | -3.02917300 | 0.23442100 |
| H | 0.10986700 | -3.04935000 | 3.32029600 |
| H | 2.45062200 | -2.97615000 | 4.27833100 |
| C | 4.78233300 | -3.10844600 | -2.43885200 |
| C | 6.55038900 | -3.03146300 | -0.77200200 |
| H | 5.91099800 | -2.99883300 | 1.27739500 |
| C | 6.14104700 | -3.07145500 | -2.11353400 |
| H | 4.48779400 | -3.13740600 | -3.49083100 |
| H | 7.61237200 | -3.00274700 | -0.51564600 |
| H | 6.89152200 | -3.07379600 | -2.91027500 |
| C | 1.90883500 | -5.79205400 | -3.15463500 |
| C | 1.88048000 | -6.18390300 | -0.84144300 |
| C | 1.97506100 | -7.17749300 | -3.38965500 |
| C | 1.88449800 | -4.74955000 | -4.19352500 |
| C | 1.94300100 | -7.56339200 | -1.01209600 |
| H | 1.84368500 | -5.73556300 | 0.15357700 |
| C | 1.99130000 | -8.06547600 | -2.31792300 |
| H | 2.01479500 | -7.55557500 | -4.41091100 |
| C | 1.82567900 | -3.39764200 | -3.73440400 |
| C | 1.92289400 | -5.04990500 | -5.56958100 |
| H | 1.95503300 | -8.22205100 | -0.14250600 |
| H | 2.04219900 | -9.14174100 | -2.49815400 |
| C | 1.80495700 | -2.39120700 | -4.72312100 |
| C | 1.90375700 | -4.02847500 | -6.51755300 |
| H | 1.96783600 | -6.08703100 | -5.91077500 |
| C | 1.84460300 | -2.69434400 | -6.08688800 |
| H | 1.76069500 | -1.34458400 | -4.41184500 |
| H | 1.93426500 | -4.26752400 | -7.58351700 |
| H | 1.82912400 | -1.88593800 | -6.82462300 |
| C | -0.88849700 | -1.76482700 | -1.84437900 |
| C | -1.24337200 | -4.08406100 | -1.84973900 |
| C | -2.27732400 | -1.55094200 | -1.91117800 |
| C | 0.13702600 | -0.70978700 | -1.80193400 |
| C | -2.62525900 | -3.93451800 | -1.91348300 |
| H | -0.77941500 | -5.07228900 | -1.82592000 |
| C | -3.14805500 | -2.63632400 | -1.94488600 |
| H | -2.67141600 | -0.53533900 | -1.93768900 |
| C | 1.49605600 | -1.14785800 | -1.74636000 |
| C | -0.18554300 | 0.66164900 | -1.82003100 |
| H | -3.26991900 | -4.81423500 | -1.93944600 |
| H | -4.22693000 | -2.47261800 | -1.99627200 |
| C | 2.48611500 | -0.14334600 | -1.70625600 |
| C | 0.82025200 | 1.62567300 | -1.78256600 |
| H | -1.22795200 | 0.98666000 | -1.86304900 |
| C | 2.16099400 | 1.21579200 | -1.72541100 |
| H | 3.53752300 | -0.43822900 | -1.66339800 |
| H | 0.56401300 | 2.68796900 | -1.79731600 |
| H | 2.95727900 | 1.96615500 | -1.69544400 |
| N | 1.86079900 | -5.32748700 | -1.87512500 |
| N | 1.88795300 | -3.09926000 | 0.45235200 |
| N | -0.40363500 | -3.03727100 | -1.81317800 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -1541.3537646
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -1539.2681362

**$Ir^{III}$ ***

Zero-point correction= 0.477445 (Hartree/Particle)
Thermal correction to Energy= 0.506712
Thermal correction to Enthalpy= 0.507657
Thermal correction to Gibbs Free Energy= 0.415791
Sum of electronic and zero-point Energies= -1539.224155
Sum of electronic and thermal Energies= -1539.194888
Sum of electronic and thermal Enthalpies= -1539.193944
Sum of electronic and thermal Free Energies= -1539.285809

| | | | |
|---|---|---|---|
| Ir | 1.77285700 | -3.15150100 | -1.77303700 |
| C | 3.14193600 | -3.05295600 | 0.91771100 |
| C | 0.82257500 | -3.01577300 | 1.26489000 |
| C | 3.35420300 | -2.98901300 | 2.30653200 |
| C | 4.20105400 | -3.10030300 | -0.10403500 |
| C | 0.96931900 | -2.95198400 | 2.64688900 |
| H | -0.16501600 | -3.02851500 | 0.79998000 |
| C | 2.26622900 | -2.93959300 | 3.17302100 |
| H | 4.36855300 | -2.97591500 | 2.70387200 |
| C | 3.77903100 | -3.14084300 | -1.46584900 |
| C | 5.57084800 | -3.10832500 | 0.22396400 |
| H | 0.08836200 | -2.91325600 | 3.28896300 |
| H | 2.42729600 | -2.89011300 | 4.25227700 |
| C | 4.78197900 | -3.19390400 | -2.45471200 |
| C | 6.53910800 | -3.15558000 | -0.77713900 |
| H | 5.89068300 | -3.07973000 | 1.26792700 |
| C | 6.13877300 | -3.19832700 | -2.12035100 |
| H | 4.48912900 | -3.22126600 | -3.50670600 |
| H | 7.59958500 | -3.15962600 | -0.51400600 |
| H | 6.89253000 | -3.23533000 | -2.91248500 |
| C | 1.92775600 | -5.76957600 | -3.19652800 |
| C | 1.86163600 | -6.16475700 | -0.85315200 |
| C | 1.99043800 | -7.18561800 | -3.41571400 |
| C | 1.94735600 | -4.76760000 | -4.19498700 |
| C | 1.93618400 | -7.54463500 | -1.02293600 |
| H | 1.81133800 | -5.72787700 | 0.14833300 |
| C | 1.99369300 | -8.06070600 | -2.35665700 |
| H | 2.03292300 | -7.56358800 | -4.43841100 |
| C | 1.84269900 | -3.35751100 | -3.74510600 |
| C | 2.04194100 | -5.02705200 | -5.60239000 |
| H | 1.94563000 | -8.20202400 | -0.15277300 |
| H | 2.03975100 | -9.13856300 | -2.52897700 |
| C | 1.79947400 | -2.34515900 | -4.72318500 |
| C | 2.00913600 | -3.98673900 | -6.50939800 |
| H | 2.13781400 | -6.05189300 | -5.96682000 |
| C | 1.88335000 | -2.62980100 | -6.08789300 |
| H | 1.71595100 | -1.30615900 | -4.39616800 |
| H | 2.08064400 | -4.20886800 | -7.57851600 |
| H | 1.86163200 | -1.82803900 | -6.82968500 |
| C | -0.89933700 | -1.77810300 | -1.81347700 |
| C | -1.23639000 | -4.10590400 | -1.81888600 |
| C | -2.29136700 | -1.57644700 | -1.82913400 |
| C | 0.11769300 | -0.71204300 | -1.79538500 |
| C | -2.61978300 | -3.96598700 | -1.83660800 |
| H | -0.75635400 | -5.08678700 | -1.81395300 |
| C | -3.15156900 | -2.67048800 | -1.84095000 |
| H | -2.69606800 | -0.56495800 | -1.83160100 |
| C | 1.48189800 | -1.12881100 | -1.77417100 |
| C | -0.21970100 | 0.65592600 | -1.79288200 |
| H | -3.25968500 | -4.84926800 | -1.84743600 |
| H | -4.23283000 | -2.51549800 | -1.85332900 |
| C | 2.46408800 | -0.12114200 | -1.73829900 |
| C | 0.77812300 | 1.62876400 | -1.76480700 |
| H | -1.26536300 | 0.97167000 | -1.81301500 |
| C | 2.12395400 | 1.23524900 | -1.73584500 |
| H | 3.51878400 | -0.40747400 | -1.71944300 |
| H | 0.51029100 | 2.68817800 | -1.76478500 |
| H | 2.91178700 | 1.99428500 | -1.71291900 |
| N | 1.84003600 | -5.29645600 | -1.86949800 |
| N | 1.87217800 | -3.06986800 | 0.43105600 |
| N | -0.40942000 | -3.04883400 | -1.80666700 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -1541.2610204
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -1539.164879

**$Ir^{IV}$**

Zero-point correction= 0.481575 (Hartree/Particle)
Thermal correction to Energy= 0.510612
Thermal correction to Enthalpy= 0.511556
Thermal correction to Gibbs Free Energy= 0.419749
Sum of electronic and zero-point Energies= -1539.125826
Sum of electronic and thermal Energies= -1539.096789
Sum of electronic and thermal Enthalpies= -1539.095845
Sum of electronic and thermal Free Energies= -1539.187653

| | | | |
|---|---|---|---|
| Ir | 1.79556100 | -3.12918400 | -1.75052100 |
| C | 3.14885800 | -3.03126200 | 0.92752100 |
| C | 0.82193800 | -3.02299500 | 1.26166200 |
| C | 3.35374900 | -2.95620000 | 2.31548400 |
| C | 4.21158400 | -3.07461500 | -0.08767600 |
| C | 0.96520200 | -2.94705900 | 2.64225400 |
| H | -0.16273700 | -3.04975800 | 0.79191100 |
| C | 2.25979200 | -2.91400500 | 3.17421300 |
| H | 4.36575200 | -2.93029400 | 2.71747000 |
| C | 3.79260700 | -3.15584100 | -1.45037100 |
| C | 5.58024300 | -3.06841200 | 0.23282700 |
| H | 0.08171400 | -2.91351600 | 3.28069300 |
| H | 2.41373800 | -2.85421900 | 4.25368500 |
| C | 4.78101700 | -3.26105900 | -2.44834900 |
| C | 6.53894800 | -3.14508600 | -0.77706200 |
| H | 5.90855800 | -3.00753500 | 1.27208500 |
| C | 6.13724900 | -3.24229500 | -2.11793600 |
| H | 4.48337100 | -3.33371200 | -3.49609900 |
| H | 7.60063700 | -3.13457300 | -0.52049700 |
| H | 6.88992500 | -3.30262400 | -2.90853800 |
| C | 1.94399800 | -5.77672300 | -3.15656800 |
| C | 1.95402100 | -6.15662600 | -0.83676400 |
| C | 2.04523400 | -7.15871700 | -3.38887300 |
| C | 1.88436100 | -4.74133800 | -4.19871200 |
| C | 2.05592500 | -7.53247000 | -1.00716900 |
| H | 1.91655000 | -5.70680000 | 0.15686600 |
| C | 2.10134900 | -8.03794800 | -2.31195500 |
| H | 2.08069500 | -7.54021000 | -4.40852800 |
| C | 1.77827600 | -3.38871700 | -3.75226000 |
| C | 1.89856400 | -5.03384800 | -5.57338800 |
| H | 2.09965800 | -8.18756500 | -0.13640800 |
| H | 2.18149800 | -9.11285800 | -2.48712500 |
| C | 1.65714700 | -2.37287000 | -4.72080900 |
| C | 1.80599400 | -4.00611300 | -6.51159300 |
| H | 1.97784800 | -6.06498400 | -5.92253600 |
| C | 1.68443300 | -2.67541500 | -6.08323000 |
| H | 1.56524500 | -1.33283500 | -4.40226400 |
| H | 1.82286900 | -4.24096800 | -7.57821400 |
| H | 1.61160300 | -1.87108500 | -6.82006600 |
| C | -0.87541100 | -1.76647800 | -1.87124700 |
| C | -1.21524900 | -4.09220300 | -1.92498000 |
| C | -2.26160300 | -1.55650400 | -1.96362900 |
| C | 0.14169000 | -0.70760900 | -1.79404800 |
| C | -2.59410500 | -3.94375500 | -2.01940300 |
| H | -0.74812800 | -5.07837800 | -1.90790200 |
| C | -3.12223000 | -2.64723800 | -2.03782600 |
| H | -2.66071400 | -0.54310300 | -1.97755900 |
| C | 1.50180700 | -1.13194900 | -1.69686400 |
| C | -0.17493500 | 0.66190500 | -1.78481100 |
| H | -3.23423000 | -4.82470900 | -2.07802300 |
| H | -4.20030400 | -2.48932900 | -2.11101400 |
| C | 2.50064500 | -0.14824200 | -1.56067200 |
| C | 0.83626900 | 1.61625700 | -1.67729200 |
| H | -1.21210800 | 0.99419600 | -1.85804200 |

| | | | |
|---|---|---|---|
| C | 2.17429800 | 1.20909600 | -1.56431000 |
| H | 3.54624000 | -0.45015300 | -1.47553800 |
| H | 0.58289400 | 2.67876600 | -1.67616100 |
| H | 2.96583400 | 1.95846000 | -1.47982200 |
| N | 1.89353300 | -5.31047800 | -1.87767100 |
| N | 1.87925300 | -3.07020800 | 0.43526800 |
| N | -0.38707400 | -3.03802500 | -1.84690200 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -1541.1651173
U□B97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -1539.0737098

**Br-Anion**
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= -0.016176
Sum of electronic and zero-point Energies= -2574.036469
Sum of electronic and thermal Energies= -2574.035053
Sum of electronic and thermal Enthalpies= -2574.034109
Sum of electronic and thermal Free Energies= -2574.052645

| | | | |
|---|---|---|---|
| Br | -4.23871500 | -2.81695000 | 0.00706700 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -2574.3697609
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -2574.0701119

**EtOH**
Zero-point correction= 0.079463 (Hartree/Particle)
Thermal correction to Energy= 0.083734
Thermal correction to Enthalpy= 0.084678
Thermal correction to Gibbs Free Energy= 0.054106
Sum of electronic and zero-point Energies= -154.851535
Sum of electronic and thermal Energies= -154.847265
Sum of electronic and thermal Enthalpies= -154.846320
Sum of electronic and thermal Free Energies= -154.876892

| | | | |
|---|---|---|---|
| O | -4.23805400 | -2.84698000 | 0.00702600 |
| H | -4.55832400 | -1.93504500 | 0.00874100 |
| C | -2.81908000 | -2.81732500 | 0.00707600 |
| H | -2.42727100 | -2.28064400 | -0.88095700 |
| H | -2.42725800 | -2.28409600 | 0.89718000 |
| C | -2.31100100 | -4.24783400 | 0.00429600 |
| H | -2.67223900 | -4.78339100 | -0.88840000 |
| H | -1.21011400 | -4.27314000 | 0.00423400 |
| H | -2.67222100 | -4.78685500 | 0.8949110 |

UB3LYP-D3/def2-TZVPP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -155.1205169
UωB97XD/def2-SVP-CPCM(acetonitrile) // UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
HF = -154.8807479

## *A2.3.b Coordinates & Energies in the study of Transition Metal-Free Photochemical C–F Activation for the Preparation of Difluorinated-Oxindole Derivatives*

**K-22**
Zero-point correction= 0.095012 (Hartree/Particle)
Thermal correction to Energy= 0.104217
Thermal correction to Enthalpy= 0.105161
Thermal correction to Gibbs Free Energy= 0.058725
Sum of electronic and zero-point Energies= -604.882779
Sum of electronic and thermal Energies= -604.873574
Sum of electronic and thermal Enthalpies= -604.872629
Sum of electronic and thermal Free Energies= -604.919065

| | | | |
|---|---|---|---|
| C | -1.06225900 | 0.49809000 | 0.00181400 |
| O | 0.13254300 | 0.63209200 | 0.00762100 |
| O | -1.74224200 | -0.63147200 | -0.00179800 |
| C | -2.04483300 | 1.69556700 | -0.00374100 |
| C | -0.97738200 | -1.86902400 | 0.00100700 |
| H | -0.33009800 | -1.86847100 | 0.89162100 |
| H | -0.32904200 | -1.87155400 | -0.88887100 |
| C | -1.95999800 | -3.01666100 | 0.00236700 |
| H | -1.40954300 | -3.96953300 | 0.00393800 |
| H | -2.60057800 | -2.98339200 | 0.89662100 |
| H | -2.60004600 | -2.98605100 | -0.89236100 |
| F | -1.37478400 | 2.84597300 | 0.00601200 |
| F | -2.81980700 | 1.66349900 | -1.09637900 |
| F | -2.84112300 | 1.65741800 | 1.07312300 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -605.7000313
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -604.7964875

**a•⁻**
Zero-point correction= 0.091431 (Hartree/Particle)
Thermal correction to Energy= 0.100856
Thermal correction to Enthalpy= 0.101800
Thermal correction to Gibbs Free Energy= 0.054908
Sum of electronic and zero-point Energies= -604.944204
Sum of electronic and thermal Energies= -604.934779
Sum of electronic and thermal Enthalpies= -604.933835
Sum of electronic and thermal Free Energies= -604.980727

| | | | |
|---|---|---|---|
| C | -0.98763700 | 0.54110500 | 0.05531800 |
| O | 0.06970000 | 0.62083600 | -0.65341900 |
| O | -1.77088500 | -0.66664300 | 0.06060800 |
| C | -1.95651200 | 1.67575500 | 0.05965400 |
| C | -1.00775000 | -1.84717100 | 0.09913700 |
| H | -0.41770700 | -1.89846500 | 1.04214500 |
| H | -0.26869100 | -1.85777300 | -0.72408800 |
| C | -1.94412200 | -3.03947000 | -0.00191900 |
| H | -1.38014600 | -3.98569800 | 0.02787300 |
| H | -2.66729000 | -3.04011000 | 0.82994500 |
| H | -2.51348800 | -3.00323800 | -0.94499300 |
| F | -1.32892800 | 2.85700400 | 0.27989900 |
| F | -2.65313400 | 1.87684900 | -1.12890600 |
| F | -2.92991800 | 1.56350000 | 0.99972000 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -605.7739675
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -604.8526834

**TS-a-b-2**
Zero-point correction= 0.090957 (Hartree/Particle)
Thermal correction to Energy= 0.100424
Thermal correction to Enthalpy= 0.101368
Thermal correction to Gibbs Free Energy= 0.055444
Sum of electronic and zero-point Energies= -604.929217
Sum of electronic and thermal Energies= -604.919750
Sum of electronic and thermal Enthalpies= -604.918806
Sum of electronic and thermal Free Energies= -604.964730

| | | | |
|---|---|---|---|
| C | -0.97637300 | 0.49528700 | 0.09732300 |
| O | -0.07927500 | 0.64238700 | -0.72192700 |
| O | -1.11933700 | -0.59917200 | 0.89801700 |

| | | | |
|---|---|---|---|
| C | -1.92833200 | 1.50305600 | 0.43998200 |
| C | -0.74274200 | -1.86184200 | 0.32838000 |
| H | -0.33038800 | -2.46331300 | 1.15402300 |
| H | 0.05822900 | -1.70115600 | -0.40960500 |
| C | -1.96377000 | -2.51224200 | -0.30838200 |
| H | -1.67571900 | -3.41053700 | -0.87928600 |
| H | -2.68976700 | -2.81239400 | 0.46546500 |
| H | -2.44752500 | -1.76299800 | -0.95687100 |
| F | -1.97599400 | 2.65440300 | -0.20461700 |
| F | -2.95983700 | 0.28334300 | -1.19162000 |
| F | -2.92567600 | 1.34165900 | 1.29009100 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -605.7694438
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -604.8320015

**b•⁻**

Zero-point correction= 0.091330 (Hartree/Particle)
Thermal correction to Energy= 0.100878
Thermal correction to Enthalpy= 0.101822
Thermal correction to Gibbs Free Energy= 0.054967
Sum of electronic and zero-point Energies= -604.933886
Sum of electronic and thermal Energies= -604.924338
Sum of electronic and thermal Enthalpies= -604.923394
Sum of electronic and thermal Free Energies= -604.970249

| | | | |
|---|---|---|---|
| C | -1.35342400 | 0.45587800 | -0.14363300 |
| O | -0.44887200 | 0.55205600 | -0.99094800 |
| O | -1.32433500 | -0.58854300 | 0.81677200 |
| C | -1.72091500 | 1.70888600 | 0.65015500 |
| C | -0.82211400 | -1.82842700 | 0.34606900 |
| H | -0.47194100 | -2.37471200 | 1.23847300 |
| H | 0.04962400 | -1.64893200 | -0.30681200 |
| C | -1.87596500 | -2.64419300 | -0.39722700 |
| H | -1.46536000 | -3.61914000 | -0.70923100 |
| H | -2.75119400 | -2.82456000 | 0.24835400 |
| H | -2.22134100 | -2.09062500 | -1.28086400 |
| F | -1.80383100 | 2.82555600 | -0.08302100 |
| F | -2.76853400 | 0.21229800 | -0.84692100 |
| F | -2.77200600 | 1.64833800 | 1.47870700 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -605.7645067
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -604.8407847

**c•**

Zero-point correction= 0.089757 (Hartree/Particle)
Thermal correction to Energy= 0.098566
Thermal correction to Enthalpy= 0.099510
Thermal correction to Gibbs Free Energy= 0.054431
Sum of electronic and zero-point Energies= -505.056123
Sum of electronic and thermal Energies= -505.047314
Sum of electronic and thermal Enthalpies= -505.046370
Sum of electronic and thermal Free Energies= -505.091448

| | | | |
|---|---|---|---|
| C | -1.12302600 | 0.51266400 | 0.01505800 |
| O | 0.08811500 | 0.63907600 | 0.00551400 |
| O | -1.79332300 | -0.64590000 | 0.00816200 |
| C | -2.03070700 | 1.64470200 | 0.08805600 |
| C | -0.99767200 | -1.85215800 | -0.00357900 |
| H | -0.33834500 | -1.84792100 | 0.87959200 |
| H | -0.35342500 | -1.84151700 | -0.89758000 |
| C | -1.94731600 | -3.02961900 | -0.00041200 |
| H | -1.37308100 | -3.96843900 | -0.00934700 |
| H | -2.58199500 | -3.01839800 | 0.89888500 |
| H | -2.59708100 | -3.01076300 | -0.88875000 |
| F | -1.57994200 | 2.86701800 | -0.03115900 |
| F | -3.32769400 | 1.54289100 | -0.06346600 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -505.7471489
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -504.9872887

**TS-c-d-2**

Zero-point correction= 0.307244 (Hartree/Particle)
Thermal correction to Energy= 0.329110
Thermal correction to Enthalpy= 0.330055
Thermal correction to Gibbs Free Energy= 0.254285
Sum of electronic and zero-point Energies= -1061.443596
Sum of electronic and thermal Energies= -1061.421730
Sum of electronic and thermal Enthalpies= -1061.420785
Sum of electronic and thermal Free Energies= -1061.496555

| | | | |
|---|---|---|---|
| C | 0.85305500 | 0.51257900 | 0.55367800 |
| C | 1.84639700 | 0.50824100 | -0.43415600 |
| C | 1.95801400 | 1.58783500 | -1.32202900 |
| C | 1.06732300 | 2.66011700 | -1.22731800 |
| C | 0.06290400 | 2.65829400 | -0.25166500 |
| C | -0.04278600 | 1.58253000 | 0.63679800 |
| H | 0.78232500 | -0.32965900 | 1.24532800 |
| H | 2.71620100 | 1.55683500 | -2.10703900 |
| H | 1.15002100 | 3.49507900 | -1.92739400 |
| H | -0.63644900 | 3.49512100 | -0.18410600 |
| H | -0.82211900 | 1.57767800 | 1.40281200 |
| N | 2.77511900 | -0.57908100 | -0.52057300 |
| C | 4.10786400 | -0.30718300 | 0.02561000 |
| H | 4.42135200 | 0.70005300 | -0.27803500 |
| H | 4.10269800 | -0.35833200 | 1.12851200 |
| H | 4.82469400 | -1.04518700 | -0.35064900 |
| C | 2.42377600 | -1.90103200 | -0.70463400 |
| O | 3.20895100 | -2.79990000 | -0.39740100 |
| C | 1.11084200 | -2.27872300 | -1.33746200 |
| C | 0.36873800 | -1.46546800 | -2.14003300 |
| H | 0.55508600 | -0.39858000 | -2.24084700 |
| H | -0.57529000 | -1.83197700 | -2.55196100 |
| C | 0.76820000 | -3.73500300 | -1.18469000 |
| H | 1.52891800 | -4.35602800 | -1.68545900 |
| H | 0.77230600 | -4.03599400 | -0.12473600 |
| H | -0.21532100 | -3.96100000 | -1.61914700 |
| C | 2.53807000 | -1.09357400 | -4.17696600 |
| O | 2.70143100 | 0.10345500 | -4.30932500 |
| O | 3.45192300 | -1.96932300 | -3.75985600 |
| C | 1.22708600 | -1.74259500 | -4.33490900 |
| C | 4.76287500 | -1.44725500 | -3.43716100 |
| H | 4.64003300 | -0.62957500 | -2.71163700 |
| H | 5.20211500 | -1.01914600 | -4.35225000 |
| C | 5.58326700 | -2.58841300 | -2.87914300 |
| H | 6.58507600 | -2.22302200 | -2.60631200 |
| H | 5.09798900 | -2.99927900 | -1.98193000 |
| H | 5.69709900 | -3.39014100 | -3.62486100 |
| F | 0.30535000 | -1.09433200 | -5.02007400 |
| F | 1.15080700 | -3.04924800 | -4.50319000 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1062.9623091
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1061.3881983

**d•**

Zero-point correction= 0.310329 (Hartree/Particle)
Thermal correction to Energy= 0.331637
Thermal correction to Enthalpy= 0.332581
Thermal correction to Gibbs Free Energy= 0.258477
Sum of electronic and zero-point Energies= -1061.490013
Sum of electronic and thermal Energies= -1061.468705
Sum of electronic and thermal Enthalpies= -1061.467761

Sum of electronic and thermal Free Energies= -1061.541865

| | | | |
|---|---|---|---|
| C | 0.76321300 | 0.40463500 | 0.41071700 |
| C | 1.81916700 | 0.53335500 | -0.50399200 |
| C | 1.92461500 | 1.69242400 | -1.28885400 |
| C | 0.97180300 | 2.70565000 | -1.16615600 |
| C | -0.09498100 | 2.56825400 | -0.26875100 |
| C | -0.19758800 | 1.41511600 | 0.51591700 |
| H | 0.69654300 | -0.49085300 | 1.03221400 |
| H | 2.73254800 | 1.77077000 | -2.01840100 |
| H | 1.05383500 | 3.60155600 | -1.78641200 |
| H | -0.84360900 | 3.35928400 | -0.18192000 |
| H | -1.02328200 | 1.30343800 | 1.22289200 |
| N | 2.79765400 | -0.50025200 | -0.62954400 |
| C | 4.13453900 | -0.18556900 | -0.12104700 |
| H | 4.40480800 | 0.83411200 | -0.42304000 |
| H | 4.16899300 | -0.25153700 | 0.98048500 |
| H | 4.86571800 | -0.89306200 | -0.52815700 |
| C | 2.45983500 | -1.84610800 | -0.71045300 |
| O | 3.23680000 | -2.70707400 | -0.28189200 |
| C | 1.21576000 | -2.24860300 | -1.39566100 |
| C | 0.53330700 | -1.43232500 | -2.45737600 |
| H | 0.51173400 | -0.35873100 | -2.23818600 |
| H | -0.50958800 | -1.76488900 | -2.58048800 |
| C | 0.77758700 | -3.66571300 | -1.23771900 |
| H | 1.03150900 | -4.24418400 | -2.14674200 |
| H | 1.26028400 | -4.15034100 | -0.38031600 |
| H | -0.31933600 | -3.72448700 | -1.13348000 |
| C | 2.60777200 | -1.02770000 | -3.90304900 |
| O | 2.86307800 | 0.13152700 | -4.11638000 |
| O | 3.47402600 | -1.98368200 | -3.61483000 |
| C | 1.15961500 | -1.56177400 | -3.84926000 |
| C | 4.87333100 | -1.61602600 | -3.49509200 |
| H | 4.93772300 | -0.70253200 | -2.88568300 |
| H | 5.25064100 | -1.37672900 | -4.50162100 |
| C | 5.59443200 | -2.78528000 | -2.86353100 |
| H | 6.65735500 | -2.53418600 | -2.72806800 |
| H | 5.15249900 | -3.01716400 | -1.88310700 |
| H | 5.52688800 | -3.67872300 | -3.50282500 |
| F | 0.41573300 | -0.83907500 | -4.72964100 |
| F | 1.12547900 | -2.85975800 | -4.26876200 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1063.007626
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1061.4457544

**TS-d-e-2**

Zero-point correction= 0.309343 (Hartree/Particle)
Thermal correction to Energy= 0.329795
Thermal correction to Enthalpy= 0.330739
Thermal correction to Gibbs Free Energy= 0.258981
Sum of electronic and zero-point Energies= -1061.467282
Sum of electronic and thermal Energies= -1061.446829
Sum of electronic and thermal Enthalpies= -1061.445885
Sum of electronic and thermal Free Energies= -1061.517644

| | | | |
|---|---|---|---|
| C | 0.93782000 | -1.14096400 | 1.18979800 |
| C | 1.76489200 | -0.07519100 | 0.68682100 |
| C | 1.31525900 | 1.23639000 | 0.63504900 |
| C | 0.00308600 | 1.53053900 | 1.05815300 |
| C | -0.85223300 | 0.49936400 | 1.48474600 |
| C | -0.39455200 | -0.81354100 | 1.57691100 |
| H | 1.42563800 | -1.97856700 | 1.69848700 |
| H | 1.95264400 | 2.02116300 | 0.22304900 |
| H | -0.35689000 | 2.56107900 | 1.02176600 |
| H | -1.87356700 | 0.73896900 | 1.79184500 |
| H | -1.03742100 | -1.59425000 | 1.99041300 |
| N | 2.92200300 | -0.55095800 | 0.04993400 |
| C | 4.11110100 | 0.25595900 | -0.15796300 |
| H | 4.93657000 | -0.41103800 | -0.43527300 |
| H | 3.95761300 | 0.98517600 | -0.97138000 |
| H | 4.36519700 | 0.79400900 | 0.76565500 |
| C | 2.74832500 | -1.76065800 | -0.59562800 |
| O | 3.65784900 | -2.37904400 | -1.13412300 |
| C | 1.30867400 | -2.22709800 | -0.58761100 |
| C | 0.38724900 | -1.53194200 | -1.56961200 |
| H | 0.52456000 | -0.44133800 | -1.53523600 |
| H | -0.66314700 | -1.74809800 | -1.31641900 |
| C | 1.11579700 | -3.70256900 | -0.38533700 |
| H | 1.48427400 | -4.26688000 | -1.25930300 |
| H | 1.66889100 | -4.06160900 | 0.49687700 |
| H | 0.04950200 | -3.94433700 | -0.25692700 |
| C | 1.98992300 | -1.61864700 | -3.54353600 |
| O | 2.44024700 | -0.50018300 | -3.45323900 |
| O | 2.60669100 | -2.68162700 | -4.02099400 |
| C | 0.56723000 | -1.92917600 | -3.02936500 |
| C | 4.00739600 | -2.53826300 | -4.38127600 |
| H | 4.39585400 | -3.56461900 | -4.34934500 |
| H | 4.49718700 | -1.94804000 | -3.59420500 |
| C | 4.17021800 | -1.91683900 | -5.75512800 |
| H | 5.23827600 | -1.89557300 | -6.02224500 |
| H | 3.63452400 | -2.50356600 | -6.51706900 |
| H | 3.78941500 | -0.88546200 | -5.76532400 |
| F | -0.30468400 | -1.20223200 | -3.79637400 |
| F | 0.25069800 | -3.23967700 | -3.21996900 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1062.9825259
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1061.4209749

**e•**

Zero-point correction= 0.311631 (Hartree/Particle)
Thermal correction to Energy= 0.331880
Thermal correction to Enthalpy= 0.332824
Thermal correction to Gibbs Free Energy= 0.261991
Sum of electronic and zero-point Energies= -1061.495942
Sum of electronic and thermal Energies= -1061.475692
Sum of electronic and thermal Enthalpies= -1061.474748
Sum of electronic and thermal Free Energies= -1061.545582

| | | | |
|---|---|---|---|
| C | 0.79232500 | -1.15342800 | 0.83947800 |
| C | 1.79459900 | -0.06185500 | 0.57551800 |
| C | 1.56083700 | 1.26442100 | 0.82980300 |
| C | 0.25472200 | 1.65672000 | 1.23364200 |
| C | -0.80700900 | 0.70722600 | 1.26031000 |
| C | -0.59969800 | -0.62728900 | 1.01289100 |
| H | 1.09524100 | -1.64502400 | 1.79411100 |
| H | 2.33955500 | 2.01310200 | 0.66976700 |
| H | 0.04946600 | 2.70727100 | 1.44836700 |
| H | -1.81975700 | 1.06106900 | 1.47425600 |
| H | -1.42798800 | -1.33987800 | 1.03968100 |
| N | 2.90995200 | -0.65137300 | -0.00477200 |
| C | 4.15053900 | 0.04273700 | -0.28581300 |
| H | 4.87107500 | -0.68710400 | -0.67415300 |
| H | 3.98512300 | 0.82542000 | -1.04321300 |
| H | 4.54618800 | 0.50388800 | 0.63092000 |
| C | 2.63428200 | -1.91846100 | -0.47343600 |
| O | 3.43334400 | -2.66023700 | -1.02040500 |
| C | 1.13005900 | -2.19789200 | -0.27073600 |
| C | 0.36192900 | -1.81230900 | -1.56435400 |
| H | 0.37373900 | -0.72065700 | -1.69313000 |
| H | -0.68945100 | -2.11719400 | -1.45644600 |
| C | 0.88774300 | -3.64846400 | 0.14251900 |
| H | 1.27646300 | -4.33668600 | -0.61821500 |
| H | 1.39156700 | -3.86694400 | 1.09643800 |
| H | -0.18920100 | -3.83871300 | 0.26902100 |
| C | 2.17113900 | -1.79828500 | -3.39522100 |
| O | 2.46220500 | -0.64218800 | -3.19225300 |
| O | 2.87428700 | -2.67461300 | -4.08619800 |

| | | | |
|---|---|---|---|
| C | 0.83375200 | -2.38740800 | -2.88726100 |
| C | 4.16177000 | -2.24382400 | -4.60155800 |
| H | 4.71791700 | -3.17856200 | -4.75098900 |
| H | 4.66200600 | -1.64886600 | -3.82350000 |
| C | 4.00913200 | -1.46583800 | -5.89482200 |
| H | 5.00505400 | -1.22037500 | -6.29514700 |
| H | 3.46959100 | -2.06105100 | -6.64727800 |
| H | 3.46311500 | -0.52697200 | -5.72301100 |
| F | -0.09470400 | -2.05112800 | -3.84625100 |
| F | 0.88040500 | -3.74697500 | -2.86633600 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1063.0112537
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1061.4594913

**MECP-e-L-2**

Zero-point correction= 0.401729 (Hartree/Particle)
Thermal correction to Energy= 0.431867
Thermal correction to Enthalpy= 0.432812
Thermal correction to Gibbs Free Energy= 0.338146
Sum of electronic and zero-point Energies= -1566.572703
Sum of electronic and thermal Energies= -1566.542564
Sum of electronic and thermal Enthalpies= -1566.541620
Sum of electronic and thermal Free Energies= -1566.636286

| | | | |
|---|---|---|---|
| C | 4.803973000 | -0.844278000 | -0.371083000 |
| C | 3.881033000 | 0.998278000 | 1.035403000 |
| C | 5.175434000 | 1.308325000 | 1.370678000 |
| C | 6.277810000 | 0.537887000 | 0.905121000 |
| C | 6.089167000 | -0.519570000 | -0.016394000 |
| H | 3.043274000 | 1.597824000 | 1.396810000 |
| H | 5.375034000 | 2.182677000 | 1.995569000 |
| H | 7.290420000 | 0.815395000 | 1.202943000 |
| H | 6.945498000 | -1.017051000 | -0.473331000 |
| N | 4.359376000 | -1.724441000 | -1.338349000 |
| C | 5.235469000 | -2.568840000 | -2.125205000 |
| H | 5.742734000 | -3.291326000 | -1.470585000 |
| H | 4.623041000 | -3.101494000 | -2.861956000 |
| H | 5.982406000 | -1.951866000 | -2.648041000 |
| C | 3.004078000 | -1.593371000 | -1.586700000 |
| O | 2.372832000 | -2.253910000 | -2.390752000 |
| C | 2.447422000 | -0.461429000 | -0.696899000 |
| C | 1.145815000 | -0.914439000 | -0.024744000 |
| H | 0.769571000 | -0.125793000 | 0.644165000 |
| H | 0.378533000 | -1.127628000 | -0.782342000 |
| H | 1.310235000 | -1.826940000 | 0.564617000 |
| C | 2.115932000 | 0.772171000 | -1.569389000 |
| H | 1.729544000 | 1.577980000 | -0.930110000 |
| H | 1.304642000 | 0.482741000 | -2.254261000 |
| C | 3.179649000 | 1.376580000 | -2.470801000 |
| C | 4.288212000 | 2.238013000 | -1.828072000 |
| O | 5.463672000 | 2.049424000 | -2.009894000 |
| O | 3.747461000 | 3.228763000 | -1.137499000 |
| C | 4.647505000 | 4.178917000 | -0.513679000 |
| H | 5.063300000 | 4.817631000 | -1.308167000 |
| H | 5.473881000 | 3.619027000 | -0.055848000 |
| C | 3.857703000 | 4.968889000 | 0.502119000 |
| H | 4.513534000 | 5.715855000 | 0.974510000 |
| H | 3.016918000 | 5.496584000 | 0.026855000 |
| H | 3.459844000 | 4.309699000 | 1.288489000 |
| F | 3.789268000 | 0.418461000 | -3.223185000 |
| F | 2.539750000 | 2.211340000 | -3.356481000 |
| C | 3.605519000 | -0.276373000 | 0.319469000 |
| H | 3.375355000 | -1.033069000 | 1.124665000 |
| C | 3.840375000 | -3.741212000 | 1.216081000 |
| O | 4.945833000 | -4.066889000 | 0.816400000 |
| O | 2.672129000 | -4.110044000 | 0.677212000 |
| C | 3.638148000 | -2.799581000 | 2.303380000 |
| C | 2.719285000 | -5.022128000 | -0.445041000 |
| H | 3.127832000 | -5.981488000 | -0.090309000 |
| H | 3.407136000 | -4.617270000 | -1.199664000 |
| C | 1.315504000 | -5.161286000 | -0.985307000 |
| H | 1.316209000 | -5.881534000 | -1.817812000 |
| H | 0.627943000 | -5.528029000 | -0.207832000 |
| H | 0.953718000 | -4.194465000 | -1.363273000 |
| F | 4.662622000 | -2.444088000 | 3.046894000 |
| F | 2.485168000 | -2.706144000 | 2.937733000 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1568.7728033
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1566.4595704

**L-2 + Est**

Zero-point correction= 0.407353 (Hartree/Particle)
Thermal correction to Energy= 0.437476
Thermal correction to Enthalpy= 0.438420
Thermal correction to Gibbs Free Energy= 0.344607
Sum of electronic and zero-point Energies= -1566.681024
Sum of electronic and thermal Energies= -1566.650901
Sum of electronic and thermal Enthalpies= -1566.649957
Sum of electronic and thermal Free Energies= -1566.743770

| | | | |
|---|---|---|---|
| C | 4.72371400 | -0.83164400 | -0.49735600 |
| C | 3.78148500 | 0.86832200 | 0.94786900 |
| C | 5.02275400 | 0.95620700 | 1.60314900 |
| C | 6.09466300 | 0.15361800 | 1.19592900 |
| C | 5.96124400 | -0.75864000 | 0.13772300 |
| H | 2.94405900 | 1.49553900 | 1.26101400 |
| H | 5.14796200 | 1.65155800 | 2.43569300 |
| H | 7.05165300 | 0.22558300 | 1.71763800 |
| H | 6.79099400 | -1.40025000 | -0.16019100 |
| N | 4.33194700 | -1.68670400 | -1.53647900 |
| C | 5.22296500 | -2.59032400 | -2.23543900 |
| H | 5.64025400 | -3.33573700 | -1.54283200 |
| H | 4.64321400 | -3.09959300 | -3.01546900 |
| H | 6.04558400 | -2.02671600 | -2.70354100 |
| C | 3.00457600 | -1.50211000 | -1.85930300 |
| O | 2.37597700 | -2.14395000 | -2.68032300 |
| C | 2.45149600 | -0.34665600 | -0.98769200 |
| C | 1.23599200 | -0.84141100 | -0.18344700 |
| H | 0.85350200 | -0.03436100 | 0.45910300 |
| H | 0.43423700 | -1.15775700 | -0.86727300 |
| H | 1.51163500 | -1.69532300 | 0.44989000 |
| C | 2.00689900 | 0.82065100 | -1.89963600 |
| H | 1.54362900 | 1.61015700 | -1.29135200 |
| H | 1.25028100 | 0.44857300 | -2.60789900 |
| C | 3.08309100 | 1.48118000 | -2.74606500 |
| C | 4.18301200 | 2.26484700 | -1.99011800 |
| O | 5.36209700 | 2.06908600 | -2.13477900 |
| O | 3.63000500 | 3.18152400 | -1.20921700 |
| C | 4.52399500 | 4.01877900 | -0.43092000 |
| H | 5.10672100 | 4.63958000 | -1.12947600 |
| H | 5.22350700 | 3.36246500 | 0.10800100 |
| C | 3.67690400 | 4.84745200 | 0.50684900 |
| H | 4.32526100 | 5.50796600 | 1.10214000 |
| H | 2.96456400 | 5.47174300 | -0.05362600 |
| H | 3.11215100 | 4.20226300 | 1.19705600 |
| F | 3.70661400 | 0.56292900 | -3.53576400 |
| F | 2.47402800 | 2.37602400 | -3.58690200 |
| C | 3.64128600 | -0.02153400 | -0.10943900 |
| H | 3.87146900 | -1.61132800 | 2.08997100 |
| C | 4.16748600 | -3.60026500 | 1.19478300 |
| O | 5.15327100 | -4.13417700 | 0.75242300 |
| O | 2.93091300 | -3.74238800 | 0.73825700 |
| C | 4.18146900 | -2.62617700 | 2.38750300 |
| C | 2.71995500 | -4.69340000 | -0.34318300 |
| H | 3.07659700 | -5.67674800 | -0.00042400 |
| H | 3.33487600 | -4.38584300 | -1.20009500 |

| | | | |
|---|---|---|---|
| C | 1.24833900 | -4.69721600 | -0.68472900 |
| H | 1.05974100 | -5.45786900 | -1.45751800 |
| H | 0.63930800 | -4.94068600 | 0.19895500 |
| H | 0.93914000 | -3.72113900 | -1.08341900 |
| F | 5.42804300 | -2.58005100 | 2.90464000 |
| F | 3.33188700 | -3.08396400 | 3.34632800 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1568.8889485
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1566.5832335

**i-2**

Zero-point correction= 0.131695 (Hartree/Particle)
Thermal correction to Energy= 0.140573
Thermal correction to Enthalpy= 0.141517
Thermal correction to Gibbs Free Energy= 0.097239
Sum of electronic and zero-point Energies= -744.487926
Sum of electronic and thermal Energies= -744.479049
Sum of electronic and thermal Enthalpies= -744.478104
Sum of electronic and thermal Free Energies= -744.522382

| | | | |
|---|---|---|---|
| C | -2.56670100 | -0.03507900 | 0.28963600 |
| C | -1.18960600 | -0.16892700 | 0.52709900 |
| C | -0.32182200 | 0.88882700 | 0.23177800 |
| C | -0.80247300 | 2.09222000 | -0.30291900 |
| C | -2.18370900 | 2.22021900 | -0.53923900 |
| C | -3.05104300 | 1.17145800 | -0.24598100 |
| H | -0.77527900 | -1.08778300 | 0.94171900 |
| H | 0.74665500 | 0.76233900 | 0.42619900 |
| H | -2.58883200 | 3.14567000 | -0.95584400 |
| H | -4.12366000 | 1.26799600 | -0.42784300 |
| S | 0.37266200 | 3.39273700 | -0.65574600 |
| H | -0.51582400 | 4.30889300 | -1.10014000 |
| O | -3.49231200 | -0.99648500 | 0.53981700 |
| C | -3.07024000 | -2.23682700 | 1.07762400 |
| H | -2.58996200 | -2.11268300 | 2.06448400 |
| H | -3.97297500 | -2.85063900 | 1.19498100 |
| H | -2.36756300 | -2.75740200 | 0.40288900 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -745.1455532
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -744.4747876

**ii-2**

Zero-point correction= 0.122424 (Hartree/Particle)
Thermal correction to Energy= 0.130459
Thermal correction to Enthalpy= 0.131403
Thermal correction to Gibbs Free Energy= 0.089120
Sum of electronic and zero-point Energies= -744.015707
Sum of electronic and thermal Energies= -744.007672
Sum of electronic and thermal Enthalpies= -744.006728
Sum of electronic and thermal Free Energies= -744.049012

| | | | |
|---|---|---|---|
| C | -1.95155400 | -0.41564300 | 0.31955500 |
| C | -0.64410600 | -0.25818500 | -0.17144800 |
| C | -0.13910400 | 1.00664900 | -0.46511700 |
| C | -0.90192700 | 2.19594800 | -0.28876100 |
| C | -2.21507800 | 1.99851700 | 0.20797100 |
| C | -2.73627800 | 0.73185000 | 0.50694900 |
| H | -0.03281900 | -1.15359400 | -0.31715300 |
| H | 0.88214400 | 1.09812500 | -0.84673900 |
| H | -2.84781400 | 2.87753300 | 0.36340200 |
| H | -3.75720700 | 0.65806600 | 0.88573600 |
| S | -0.25665800 | 3.78904300 | -0.66274100 |
| O | -2.35908700 | -1.69974000 | 0.57939700 |
| C | -3.66382300 | -1.90710400 | 1.07240600 |
| H | -4.43662400 | -1.55158900 | 0.36530200 |
| H | -3.78393800 | -2.99066100 | 1.21126800 |
| H | -3.82583400 | -1.40430700 | 2.04427100 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -744.6745878
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -743.994557

**ii*-2**

UB3LYP-D3/def2-SVP-CPCM(DMSO)
Excitation energies and oscillator strengths:
Excited State 1: 3.000-?Sym 2.8303 eV 438.06 nm f=0.0000 <S**2>=2.000
37A -> 38A 0.69116
37B -> 38B -0.69116
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -744.034119982

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
Excited State 1: 3.000-?Sym 2.9628 eV 418.47 nm f=0.0000 <S**2>=2.000
35A -> 38A 0.11311
37A -> 38A 0.66766
37A -> 39A -0.18869
35B -> 38B -0.11311
37B -> 38B -0.66766
37B -> 39B 0.18869
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -744.565707516

UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
Excited State 1: 3.000-?Sym 3.1032 eV 399.54 nm f=0.0000 <S**2>=2.000
34A -> 38A 0.15400
35A -> 38A 0.16864
35A -> 39A -0.11936
37A -> 38A -0.45560
37A -> 39A 0.46933
34B -> 38B -0.15400
35B -> 38B -0.16864
35B -> 39B 0.11936
37B -> 38B 0.45560
37B -> 39B -0.46933
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -743.880518206

**iii-2**

Zero-point correction= 0.117055 (Hartree/Particle)
Thermal correction to Energy= 0.126131
Thermal correction to Enthalpy= 0.127075
Thermal correction to Gibbs Free Energy= 0.081874
Sum of electronic and zero-point Energies= -743.921281
Sum of electronic and thermal Energies= -743.912205
Sum of electronic and thermal Enthalpies= -743.911261
Sum of electronic and thermal Free Energies= -743.956462

| | | | |
|---|---|---|---|
| C | -1.97948400 | -0.38539600 | 0.32329100 |
| C | -0.61439800 | -0.28825200 | -0.18637400 |
| C | -0.09962000 | 1.00154500 | -0.47789800 |
| C | -0.85555700 | 2.16763500 | -0.28460500 |
| C | -2.23574300 | 2.04106600 | 0.24325600 |
| C | -2.76481600 | 0.73345800 | 0.53105700 |
| H | -0.03947800 | -1.20386600 | -0.32914000 |
| H | 0.91835300 | 1.10425700 | -0.86759300 |
| H | -2.83236800 | 2.94041400 | 0.39894800 |
| H | -3.78332200 | 0.64063600 | 0.91152000 |

| | | | |
|---|---|---|---|
| S | -0.25796700 | 3.74632800 | -0.63568400 |
| O | -2.37634400 | -1.66447300 | 0.56084800 |
| C | -3.67851000 | -1.90514900 | 1.05511000 |
| H | -4.45267100 | -1.54194100 | 0.35521900 |
| H | -3.77941900 | -2.99282400 | 1.17208000 |
| H | -3.83836300 | -1.41853000 | 2.03426300 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -744.5718713
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -743.8903174

**iv-2**

Zero-point correction= 0.123354 (Hartree/Particle)
Thermal correction to Energy= 0.131388
Thermal correction to Enthalpy= 0.132332
Thermal correction to Gibbs Free Energy= 0.089507
Sum of electronic and zero-point Energies= -743.872507
Sum of electronic and thermal Energies= -743.864473
Sum of electronic and thermal Enthalpies= -743.863529
Sum of electronic and thermal Free Energies= -743.906355

| | | | |
|---|---|---|---|
| C | -2.59188700 | -0.03291000 | 0.30740100 |
| C | -1.20011600 | -0.14165100 | 0.52926800 |
| C | -0.37511900 | 0.93811500 | 0.25116500 |
| C | -0.88928000 | 2.16689100 | -0.25622200 |
| C | -2.30075600 | 2.24751800 | -0.47014700 |
| C | -3.12837900 | 1.17833200 | -0.19619500 |
| H | -0.76504100 | -1.06267100 | 0.91628000 |
| H | 0.70021700 | 0.85410600 | 0.42250700 |
| H | -2.71915300 | 3.17855600 | -0.85832500 |
| H | -4.20653900 | 1.23584000 | -0.35844000 |
| S | 0.14525900 | 3.49480200 | -0.59617400 |
| O | -3.47528900 | -1.01105700 | 0.54078500 |
| C | -3.03648900 | -2.26899000 | 1.04540600 |
| H | -2.55495300 | -2.15757700 | 2.03078800 |
| H | -3.93612900 | -2.88778900 | 1.14866100 |
| H | -2.33605200 | -2.75660600 | 0.34754000 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -744.520087
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -743.84685

**v-2**

Zero-point correction= 0.248805 (Hartree/Particle)
Thermal correction to Energy= 0.266251
Thermal correction to Enthalpy= 0.267196
Thermal correction to Gibbs Free Energy= 0.200236
Sum of electronic and zero-point Energies= -1487.802139
Sum of electronic and thermal Energies= -1487.784693
Sum of electronic and thermal Enthalpies= -1487.783749
Sum of electronic and thermal Free Energies= -1487.850708

| | | | |
|---|---|---|---|
| C | -1.66568100 | 1.34433200 | -0.37426000 |
| C | -0.92024100 | 0.32767300 | -1.00769700 |
| C | 0.46456900 | 0.40615200 | -1.06942800 |
| C | 1.14277500 | 1.50212600 | -0.50012500 |
| C | 0.39809500 | 2.51145800 | 0.12709000 |
| C | -0.99649100 | 2.43981300 | 0.19753400 |
| H | -1.45936700 | -0.51601900 | -1.44358900 |
| H | 1.03413300 | -0.38220200 | -1.56666000 |
| H | 0.91424400 | 3.36970500 | 0.56191100 |
| H | -1.54507500 | 3.24130000 | 0.69127000 |
| O | -3.00594600 | 1.17765400 | -0.36739000 |
| C | -3.82928600 | 2.15897500 | 0.24359600 |
| H | -3.71874700 | 3.14255900 | -0.24494000 |
| H | -4.86423900 | 1.81343900 | 0.12496800 |
| H | -3.60500300 | 2.26447000 | 1.31916400 |
| S | 2.91670700 | 1.63791800 | -0.59118500 |
| S | 3.18542200 | 2.58230900 | -2.50084100 |
| C | 2.56126200 | 4.22083600 | -2.18577800 |
| C | 1.22238000 | 4.52325000 | -2.47289400 |
| C | 3.38302200 | 5.22020100 | -1.62788500 |
| C | 0.70066300 | 5.79551900 | -2.21946500 |
| H | 0.57528000 | 3.75196700 | -2.89536400 |
| C | 2.87316900 | 6.48520500 | -1.36843800 |
| H | 4.42551600 | 4.99341700 | -1.39353900 |
| C | 1.52608700 | 6.78615700 | -1.66078000 |
| H | -0.34409500 | 5.99728900 | -2.45387200 |
| H | 3.49818600 | 7.26978000 | -0.93684200 |
| O | 1.12497400 | 8.04288100 | -1.37124800 |
| C | -0.21734000 | 8.42490300 | -1.62886100 |
| H | -0.30781600 | 9.47250800 | -1.31433800 |
| H | -0.46210000 | 8.34790000 | -2.70235800 |
| H | -0.93139700 | 7.81178600 | -1.05221500 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1489.1004792
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1487.759139

**HCOONa**

Zero-point correction= 0.021982 (Hartree/Particle)
Thermal correction to Energy= 0.026698
Thermal correction to Enthalpy= 0.027642
Thermal correction to Gibbs Free Energy= -0.005742
Sum of electronic and zero-point Energies= -351.352880
Sum of electronic and thermal Energies= -351.348164
Sum of electronic and thermal Enthalpies= -351.347220
Sum of electronic and thermal Free Energies= -351.380604

| | | | |
|---|---|---|---|
| O | -0.84574300 | 0.97696500 | 1.56679500 |
| C | 0.39777800 | 1.14315500 | 1.50722400 |
| H | 0.76362200 | 2.21135800 | 1.46834900 |
| O | 1.27667900 | 0.24658500 | 1.48578100 |
| Na | -0.46116800 | -1.33521400 | 1.57766300 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -351.6648884
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -351.2948563

**$CO_2^{\bullet-}$ Radical Anion**

Zero-point correction= 0.008776 (Hartree/Particle)
Thermal correction to Energy= 0.011715
Thermal correction to Enthalpy= 0.012659
Thermal correction to Gibbs Free Energy= -0.015228
Sum of electronic and zero-point Energies= -188.492593
Sum of electronic and thermal Energies= -188.489655
Sum of electronic and thermal Enthalpies= -188.488711
Sum of electronic and thermal Free Energies= -188.516598

| | | | |
|---|---|---|---|
| O | -0.85384600 | 1.30246100 | 1.49916800 |
| C | 0.37252100 | 1.11745100 | 1.50562800 |
| O | 1.09492900 | 0.11004500 | 1.54080800 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -188.7465999
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -188.4380354

**$CO_2$**

Zero-point correction= 0.011678 (Hartree/Particle)
Thermal correction to Energy= 0.014316
Thermal correction to Enthalpy= 0.015260
Thermal correction to Gibbs Free Energy= -0.009027
Sum of electronic and zero-point Energies= -188.434130
Sum of electronic and thermal Energies= -188.431491

Sum of electronic and thermal Enthalpies= -188.430547
Sum of electronic and thermal Free Energies= -188.454835

| | | | |
|---|---|---|---|
| C | 0.38648600 | 1.25634400 | 1.50077800 |
| O | 1.54975800 | 1.25634400 | 1.50077800 |
| O | -0.77678600 | 1.25634400 | 1.50077800 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -188.6725431
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -188.3832588

**AlkSM**
Zero-point correction= 0.215412 (Hartree/Particle)
Thermal correction to Energy= 0.228232
Thermal correction to Enthalpy= 0.229176
Thermal correction to Gibbs Free Energy= 0.175093
Sum of electronic and zero-point Energies= -556.377104
Sum of electronic and thermal Energies= -556.364284
Sum of electronic and thermal Enthalpies= -556.363340
Sum of electronic and thermal Free Energies= -556.417423

| | | | |
|---|---|---|---|
| C | 0.59432200 | 0.28276100 | 0.61169600 |
| C | 1.85768300 | 0.13621500 | 0.02136300 |
| C | 2.48671900 | 1.24881600 | -0.55528400 |
| C | 1.85079800 | 2.49275700 | -0.55130800 |
| C | 0.58071500 | 2.63406700 | 0.02047800 |
| C | -0.04558900 | 1.52525900 | 0.59978900 |
| H | 0.11558000 | -0.58259500 | 1.07529900 |
| H | 3.46848200 | 1.13028200 | -1.01931800 |
| H | 2.34588700 | 3.35365900 | -1.00734300 |
| H | 0.08232800 | 3.60641500 | 0.01668000 |
| H | -1.03396800 | 1.62800800 | 1.05456800 |
| N | 2.51840100 | -1.13276500 | 0.03414500 |
| C | 3.71938800 | -1.25601700 | 0.86251400 |
| H | 3.45721000 | -1.43427200 | 1.91993100 |
| H | 4.32537600 | -2.09911100 | 0.50910100 |
| H | 4.30542000 | -0.33052900 | 0.79787100 |
| C | 1.92799300 | -2.29461800 | -0.40556900 |
| O | 2.34479500 | -3.39820400 | -0.06141000 |
| C | 0.78312300 | -2.20626400 | -1.38684000 |
| C | 0.86682000 | -1.43087600 | -2.47706700 |
| H | 1.71637200 | -0.76470400 | -2.64473700 |
| H | 0.08213000 | -1.44329700 | -3.23954200 |
| C | -0.35202300 | -3.15515600 | -1.11516000 |
| H | 0.03299400 | -4.18063500 | -1.00163700 |
| H | -0.85638300 | -2.89811800 | -0.16733200 |
| H | -1.09747700 | -3.13560800 | -1.92276200 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -557.211362
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -556.3928833

**NaF**
Zero-point correction= 0.001090 (Hartree/Particle)
Thermal correction to Energy= 0.003691
Thermal correction to Enthalpy= 0.004635
Thermal correction to Gibbs Free Energy= -0.020146
Sum of electronic and zero-point Energies= -262.093149
Sum of electronic and thermal Energies= -262.090548
Sum of electronic and thermal Enthalpies= -262.089604
Sum of electronic and thermal Free Energies= -262.114384

| | | | |
|---|---|---|---|
| F | -1.05199600 | -0.09864300 | -0.92600600 |
| Na | -3.01608400 | -0.09864300 | -0.92600600 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -262.2970078
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -262.0494951

**$HCO_3$-**
Zero-point correction= 0.026496 (Hartree/Particle)
Thermal correction to Energy= 0.029997
Thermal correction to Enthalpy= 0.030941
Thermal correction to Gibbs Free Energy= 0.000748
Sum of electronic and zero-point Energies= -264.314546
Sum of electronic and thermal Energies= -264.311045
Sum of electronic and thermal Enthalpies= -264.310101
Sum of electronic and thermal Free Energies= -264.340294

| | | | |
|---|---|---|---|
| O | -0.74100800 | 1.07561400 | 1.73888100 |
| C | 0.46452000 | 1.34907700 | 1.56081300 |
| O | 1.00852800 | 2.39337800 | 1.16683600 |
| O | 1.37093600 | 0.30029300 | 1.85433200 |
| H | 0.81315100 | -0.43591800 | 2.14436000 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -264.6796935
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -264.2593954

**$H_2CO_3$**
Zero-point correction= 0.039606 (Hartree/Particle)
Thermal correction to Energy= 0.043314
Thermal correction to Enthalpy= 0.044258
Thermal correction to Gibbs Free Energy= 0.013718
Sum of electronic and zero-point Energies= -264.779367
Sum of electronic and thermal Energies= -264.775658
Sum of electronic and thermal Enthalpies= -264.774714
Sum of electronic and thermal Free Energies= -264.805254

| | | | |
|---|---|---|---|
| O | -0.86203900 | 1.35089400 | 1.11022600 |
| C | 0.27719000 | 1.13620900 | 1.44946700 |
| O | 0.72330700 | 0.00808600 | 2.00557800 |
| H | -0.02811300 | -0.60184900 | 2.08604800 |
| O | 1.29777300 | 1.98783700 | 1.33005400 |
| H | 0.95966400 | 2.80294800 | 0.92462200 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -265.1409055
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -264.7377114

**MECP-e-L-2-Inta**
Zero-point correction= 0.402426 (Hartree/Particle)
Thermal correction to Energy= 0.432861
Thermal correction to Enthalpy= 0.433805
Thermal correction to Gibbs Free Energy= 0.338480
Sum of electronic and zero-point Energies= -1666.464082
Sum of electronic and thermal Energies= -1666.433647
Sum of electronic and thermal Enthalpies= -1666.432703
Sum of electronic and thermal Free Energies= -1666.528029

| | | | |
|---|---|---|---|
| C | 5.093120000 | -1.672665000 | -1.427395000 |
| C | 3.798790000 | 0.436379000 | -1.706848000 |
| C | 4.952522000 | 1.009252000 | -2.183697000 |
| C | 6.186620000 | 0.302667000 | -2.236571000 |
| C | 6.233668000 | -1.078180000 | -1.896926000 |
| H | 2.867566000 | 1.001277000 | -1.672857000 |
| H | 4.925135000 | 2.040793000 | -2.546697000 |
| H | 7.083796000 | 0.798032000 | -2.612907000 |
| H | 7.144472000 | -1.657954000 | -2.061471000 |
| N | 4.852424000 | -3.020667000 | -1.201167000 |
| C | 5.880637000 | -4.037015000 | -1.147454000 |
| H | 6.596866000 | -3.800877000 | -0.347232000 |
| H | 5.396798000 | -4.998568000 | -0.938442000 |
| H | 6.417224000 | -4.100395000 | -2.107335000 |
| C | 3.510228000 | -3.294612000 | -1.077166000 |
| O | 3.031427000 | -4.402344000 | -0.896749000 |

| | | | |
|---|---|---|---|
| C | 2.714911000 | -1.985371000 | -1.293030000 |
| C | 2.235683000 | -2.062660000 | -2.770123000 |
| H | 1.986950000 | -3.104780000 | -3.023822000 |
| H | 3.057613000 | -1.753730000 | -3.431338000 |
| C | 1.585008000 | -1.895509000 | -0.265779000 |
| H | 1.021672000 | -0.960236000 | -0.381255000 |
| H | 2.007300000 | -1.916936000 | 0.747626000 |
| C | 3.837874000 | -0.923845000 | -1.085619000 |
| H | 3.889124000 | -0.783710000 | 0.025268000 |
| H | 0.887848000 | -2.737237000 | -0.382998000 |
| C | 1.001265000 | -1.270635000 | -3.162479000 |
| C | 0.841165000 | -1.169680000 | -4.695903000 |
| O | -0.050507000 | -1.699709000 | -5.311245000 |
| O | 1.821310000 | -0.445445000 | -5.206876000 |
| C | 1.844838000 | -0.259777000 | -6.645133000 |
| H | 1.845960000 | -1.252257000 | -7.119921000 |
| H | 0.919004000 | 0.257953000 | -6.938836000 |
| C | 3.081095000 | 0.539685000 | -6.983560000 |
| H | 3.991300000 | 0.004546000 | -6.672270000 |
| H | 3.126300000 | 0.702102000 | -8.070919000 |
| H | 3.062507000 | 1.520501000 | -6.485644000 |
| F | -0.127325000 | -1.853673000 | -2.671816000 |
| F | 1.012367000 | 0.010148000 | -2.671427000 |
| C | 4.458630000 | -0.746284000 | 2.282144000 |
| O | 5.220182000 | 0.206541000 | 2.643157000 |
| O | 3.076789000 | -0.749527000 | 2.646404000 |
| C | 4.956294000 | -2.148958000 | 2.350699000 |
| C | 2.433702000 | 0.490742000 | 2.432351000 |
| H | 2.478605000 | 0.758094000 | 1.356481000 |
| H | 2.967411000 | 1.289862000 | 2.976419000 |
| C | 0.993996000 | 0.387207000 | 2.897563000 |
| H | 0.477325000 | 1.352302000 | 2.771685000 |
| H | 0.445997000 | -0.375234000 | 2.321663000 |
| H | 0.951732000 | 0.109000000 | 3.963045000 |
| F | 6.140315000 | -2.279773000 | 1.699881000 |
| F | 5.216313000 | -2.626147000 | 3.627118000 |
| F | 4.108450000 | -3.063612000 | 1.816045000 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1668.7973434
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1666.3285172

**MECP-e-L-2-$CO_2$**

Zero-point correction= 0.319728 (Hartree/Particle)
Thermal correction to Energy= 0.343039
Thermal correction to Enthalpy= 0.343983
Thermal correction to Gibbs Free Energy= 0.265705
Sum of electronic and zero-point Energies= -1250.003058
Sum of electronic and thermal Energies= -1249.979747
Sum of electronic and thermal Enthalpies= -1249.978803
Sum of electronic and thermal Free Energies= -1250.057082

| | | | |
|---|---|---|---|
| C | 4.957717000 | -1.447284000 | -1.131096000 |
| C | 3.904271000 | 0.797056000 | -1.226852000 |
| C | 5.174688000 | 1.324998000 | -1.278731000 |
| C | 6.338920000 | 0.514527000 | -1.197110000 |
| C | 6.214113000 | -0.902922000 | -1.179759000 |
| H | 3.031335000 | 1.446470000 | -1.294348000 |
| H | 5.297318000 | 2.405788000 | -1.403944000 |
| H | 7.329507000 | 0.972415000 | -1.233725000 |
| H | 7.099169000 | -1.538574000 | -1.257285000 |
| N | 4.588891000 | -2.780178000 | -1.256689000 |
| C | 5.510941000 | -3.891742000 | -1.196103000 |
| H | 6.018096000 | -3.913061000 | -0.219220000 |
| H | 4.938165000 | -4.816795000 | -1.332522000 |
| H | 6.270564000 | -3.811850000 | -1.990207000 |
| C | 3.237949000 | -2.928593000 | -1.456600000 |
| O | 2.658742000 | -3.992840000 | -1.607292000 |
| C | 2.600544000 | -1.523734000 | -1.571909000 |
| C | 2.477357000 | -1.283610000 | -3.103775000 |
| H | 2.228153000 | -2.228448000 | -3.608148000 |
| H | 3.453480000 | -0.956556000 | -3.494927000 |
| C | 1.262499000 | -1.504382000 | -0.831564000 |
| H | 0.813934000 | -0.501864000 | -0.845986000 |
| H | 1.424471000 | -1.810091000 | 0.210358000 |
| C | 3.709620000 | -0.647372000 | -0.914068000 |
| H | 3.505325000 | -0.752475000 | 0.202319000 |
| C | 3.572494000 | -1.879008000 | 2.046231000 |
| O | 3.178022000 | -2.973716000 | 1.645369000 |
| O | 4.104268000 | -1.429449000 | 3.057994000 |
| H | 0.557043000 | -2.205994000 | -1.297983000 |
| C | 1.426644000 | -0.301130000 | -3.590463000 |
| C | 1.636088000 | 0.075290000 | -5.072821000 |
| O | 1.924329000 | 1.185437000 | -5.445228000 |
| O | 1.479516000 | -0.989277000 | -5.841520000 |
| C | 1.672574000 | -0.816184000 | -7.269792000 |
| H | 0.958054000 | -0.057162000 | -7.622018000 |
| H | 2.689889000 | -0.429384000 | -7.432414000 |
| C | 1.456289000 | -2.156608000 | -7.931029000 |
| H | 0.436563000 | -2.526943000 | -7.743671000 |
| H | 1.594249000 | -2.052928000 | -9.018153000 |
| H | 2.177241000 | -2.900147000 | -7.558404000 |
| F | 0.168388000 | -0.837108000 | -3.474078000 |
| F | 1.413558000 | 0.857326000 | -2.877495000 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1251.7626414
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1249.9054008

**TS-e-L-2*-Intc**

Zero-point correction= 0.398021 (Hartree/Particle)
Thermal correction to Energy= 0.427977
Thermal correction to Enthalpy= 0.428921
Thermal correction to Gibbs Free Energy= 0.336031
Sum of electronic and zero-point Energies= -1566.544569
Sum of electronic and thermal Energies= -1566.514612
Sum of electronic and thermal Enthalpies= -1566.513668
Sum of electronic and thermal Free Energies= -1566.606559

| | | | |
|---|---|---|---|
| C | 4.79057000 | -0.88511600 | -0.45221900 |
| C | 3.88593400 | 0.91184200 | 1.06520300 |
| C | 5.17651900 | 1.14333200 | 1.43637000 |
| C | 6.28563500 | 0.34729100 | 0.94624900 |
| C | 6.07900000 | -0.64263300 | -0.04183400 |
| H | 3.06424500 | 1.52696600 | 1.43571100 |
| H | 5.39858200 | 1.97100500 | 2.11559100 |
| H | 7.29501300 | 0.56491800 | 1.29768600 |
| H | 6.92157400 | -1.17573500 | -0.48527600 |
| N | 4.30988700 | -1.73575100 | -1.42146800 |
| C | 5.14549400 | -2.61750300 | -2.21337400 |
| H | 5.68858900 | -3.30860400 | -1.55241500 |
| H | 4.49765900 | -3.18254800 | -2.89412900 |
| H | 5.86763500 | -2.02707600 | -2.79844500 |
| C | 2.94592500 | -1.57477500 | -1.64739100 |
| O | 2.29566900 | -2.21599000 | -2.44902300 |
| C | 2.42248400 | -0.43472900 | -0.74323700 |
| C | 1.11563400 | -0.86221000 | -0.05026900 |
| H | 0.76873200 | -0.06924700 | 0.62919500 |
| H | 0.33356600 | -1.04890900 | -0.80035300 |
| H | 1.25920100 | -1.78303000 | 0.52916100 |
| C | 2.09019200 | 0.81153600 | -1.61687400 |
| H | 1.70998200 | 1.61581700 | -0.97184700 |
| H | 1.28203100 | 0.53167500 | -2.30991700 |
| C | 3.17037300 | 1.41658300 | -2.50133700 |
| C | 4.28177700 | 2.24608800 | -1.81635900 |
| O | 5.45794600 | 2.04819600 | -1.97820800 |
| O | 3.73656600 | 3.21334400 | -1.09336300 |
| C | 4.63129800 | 4.12539400 | -0.40891300 |

| | | | |
|---|---|---|---|
| H | 5.10929500 | 4.76557600 | -1.16741600 |
| H | 5.41774800 | 3.53386200 | 0.08150200 |
| C | 3.80977800 | 4.91989300 | 0.58002500 |
| H | 4.45714400 | 5.63915500 | 1.10405100 |
| H | 3.01027100 | 5.47835400 | 0.06989700 |
| H | 3.35225300 | 4.25449300 | 1.32804900 |
| F | 3.77576900 | 0.45969000 | -3.25876200 |
| F | 2.55283100 | 2.27449100 | -3.37764300 |
| C | 3.59511000 | -0.26206700 | 0.21686100 |
| H | 3.46820200 | -1.29597600 | 1.14428200 |
| C | 3.88472800 | -3.54087200 | 1.19046400 |
| O | 4.97361700 | -4.04020000 | 1.01884500 |
| O | 2.75031000 | -3.91083000 | 0.59856100 |
| C | 3.64294400 | -2.29546100 | 2.00563400 |
| C | 2.80459700 | -5.03292800 | -0.31915500 |
| H | 3.09459500 | -5.92914000 | 0.25147600 |
| H | 3.59279700 | -4.83650600 | -1.06126500 |
| C | 1.44199500 | -5.16750700 | -0.95944200 |
| H | 1.44395400 | -6.02699500 | -1.64703100 |
| H | 0.66584200 | -5.33463300 | -0.19709200 |
| H | 1.19924200 | -4.26069300 | -1.53180500 |
| F | 4.67732600 | -1.97019500 | 2.78638400 |
| F | 2.50868400 | -2.31515600 | 2.73077600 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1568.7381923
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1566.4312041

**TS-e-L-2*-$CO_2$**

Zero-point correction= 0.315925 (Hartree/Particle)
Thermal correction to Energy= 0.340316
Thermal correction to Enthalpy= 0.341260
Thermal correction to Gibbs Free Energy= 0.258340
Sum of electronic and zero-point Energies= -1249.975290
Sum of electronic and thermal Energies= -1249.950900
Sum of electronic and thermal Enthalpies= -1249.949955
Sum of electronic and thermal Free Energies= -1250.032875

| | | | |
|---|---|---|---|
| C | 5.01383500 | -1.47033800 | -1.07476100 |
| C | 3.89554500 | 0.76172100 | -1.03423000 |
| C | 5.13065600 | 1.31543600 | -0.83388900 |
| C | 6.32611000 | 0.50720700 | -0.70679300 |
| C | 6.24889900 | -0.90570900 | -0.85598500 |
| H | 3.01060100 | 1.39219100 | -1.12876400 |
| H | 5.22857600 | 2.40350300 | -0.76795100 |
| H | 7.29115500 | 0.98679700 | -0.53235000 |
| H | 7.14970400 | -1.52247000 | -0.81545900 |
| N | 4.68586300 | -2.79323300 | -1.30021100 |
| C | 5.60170500 | -3.90299300 | -1.15270900 |
| H | 5.95032400 | -3.97370100 | -0.10978400 |
| H | 5.07095700 | -4.82417900 | -1.42327800 |
| H | 6.47454000 | -3.77492200 | -1.81147100 |
| C | 3.34149400 | -2.95403700 | -1.58503300 |
| O | 2.79214200 | -4.02651700 | -1.78624600 |
| C | 2.68200100 | -1.55768700 | -1.69968000 |
| C | 2.52876800 | -1.33322200 | -3.25099700 |
| H | 2.19253600 | -2.26836400 | -3.72311100 |
| H | 3.51786100 | -1.09034900 | -3.67018200 |
| C | 1.32143600 | -1.56528100 | -0.98424700 |
| H | 0.87854300 | -0.55959800 | -0.98283600 |
| H | 1.45616800 | -1.90045400 | 0.05280500 |
| C | 3.74670000 | -0.69675300 | -1.04756600 |
| H | 3.63107600 | -1.01366400 | 0.53724200 |
| C | 3.70232900 | -1.53125500 | 1.68474600 |
| O | 3.30327700 | -2.70414200 | 1.66085300 |
| O | 4.13310600 | -0.77162600 | 2.55645200 |
| H | 0.62246800 | -2.24756600 | -1.48893000 |
| C | 1.54940700 | -0.27281600 | -3.72033800 |
| C | 1.72605900 | 0.04741500 | -5.22106600 |
| O | 2.17823300 | 1.08447700 | -5.63738600 |
| O | 1.35490400 | -0.99270700 | -5.95710200 |
| C | 1.50301000 | -0.87711100 | -7.39428200 |
| H | 0.90103200 | -0.02088800 | -7.73730900 |
| H | 2.55848000 | -0.65503100 | -7.61758500 |
| C | 1.04779800 | -2.18096000 | -8.00948900 |
| H | -0.00579300 | -2.38312600 | -7.76334700 |
| H | 1.14495100 | -2.12693800 | -9.10439400 |
| H | 1.66090100 | -3.02014000 | -7.64689600 |
| F | 0.25507200 | -0.68469300 | -3.52721600 |
| F | 1.68854800 | 0.89562100 | -3.03388300 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1251.73021
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1249.8711735

**TS-e-L-2*-Inta**

Zero-point correction= 0.398821 (Hartree/Particle)
Thermal correction to Energy= 0.429924
Thermal correction to Enthalpy= 0.430869
Thermal correction to Gibbs Free Energy= 0.333801
Sum of electronic and zero-point Energies= -1666.434562
Sum of electronic and thermal Energies= -1666.403458
Sum of electronic and thermal Enthalpies= -1666.402514
Sum of electronic and thermal Free Energies= -1666.499582

| | | | |
|---|---|---|---|
| C | 5.11461000 | -1.76977200 | -1.33071900 |
| C | 3.82221800 | 0.34880900 | -1.45166800 |
| C | 5.01123400 | 1.00024300 | -1.66389800 |
| C | 6.27052600 | 0.30921700 | -1.66113200 |
| C | 6.30150100 | -1.11556500 | -1.54218100 |
| H | 2.87674900 | 0.89107900 | -1.46901500 |
| H | 5.00744900 | 2.07938900 | -1.84919300 |
| H | 7.19814200 | 0.86289100 | -1.82112200 |
| H | 7.24176700 | -1.66478000 | -1.62746600 |
| N | 4.87879400 | -3.13430800 | -1.24493800 |
| C | 5.91281900 | -4.14366800 | -1.18049700 |
| H | 6.53563600 | -3.99019900 | -0.28588100 |
| H | 5.42841600 | -5.12671100 | -1.12740600 |
| H | 6.55415900 | -4.10001600 | -2.07495100 |
| C | 3.53023000 | -3.41947500 | -1.16256900 |
| O | 3.05518600 | -4.54176600 | -1.06233700 |
| C | 2.73100400 | -2.10194500 | -1.30495100 |
| C | 2.18876000 | -2.14153200 | -2.78637500 |
| H | 1.89448600 | -3.17291500 | -3.03668000 |
| H | 3.00350400 | -1.85195600 | -3.46510900 |
| C | 1.59008700 | -2.06718800 | -0.27622100 |
| H | 1.03356200 | -1.12310200 | -0.35017000 |
| H | 1.99973200 | -2.13857600 | 0.73837700 |
| C | 3.83313200 | -1.07672200 | -1.09638400 |
| H | 4.13947200 | -0.89508200 | 0.46734900 |
| H | 0.88895000 | -2.89658100 | -0.44963400 |
| C | 0.97513600 | -1.29464900 | -3.12374200 |
| C | 0.77263200 | -1.14265100 | -4.64648100 |
| O | -0.14041800 | -1.63796200 | -5.26017300 |
| O | 1.76092400 | -0.42253200 | -5.16663100 |
| C | 1.74835400 | -0.20692200 | -6.59842800 |
| H | 1.73980300 | -1.18834300 | -7.09850800 |
| H | 0.81359800 | 0.31189100 | -6.86400900 |
| C | 2.97407400 | 0.60573800 | -6.94993700 |
| H | 3.89321800 | 0.06829600 | -6.67062900 |
| H | 2.99623600 | 0.79322200 | -8.03416100 |
| H | 2.96272900 | 1.57530900 | -6.42900700 |
| F | -0.16083400 | -1.84688100 | -2.61240500 |
| F | 1.05930400 | -0.02863300 | -2.59178500 |
| C | 4.41503000 | -0.68935400 | 1.70656700 |
| O | 5.23346200 | 0.28058800 | 1.85306200 |
| O | 3.10667600 | -0.59564800 | 2.29751300 |

| | | | |
|---|---|---|---|
| C | 4.93285300 | -2.06849900 | 2.16266000 |
| C | 2.45661300 | 0.63855300 | 2.05805300 |
| H | 2.43657600 | 0.85042900 | 0.97095100 |
| H | 3.02223300 | 1.46401900 | 2.52798000 |
| C | 1.04713700 | 0.55782300 | 2.61412600 |
| H | 0.52191400 | 1.51663500 | 2.47925700 |
| H | 0.47165600 | -0.22940400 | 2.10210700 |
| H | 1.06952900 | 0.32249600 | 3.69035100 |
| F | 6.12750000 | -2.33936600 | 1.60034100 |
| F | 5.10879800 | -2.14275700 | 3.50041500 |
| F | 4.10343200 | -3.08208300 | 1.82392700 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1668.7613853
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1666.2940773

**L-2*-Est**

Zero-point correction= 0.401927 (Hartree/Particle)
Thermal correction to Energy= 0.432775
Thermal correction to Enthalpy= 0.433719
Thermal correction to Gibbs Free Energy= 0.337892
Sum of electronic and zero-point Energies= -1566.564481
Sum of electronic and thermal Energies= -1566.533633
Sum of electronic and thermal Enthalpies= -1566.532689
Sum of electronic and thermal Free Energies= -1566.628516

| | | | |
|---|---|---|---|
| C | 4.66784300 | -0.67468300 | -0.38998600 |
| C | 3.45972900 | 0.94142400 | 1.08441900 |
| C | 4.64442200 | 1.10137000 | 1.76964600 |
| C | 5.89073200 | 0.39248700 | 1.36291700 |
| C | 5.86656500 | -0.50180200 | 0.29164700 |
| H | 2.56301700 | 1.48176000 | 1.39630500 |
| H | 4.68697600 | 1.76766600 | 2.63397900 |
| H | 6.79999400 | 0.54604100 | 1.94360800 |
| H | 6.75608600 | -1.06612700 | 0.00700100 |
| N | 4.35007300 | -1.49204100 | -1.43310400 |
| C | 5.30142600 | -2.33525200 | -2.13489800 |
| H | 5.74475300 | -3.06351200 | -1.44099700 |
| H | 4.76747300 | -2.86015700 | -2.93563300 |
| H | 6.09478300 | -1.70655800 | -2.56606600 |
| C | 2.99471300 | -1.41513600 | -1.79407800 |
| O | 2.47153900 | -2.13528800 | -2.62401100 |
| C | 2.30182300 | -0.32701100 | -0.94700000 |
| C | 1.09735900 | -0.94071300 | -0.19181700 |
| H | 0.62377200 | -0.17769700 | 0.44379600 |
| H | 0.34889900 | -1.31428100 | -0.90672800 |
| H | 1.42406300 | -1.77648100 | 0.44126800 |
| C | 1.76275800 | 0.82616200 | -1.83976000 |
| H | 1.35389300 | 1.61450500 | -1.19100200 |
| H | 0.94945000 | 0.46046200 | -2.48586700 |
| C | 2.77574000 | 1.48135900 | -2.76229600 |
| C | 4.05554000 | 2.03048000 | -2.09004500 |
| O | 5.15985200 | 1.59312800 | -2.30905700 |
| O | 3.76025300 | 3.04833200 | -1.29111600 |
| C | 4.86519800 | 3.68803400 | -0.60323700 |
| H | 5.49232800 | 4.18955700 | -1.35765200 |
| H | 5.47355700 | 2.90716200 | -0.12249200 |
| C | 4.28461000 | 4.65997600 | 0.39761400 |
| H | 5.10041100 | 5.17867100 | 0.92358100 |
| H | 3.65818200 | 5.41409200 | -0.10275600 |
| H | 3.67293400 | 4.12947400 | 1.14276500 |
| F | 3.17345800 | 0.59995700 | -3.72408000 |
| F | 2.16395400 | 2.51962100 | -3.41212800 |
| C | 3.42482000 | 0.08680800 | -0.04003600 |
| H | 3.71141300 | -1.62116000 | 2.09931600 |
| C | 4.21443900 | -3.54871200 | 1.15930200 |
| O | 5.24064500 | -4.04195500 | 0.76293800 |
| O | 3.00783600 | -3.73085300 | 0.63943100 |
| C | 4.12031300 | -2.60693800 | 2.37328300 |
| C | 2.87897700 | -4.69042200 | -0.44729100 |
| H | 3.28786800 | -5.65098700 | -0.09856800 |
| H | 3.49102500 | -4.34321900 | -1.29109600 |
| C | 1.41773700 | -4.78141400 | -0.81941600 |
| H | 1.29139800 | -5.54492300 | -1.60201000 |
| H | 0.80751400 | -5.06952000 | 0.04990300 |
| H | 1.05862000 | -3.82147300 | -1.21550400 |
| F | 5.34778900 | -2.45253900 | 2.91191100 |
| F | 3.30789200 | -3.17558800 | 3.30610400 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1568.7665357
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1566.4553869

**L-2*-$CO_2$**

Zero-point correction= 0.318405 (Hartree/Particle)
Thermal correction to Energy= 0.343952
Thermal correction to Enthalpy= 0.344896
Thermal correction to Gibbs Free Energy= 0.258477
Sum of electronic and zero-point Energies= -1249.978089
Sum of electronic and thermal Energies= -1249.952543
Sum of electronic and thermal Enthalpies= -1249.951599
Sum of electronic and thermal Free Energies= -1250.038017

| | | | |
|---|---|---|---|
| C | 5.05740400 | -1.29722600 | -0.99927100 |
| C | 4.00733900 | 0.94211400 | -1.28203300 |
| C | 5.12966800 | 1.47619700 | -0.67449100 |
| C | 6.25705200 | 0.61592400 | -0.20478000 |
| C | 6.18176500 | -0.76435300 | -0.37145300 |
| H | 3.19529000 | 1.59637700 | -1.60165100 |
| H | 5.20018900 | 2.55570700 | -0.51933300 |
| H | 7.11381700 | 1.07961200 | 0.28545000 |
| H | 6.96952000 | -1.42302800 | -0.00172000 |
| N | 4.73259200 | -2.59136700 | -1.25049800 |
| C | 5.52012400 | -3.73224300 | -0.82282800 |
| H | 5.53189700 | -3.74389200 | 0.28159200 |
| H | 5.04582500 | -4.63913400 | -1.21614000 |
| H | 6.54390300 | -3.64566200 | -1.21728300 |
| C | 3.46640100 | -2.72967700 | -1.81723600 |
| O | 2.95918000 | -3.80073100 | -2.11408400 |
| C | 2.82901400 | -1.33715900 | -2.02388000 |
| C | 2.55050200 | -1.21627400 | -3.55653400 |
| H | 2.11293500 | -2.16074000 | -3.91149000 |
| H | 3.50682600 | -1.08130100 | -4.08450600 |
| C | 1.52521500 | -1.26471500 | -1.18962900 |
| H | 1.09719100 | -0.25376700 | -1.23895500 |
| H | 1.75823900 | -1.51959800 | -0.14657600 |
| C | 3.91961500 | -0.44654200 | -1.49203600 |
| H | 3.79648800 | -1.62437700 | 2.89966300 |
| C | 4.05670800 | -2.43264200 | 2.13429800 |
| O | 3.17075500 | -2.68688600 | 1.28940500 |
| O | 5.19416400 | -2.94152200 | 2.26345900 |
| H | 0.77969200 | -1.97421500 | -1.57961700 |
| C | 1.60507800 | -0.12404600 | -4.02043800 |
| C | 1.63684700 | 0.06415500 | -5.55485800 |
| O | 2.01389500 | 1.06891300 | -6.10246100 |
| O | 1.21656800 | -1.04177700 | -6.15446300 |
| C | 1.20462700 | -1.05113200 | -7.60439800 |
| H | 0.53271800 | -0.24964800 | -7.94979100 |
| H | 2.21949500 | -0.81484400 | -7.96070200 |
| C | 0.74253200 | -2.41931000 | -8.05142700 |
| H | -0.26861300 | -2.63403200 | -7.67335800 |
| H | 0.71861900 | -2.45990200 | -9.15094100 |
| H | 1.42711300 | -3.20144500 | -7.68925700 |
| F | 0.31042400 | -0.41187000 | -3.66964600 |
| F | 1.89886600 | 1.07975700 | -3.45426300 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1251.7353466

UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1249.8767345

**L-2*-Alkoxide**

Zero-point correction= 0.401351 (Hartree/Particle)
Thermal correction to Energy= 0.433094
Thermal correction to Enthalpy= 0.434038
Thermal correction to Gibbs Free Energy= 0.334639
Sum of electronic and zero-point Energies= -1666.432915
Sum of electronic and thermal Energies= -1666.401172
Sum of electronic and thermal Enthalpies= -1666.400228
Sum of electronic and thermal Free Energies= -1666.499627

| | | | |
|---|---|---|---|
| C | 5.13022700 | -1.67973200 | -1.29189500 |
| C | 3.83998600 | 0.44652100 | -1.32731900 |
| C | 5.03811400 | 1.11354600 | -1.25930700 |
| C | 6.30484000 | 0.41041800 | -1.19319700 |
| C | 6.33081200 | -1.00874900 | -1.24190700 |
| H | 2.89913100 | 0.99382300 | -1.38938800 |
| H | 5.04681100 | 2.20773800 | -1.26497000 |
| H | 7.23695100 | 0.97428400 | -1.12503800 |
| H | 7.27620900 | -1.55453600 | -1.20824600 |
| N | 4.88556500 | -3.04035300 | -1.29963200 |
| C | 5.90616500 | -4.05911000 | -1.17992400 |
| H | 6.43204400 | -3.96027400 | -0.21822500 |
| H | 5.41714200 | -5.03978600 | -1.23212900 |
| H | 6.63800400 | -3.96947800 | -1.99788300 |
| C | 3.53025900 | -3.32409700 | -1.31577000 |
| O | 3.05094500 | -4.45256200 | -1.28592200 |
| C | 2.73169500 | -2.00653500 | -1.44303300 |
| C | 2.12259800 | -2.05456300 | -2.90347400 |
| H | 1.74665900 | -3.07258300 | -3.09109000 |
| H | 2.92729900 | -1.85597400 | -3.62487400 |
| C | 1.61835900 | -1.96459500 | -0.37616400 |
| H | 1.07054900 | -1.01353300 | -0.42941700 |
| H | 2.05856200 | -2.04732000 | 0.62615300 |
| C | 3.82739500 | -0.99423100 | -1.25697700 |
| H | 4.27025300 | -0.91745400 | 0.62823800 |
| H | 0.90130800 | -2.78479400 | -0.53086100 |
| C | 0.97036700 | -1.12486800 | -3.22769400 |
| C | 0.67954400 | -1.05861700 | -4.73975500 |
| O | -0.31135500 | -1.51496900 | -5.25830500 |
| O | 1.68876900 | -0.47001400 | -5.37715400 |
| C | 1.59503600 | -0.37091500 | -6.81787400 |
| H | 1.46989400 | -1.38483700 | -7.23013200 |
| H | 0.69041800 | 0.20503900 | -7.07007800 |
| C | 2.85617900 | 0.29830100 | -7.31618000 |
| H | 3.74508300 | -0.29403700 | -7.05021400 |
| H | 2.81706100 | 0.39384700 | -8.41190600 |
| H | 2.96250100 | 1.30455200 | -6.88283200 |
| F | -0.17621100 | -1.52854500 | -2.61054800 |
| F | 1.21369300 | 0.15778400 | -2.78863700 |
| C | 4.49602600 | -0.77075400 | 1.76034400 |
| O | 5.33268900 | 0.19543300 | 1.95221300 |
| O | 3.19959400 | -0.67834900 | 2.38634700 |
| C | 5.00802400 | -2.16074200 | 2.21120700 |
| C | 2.52542600 | 0.54036700 | 2.12987100 |
| H | 2.45833100 | 0.71344900 | 1.03887900 |
| H | 3.09827100 | 1.38723100 | 2.55038800 |
| C | 1.14009500 | 0.46252000 | 2.74378200 |
| H | 0.59770100 | 1.41007500 | 2.59767700 |
| H | 0.55478300 | -0.34795300 | 2.28107800 |
| H | 1.20717300 | 0.26358700 | 3.82550600 |
| F | 6.22467200 | -2.41533100 | 1.69241900 |
| F | 5.12506000 | -2.25854300 | 3.54929600 |
| F | 4.19518400 | -3.16390000 | 1.80919800 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1668.7631322

UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1666.2907636

**L-2 + $CO_2H$**

Zero-point correction= 0.324080 (Hartree/Particle)
Thermal correction to Energy= 0.348794
Thermal correction to Enthalpy= 0.349739
Thermal correction to Gibbs Free Energy= 0.266390
Sum of electronic and zero-point Energies= -1250.094714
Sum of electronic and thermal Energies= -1250.069999
Sum of electronic and thermal Enthalpies= -1250.069055
Sum of electronic and thermal Free Energies= -1250.152403

| | | | |
|---|---|---|---|
| C | 4.97948800 | -1.29187600 | -1.04079700 |
| C | 4.01139800 | 0.91032300 | -1.28292400 |
| C | 5.16393600 | 1.45107900 | -0.68434500 |
| C | 6.20520500 | 0.61394700 | -0.26945000 |
| C | 6.12596500 | -0.77675100 | -0.43910600 |
| H | 3.19717400 | 1.56323100 | -1.59715500 |
| H | 5.24195500 | 2.53122300 | -0.53846900 |
| H | 7.09309200 | 1.04487000 | 0.20091700 |
| H | 6.92321800 | -1.43388200 | -0.09132000 |
| N | 4.68338300 | -2.63238900 | -1.30442000 |
| C | 5.49347700 | -3.74629200 | -0.85554400 |
| H | 5.55553200 | -3.72386200 | 0.24539400 |
| H | 5.00522600 | -4.67106100 | -1.18845600 |
| H | 6.50110800 | -3.69032400 | -1.29828600 |
| C | 3.42850700 | -2.76464400 | -1.83288900 |
| O | 2.88211900 | -3.81360700 | -2.13443900 |
| C | 2.81601000 | -1.34937400 | -2.01588800 |
| C | 2.55453900 | -1.20577500 | -3.53607700 |
| H | 2.12603300 | -2.14795900 | -3.90851600 |
| H | 3.51189500 | -1.05599900 | -4.05905000 |
| C | 1.53730600 | -1.27495000 | -1.15760300 |
| H | 1.10010200 | -0.26807100 | -1.20288400 |
| H | 1.79216900 | -1.52543100 | -0.11804000 |
| C | 3.92305700 | -0.46465300 | -1.46818000 |
| H | 3.80413400 | -1.51734100 | 2.85898900 |
| C | 4.05951400 | -2.37073000 | 2.14054600 |
| O | 3.15929900 | -2.68231800 | 1.32984000 |
| O | 5.20279700 | -2.86038200 | 2.28127700 |
| H | 0.79364000 | -1.99521200 | -1.52963300 |
| C | 1.59779300 | -0.11791300 | -3.98963200 |
| C | 1.61874500 | 0.08314600 | -5.52366300 |
| O | 1.93231300 | 1.11332900 | -6.06290200 |
| O | 1.25781600 | -1.03903800 | -6.13010600 |
| C | 1.23259000 | -1.03664600 | -7.58043700 |
| H | 0.52040000 | -0.26475400 | -7.91200400 |
| H | 2.23200600 | -0.74976300 | -7.94310100 |
| C | 0.83133900 | -2.42131200 | -8.03512900 |
| H | -0.16525500 | -2.68631200 | -7.65042600 |
| H | 0.79967300 | -2.45377900 | -9.13470300 |
| H | 1.55511300 | -3.17332000 | -7.68564000 |
| F | 0.30782000 | -0.42596300 | -3.63839800 |
| F | 1.87584600 | 1.08423500 | -3.41551200 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1251.8579692
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1250.0047732

**L-2 + Alkoxide**

Zero-point correction= 0.407302 (Hartree/Particle)
Thermal correction to Energy= 0.438687
Thermal correction to Enthalpy= 0.439631
Thermal correction to Gibbs Free Energy= 0.340993
Sum of electronic and zero-point Energies= -1666.538602
Sum of electronic and thermal Energies= -1666.507218
Sum of electronic and thermal Enthalpies= -1666.506274

Sum of electronic and thermal Free Energies= -1666.604912

| | | | |
|---|---|---|---|
| C | 1.86049500 | -0.27368400 | -0.24075300 |
| C | 0.70474100 | 1.83338100 | -0.47627400 |
| C | 1.93556100 | 2.49193600 | -0.30659400 |
| C | 3.11060500 | 1.76046000 | -0.10693400 |
| C | 3.08990900 | 0.35813800 | -0.06898600 |
| H | -0.21047300 | 2.40660300 | -0.62119000 |
| H | 1.97105900 | 3.58379800 | -0.32494100 |
| H | 4.06008100 | 2.28453900 | 0.02936900 |
| H | 4.00071200 | -0.21464300 | 0.10991400 |
| N | 1.59614700 | -1.64883200 | -0.20717000 |
| C | 2.58567100 | -2.66375400 | 0.08092500 |
| H | 3.03414900 | -2.48465300 | 1.06952200 |
| H | 2.08194200 | -3.63838000 | 0.07907000 |
| H | 3.37936400 | -2.66224000 | -0.68285100 |
| C | 0.25533600 | -1.89929100 | -0.34826100 |
| O | -0.27189700 | -2.99861100 | -0.33967500 |
| C | -0.48188500 | -0.54537800 | -0.53084400 |
| C | -1.16583400 | -0.63102200 | -1.91982800 |
| H | -1.60217600 | -1.63633000 | -2.03128400 |
| H | -0.40960300 | -0.51005200 | -2.70767900 |
| C | -1.46974500 | -0.38198600 | 0.64144700 |
| H | -1.99951800 | 0.57684200 | 0.56511200 |
| H | -0.93145000 | -0.39918500 | 1.59916000 |
| C | 0.66873700 | 0.44434600 | -0.45183200 |
| H | 1.41399900 | 0.90095200 | 2.30563000 |
| H | -2.21187900 | -1.19364100 | 0.62312800 |
| C | -2.29767800 | 0.33904600 | -2.20684600 |
| C | -2.71464900 | 0.35229200 | -3.69886700 |
| O | -3.80920800 | 0.03863500 | -4.09074600 |
| O | -1.69858300 | 0.74989700 | -4.45116000 |
| C | -1.91605300 | 0.82628400 | -5.88339400 |
| H | -2.24013700 | -0.16495600 | -6.23705700 |
| H | -2.73805700 | 1.53509000 | -6.06996300 |
| C | -0.61921400 | 1.26930100 | -6.52129600 |
| H | 0.18527500 | 0.54664600 | -6.31603200 |
| H | -0.75051500 | 1.34293100 | -7.61144500 |
| H | -0.31247600 | 2.25532400 | -6.14040200 |
| F | -3.40401700 | 0.02774600 | -1.47979300 |
| F | -1.96388300 | 1.62823200 | -1.87124600 |
| C | 1.34083400 | 0.63886900 | 3.40618400 |
| O | 1.99108600 | 1.37385900 | 4.23788700 |
| O | -0.14466900 | 0.53888100 | 3.63209500 |
| C | 1.73639000 | -0.86147000 | 3.45759700 |
| C | -0.77246900 | 1.78381400 | 3.48434600 |
| H | -0.67693200 | 2.14953100 | 2.43627300 |
| H | -0.27212400 | 2.53843700 | 4.12324800 |
| C | -2.24157500 | 1.65836700 | 3.85388200 |
| H | -2.75409800 | 2.63129000 | 3.77655100 |
| H | -2.75256800 | 0.94528900 | 3.18645800 |
| H | -2.34665000 | 1.29027800 | 4.88759600 |
| F | 3.02644600 | -1.01745600 | 3.05743200 |
| F | 1.65436200 | -1.38835900 | 4.69549700 |
| F | 1.00458500 | -1.67070300 | 2.64553900 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1668.8830096
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1666.4138105

**F**

Zero-point correction= 0.313725 (Hartree/Particle)
Thermal correction to Energy= 0.334122
Thermal correction to Enthalpy= 0.335067
Thermal correction to Gibbs Free Energy= 0.263823
Sum of electronic and zero-point Energies= -1061.336352
Sum of electronic and thermal Energies= -1061.315955
Sum of electronic and thermal Enthalpies= -1061.315011
Sum of electronic and thermal Free Energies= -1061.386254

| | | | |
|---|---|---|---|
| C | 0.73733500 | -1.09837100 | 0.76771200 |
| C | 1.82334900 | -0.09622200 | 0.55747100 |
| C | 1.63310600 | 1.26831600 | 0.83179700 |
| C | 0.33650200 | 1.68362600 | 1.07435900 |
| C | -0.79981400 | 0.79963400 | 1.06551600 |
| C | -0.63259100 | -0.53511800 | 0.87889700 |
| H | 0.93047000 | -1.48506000 | 1.79591600 |
| H | 2.45280700 | 1.98320300 | 0.76495900 |
| H | 0.15622800 | 2.74861600 | 1.24239000 |
| H | -1.79362400 | 1.22205600 | 1.21955700 |
| H | -1.47792400 | -1.22609900 | 0.90655200 |
| N | 2.90602600 | -0.69061900 | 0.05111400 |
| C | 4.20052900 | -0.06955700 | -0.20392300 |
| H | 4.92260100 | -0.87312800 | -0.38922800 |
| H | 4.12911800 | 0.56809800 | -1.09652900 |
| H | 4.51227600 | 0.51932000 | 0.66767400 |
| C | 2.61210800 | -2.02285400 | -0.36421000 |
| O | 3.43764700 | -2.79133400 | -0.77510700 |
| C | 1.09853600 | -2.24392600 | -0.22331200 |
| C | 0.38610400 | -1.94691800 | -1.57696700 |
| H | 0.35299300 | -0.86474400 | -1.76273100 |
| H | -0.65122100 | -2.30307800 | -1.50338600 |
| C | 0.80189200 | -3.65120000 | 0.29781900 |
| H | 1.15543900 | -4.40032400 | -0.42038700 |
| H | 1.30105800 | -3.82634000 | 1.26187100 |
| H | -0.28110100 | -3.78326500 | 0.43513700 |
| C | 2.27091700 | -1.88720100 | -3.32929100 |
| O | 2.58528600 | -0.77588400 | -2.96687900 |
| O | 2.92098200 | -2.65044200 | -4.17988600 |
| C | 0.96530500 | -2.56454100 | -2.84010300 |
| C | 4.14684800 | -2.12520900 | -4.76649000 |
| H | 4.69425000 | -3.02098800 | -5.08606000 |
| H | 4.71599000 | -1.61587600 | -3.97538000 |
| C | 3.84182500 | -1.20023400 | -5.92864500 |
| H | 4.78520900 | -0.87918400 | -6.39654500 |
| H | 3.23426600 | -1.71487500 | -6.68833400 |
| H | 3.30329900 | -0.30467200 | -5.58593900 |
| F | 0.05421900 | -2.38858000 | -3.84643400 |
| F | 1.15306600 | -3.90476900 | -2.71075100 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1062.8522237
UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1061.2990665

**L-2**

Zero-point correction= 0.302016 (Hartree/Particle)
Thermal correction to Energy= 0.322039
Thermal correction to Enthalpy= 0.322983
Thermal correction to Gibbs Free Energy= 0.253523
Sum of electronic and zero-point Energies= -1060.962266
Sum of electronic and thermal Energies= -1060.942244
Sum of electronic and thermal Enthalpies= -1060.941299
Sum of electronic and thermal Free Energies= -1061.010760

| | | | |
|---|---|---|---|
| C | 4.73006600 | -0.86752900 | -0.50154800 |
| C | 3.82191800 | 0.87771400 | 0.91111800 |
| C | 5.06619100 | 0.95970900 | 1.56065100 |
| C | 6.12346900 | 0.13157700 | 1.16690200 |
| C | 5.97085000 | -0.80197100 | 0.12911500 |
| H | 2.99769700 | 1.52943000 | 1.20972900 |
| H | 5.20694700 | 1.67376400 | 2.37509700 |
| H | 7.08718600 | 0.20674900 | 1.67672000 |
| H | 6.79537000 | -1.45128500 | -0.16902600 |
| N | 4.32898500 | -1.71689900 | -1.54130500 |
| C | 5.18120700 | -2.69806000 | -2.17624800 |
| H | 5.54783800 | -3.43236000 | -1.44154000 |
| H | 4.59040800 | -3.21518100 | -2.94269400 |

| | | | |
|---|---|---|---|
| H | 6.04731300 | -2.20998400 | -2.65141900 |
| C | 3.02005100 | -1.48430300 | -1.90082100 |
| O | 2.39534400 | -2.08418500 | -2.75550300 |
| C | 2.47399400 | -0.33887600 | -1.01199800 |
| C | 1.26812900 | -0.86989000 | -0.21453200 |
| H | 0.86281000 | -0.08076300 | 0.43643000 |
| H | 0.47794600 | -1.20402900 | -0.90355600 |
| H | 1.56562600 | -1.72068000 | 0.41625000 |
| C | 2.01399700 | 0.84146100 | -1.89519800 |
| H | 1.54673800 | 1.61586500 | -1.27048800 |
| H | 1.25781700 | 0.47785800 | -2.60841000 |
| C | 3.08213900 | 1.52516300 | -2.73333500 |
| C | 4.17137000 | 2.31709200 | -1.97080500 |
| O | 5.35308400 | 2.14043800 | -2.11844000 |
| O | 3.60636200 | 3.22224500 | -1.18455800 |
| C | 4.49016300 | 4.06813000 | -0.40472300 |
| H | 5.07107300 | 4.69219100 | -1.10194900 |
| H | 5.19271700 | 3.41855100 | 0.13847200 |
| C | 3.63268700 | 4.89229400 | 0.52767800 |
| H | 4.27317900 | 5.55932500 | 1.12422900 |
| H | 2.91780000 | 5.50965900 | -0.03725800 |
| H | 3.06993900 | 4.24437000 | 1.21701400 |
| F | 3.71889000 | 0.62382700 | -3.53156200 |
| F | 2.46238500 | 2.42094500 | -3.56639900 |
| C | 3.66426600 | -0.02902700 | -0.12857400 |

UB3LYP-D3/def2-TZVPP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1062.4678667

UωB97XD/def2-SVP-CPCM(DMSO) // UB3LYP-D3/def2-SVP-CPCM(DMSO)
HF = -1060.916768

# Appendix 3: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 3 (Access to Chiral Diamine Derivatives through Stereoselective Cu-Catalyzed Reductive Coupling of Imines and Allenamides)

## A3.1 Computational Methods

All optimizations of intermediates and transition states were calculated using B3LYP/def2-SVP[226,227] level of the theory, with dispersion correction ("empiricaldispersion=gd3"[228] keyword) in implicit solvent (toluene) using CPCM as the solvation model[229] with the "guess=mix" keyword and with an ultrafine grid size, as implemented in Gaussian16.[230] Frequency calculations (using the same level of theory) were used to obtain thermal corrections (at 298K) and to characterize optimized structures as transition states (if only a single imaginary frequency was found) or intermediates (if no imaginary frequencies were found). Single point energy calculations in the gas phase using M06-L/def2-SVP[184] and B3LYP-D3/def2-TZVPP[226,227] with an ultrafine grid size were also performed to compare energetics. All 3-D structures were generated using CYLview.[185] In order to elucidate the mechanism of this reaction and determine the lowest energy pathway, we performed exhaustive conformational searches for the key transition states: hydrocupration, isomerization, and C-C bond formation. These conformational searches and additional computational results are outlined in the figures below.

## A3.2 Supplementary Figures

Consider the hydrocupration of allene **A-3** as shown in **Figure A3.2.1** below. This allene can hypothetically undergo hydrocupration in to yield 4 unique regioisomers: Cu attaches on C1 with H on C2 ("Cu Branched"), Cu attaches on C2 with H on C1 ("Cu Vinyl Terminal"), Cu attaches on C2 with H on C3 ("Cu Vinyl Internal"), or Cu attaches on C3 with H on C2 ("Cu Terminal"). Based on our calculations, we found that the preferred pathway for this reaction is the Cu Branched Pathway ($\Delta G^{\ddagger}$ = 10.4 kcal/mol) as the other pathways were all significantly higher in energy (> 3 kcal/mol).

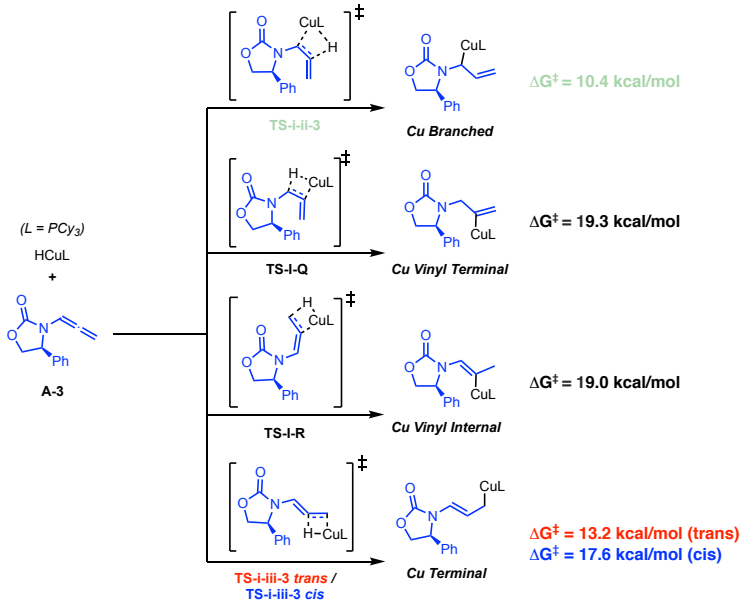



**Figure A3.2.1.** Potential hydrocupration transition states for starting allene **A-3**. Optimizations performed at B3LYP-D3/def2-SVP-CPCM(toluene) level of theory, $\Delta G^{\ddagger}$ reported in kcal/mol with respect to separate LCuH catalyst and reactants.

**Figure A3.2.2** below shows conformations of transition states located and their respective energies.

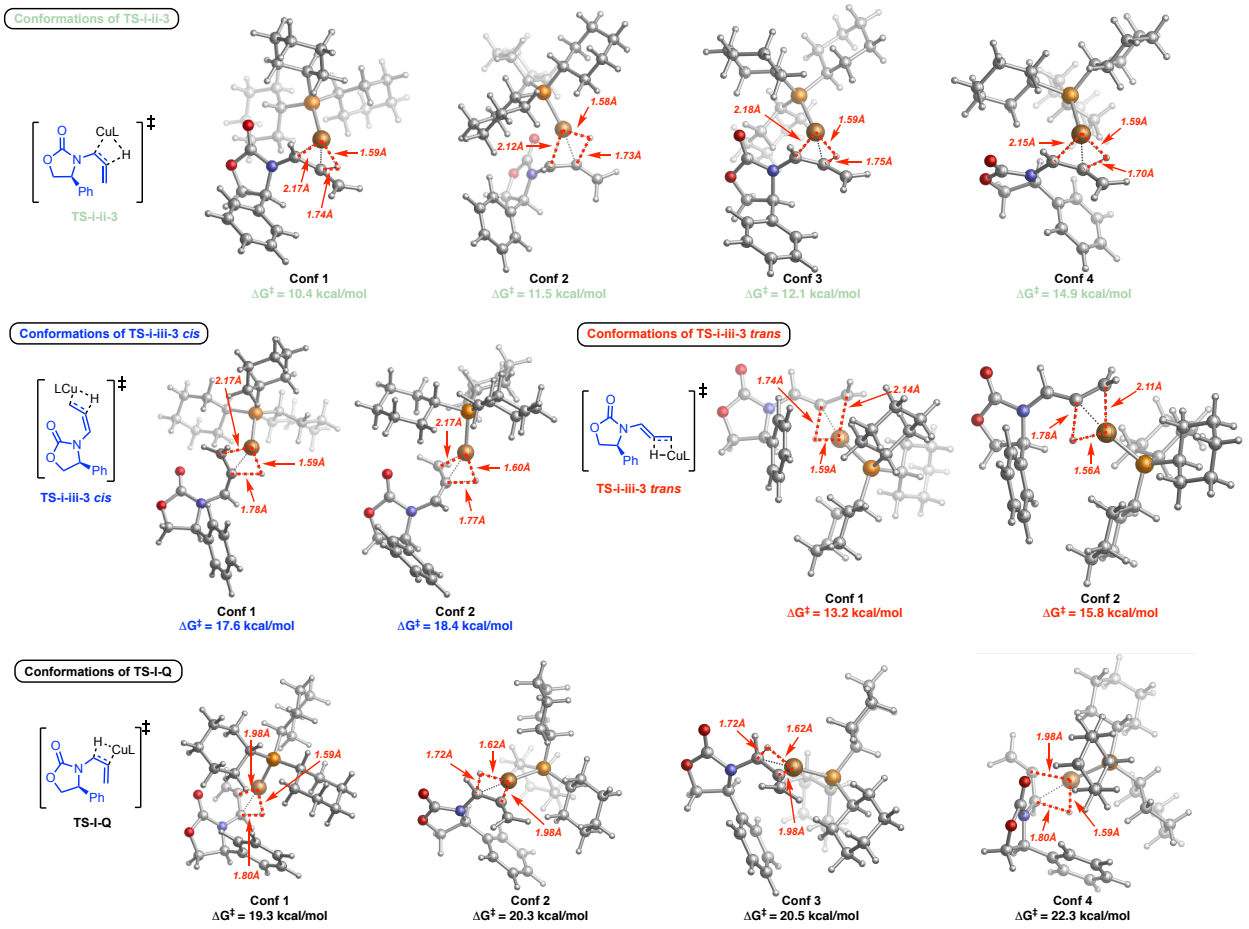



**Figure A3.2.2.** Conformational search for hydrocupration transition state for starting allene **15a**. Optimizations performed at B3LYP-D3/def2-SVP-CPCM(toluene) level of theory, $\Delta G^{\ddagger}$ reported in kcal/mol with respect to separate LCuH catalyst and reactants.

Following the conformational search of the hydrocupration transition states, we sought to understand why the isomerization from branched allylcopper species **ii-3** to **iii-3** ***cis*** was favored over the same isomerization to **iii-3** ***trans***. We recognized that there seemed to be coordination between the copper and the oxazolidinone in the *cis* transition state, as evidenced by the relatively short O-Cu distance (2.33Å) compared to the *trans* transition state (2.88Å) (see **Figure A3.2.3**). We then optimized a transition state structure that would yield the *cis* isomer, but which did not have the coordination. As seen in **Figure A3.2.3**, this coordination seems to stabilize the transition state by 2.7 kcal/mol (**TS-ii-iii-3** ***cis*** *vs.* **TS-ii-iii-3** ***cis*** **No Coordination**). As such, we propose

that the *cis* isomer is benefitting from this coordination between the copper and oxazolidinone. This also provides justification for why the *cis* isomer **iii'-3** ***cis*** becomes unfavorable once the imine is attached to the copper, as this coordination is no longer possible.

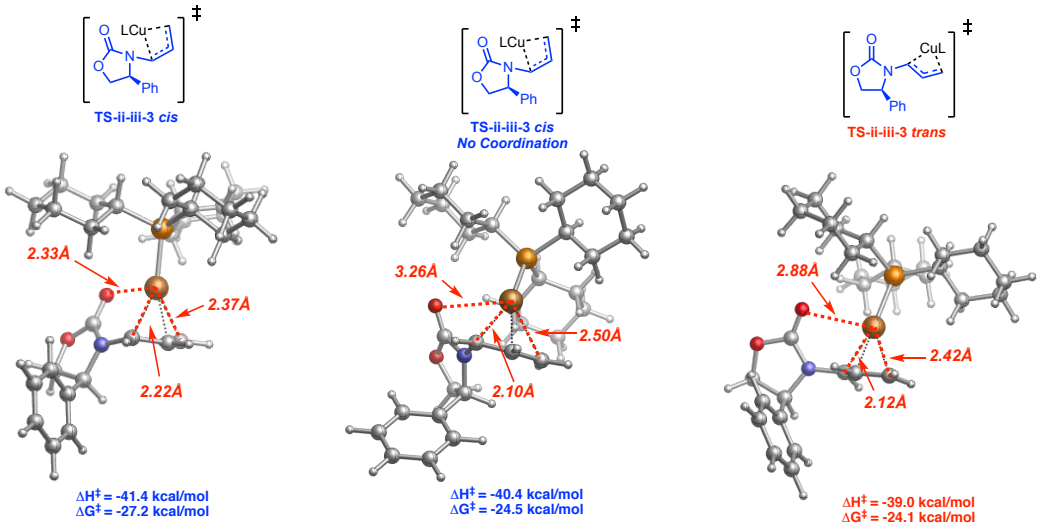



**Figure A3.2.3.** Determination of the effect of coordination between copper and oxazolidinone on energies of isomerization transition states **TS-ii-iii-3** ***cis*** and **TS-ii-iii-3** ***trans***. Optimizations performed at B3LYP-D3/def2-SVP-CPCM(toluene) level of theory, $\Delta H^{\ddagger}/\Delta G^{\ddagger}$ reported in kcal/mol.

Prior to the isomerization from branched to linear allylcopper species (**TS-ii-iii-3**), it is possible for the branched allylcopper intermediate to coordinate to the imine and undergo C-C bond formation directly. To assess this possibility, we performed calculations on this pathway. As seen in **Figure A3.2.4**, coordination of the imine to the branched allylcopper species (**ii'-3**) is energetically unfavorable by 5.1 kcal/mol compared to imine coordination to the linear allylcopper species (**iii'-3** ***trans***). In addition, the transition state from branched allylcopper species **ii'-3** C-C bond formation (**TS-ii'-X**) is 3.3 kcal/mol higher in energy than the lowest energy *(S,S,S)* branched C-C bond formation transition state **TS-iii'-iv-3** ***trans (S,S,S)***. Based on these results, the pathway to form the linear product is unfavorable compared to the branched product, which aligns with the experimental observation that no linear product is formed.

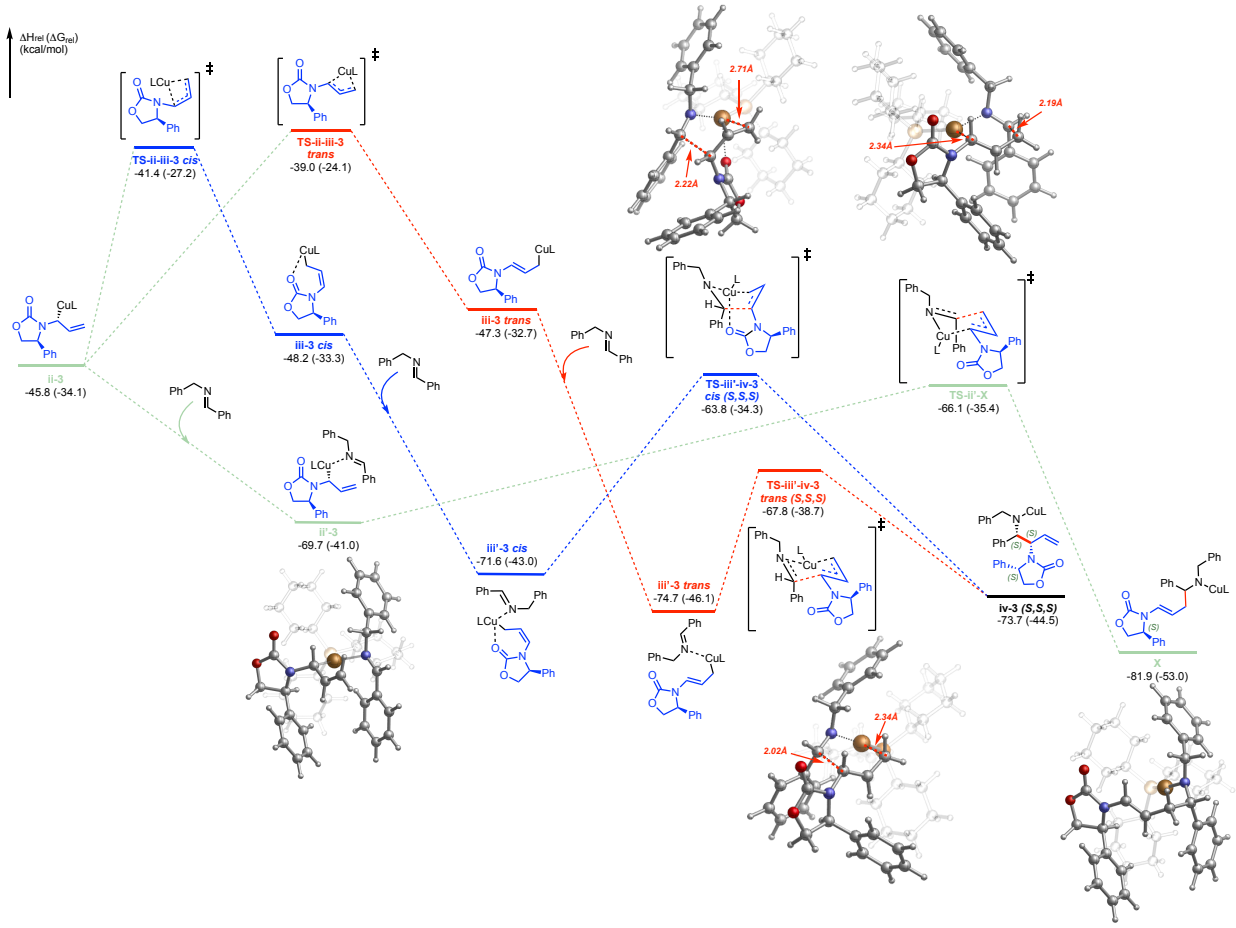



**Figure A3.2.4.** Comparison of linear vs. branched C-C bond formation pathways. Optimizations performed at B3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔH (ΔG; in parentheses) reported in kcal/mol with respect to separate LCuH catalyst and reactants.

Following the isomerization to linear allylcopper species, the C-C bond formation can proceed via numerous pathways. In order to find the lowest energy transition states for the desired stereochemical outcome (*(S,S,S)* stereochemistry), we performed an extensive conformational search. These conformations' geometries and their respective energies are shown in **Figure A3.2.5** below.

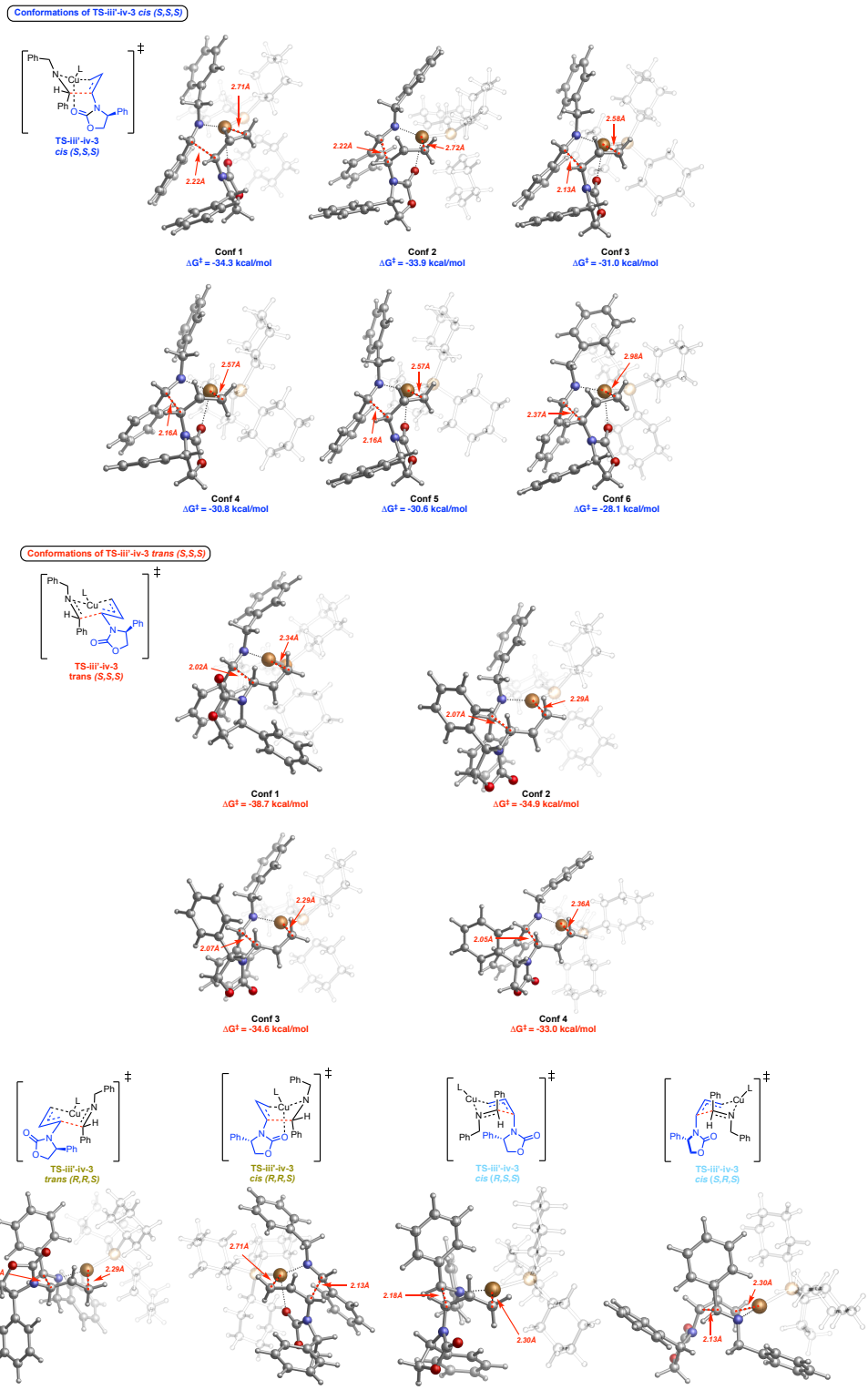



**Figure A3.2.5.** Conformational search for branched C-C bond formation transition states. Optimizations performed at B3LYP-D3/def2-SVP-CPCM(toluene) level of theory, $\Delta G^{\ddagger}$ reported in kcal/mol with respect to separate LCuH catalyst and reactants.

## A3.3 Coordinates & Energies

**i-3 *cis***

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.697561 (Hartree/Particle)

Thermal correction to Energy= 0.733143

Thermal correction to Enthalpy= 0.734087

Thermal correction to Gibbs Free Energy= 0.626652

Sum of electronic and zero-point Energies= -3355.517076

Sum of electronic and thermal Energies= -3355.481494

Sum of electronic and thermal Enthalpies= -3355.480550

Sum of electronic and thermal Free Energies= -3355.587985

| | | | |
|---|---|---|---|
| O | -2.00170300 | -1.58853400 | 0.38978800 |
| C | -0.93048800 | -1.31579700 | 1.30150600 |
| C | -1.61495000 | -0.75508400 | 2.56861900 |
| H | -0.37722400 | -2.24578500 | 1.48650600 |
| H | -0.25636100 | -0.57113800 | 0.84836100 |
| H | -1.04554600 | 0.10472800 | 2.96197600 |
| N | -2.87386500 | -0.28480900 | 1.98312100 |
| C | -3.11846500 | -0.90380000 | 0.76707300 |
| O | -4.13437400 | -0.89929200 | 0.11327000 |
| C | -3.86446900 | 0.42593700 | 2.69780100 |
| H | -4.13565900 | 0.03446300 | 3.68282300 |
| C | -4.47708300 | 1.44778800 | 2.10277900 |
| H | -6.03348400 | 1.87681400 | 4.01517100 |
| C | -4.71054800 | 2.07137500 | 0.92465700 |
| H | -4.45926400 | 3.13351400 | 0.78272400 |
| H | -4.93311500 | 1.47106600 | 0.02737600 |
| Cu | -6.38426500 | 1.97002500 | 2.31411000 |
| P | -8.48086600 | 1.89350100 | 1.55983900 |
| C | -8.52034400 | 0.44782700 | 0.35809900 |
| C | -9.03872200 | 3.39428500 | 0.57825400 |
| C | -9.86201600 | 1.56956100 | 2.79948300 |
| C | -8.03966900 | 0.80429000 | -1.06236600 |
| C | -7.65224400 | -0.71054800 | 0.90378700 |
| H | -9.57382600 | 0.11243900 | 0.28363900 |
| C | -9.83918500 | 4.45033500 | 1.36492800 |
| C | -7.81438900 | 4.06641300 | -0.07928800 |
| H | -9.70194000 | 3.00764700 | -0.21303200 |
| C | -10.05116600 | 0.08928200 | 3.18262700 |
| C | -9.61277100 | 2.40066300 | 4.07579000 |
| H | -10.78835100 | 1.91113300 | 2.31722900 |
| C | -8.07661000 | -0.42079700 | -1.98853200 |
| H | -7.00330000 | 1.17693900 | -0.99871900 |
| H | -8.65003400 | 1.60894800 | -1.49983000 |
| C | -7.70004300 | -1.94004100 | -0.01132700 |
| H | -6.60542900 | -0.36556000 | 0.96405100 |
| H | -7.95042600 | -0.98761000 | 1.92407100 |
| C | -10.26542600 | 5.61017600 | 0.45216100 |
| H | -9.21262900 | 4.85120700 | 2.18116000 |
| H | -10.73117800 | 4.00784100 | 1.83293600 |
| C | -8.22553900 | 5.23116700 | -0.98776000 |
| H | -7.15223100 | 4.43352200 | 0.72614300 |
| H | -7.21454000 | 3.33831700 | -0.64064300 |
| C | -11.19374800 | -0.08038800 | 4.19483400 |
| H | -9.11641100 | -0.29125100 | 3.63125500 |
| H | -10.25553900 | -0.52688700 | 2.29428000 |
| C | -10.74432200 | 2.23380000 | 5.09767800 |
| H | -8.65455600 | 2.06690300 | 4.51297400 |
| H | -9.47864900 | 3.46529600 | 3.83725100 |
| C | -7.24935100 | -1.58429200 | -1.43148700 |
| H | -7.71420600 | -0.13314100 | -2.98999000 |
| H | -9.12686000 | -0.74403600 | -2.11575700 |
| H | -7.05689700 | -2.73179700 | 0.40724300 |
| H | -8.73000500 | -2.34360900 | -0.03447100 |
| C | -9.06107000 | 6.26804900 | -0.22977100 |
| H | -10.83168400 | 6.35329100 | 1.03836600 |
| H | -10.95735500 | 5.22528800 | -0.31957800 |
| H | -7.32674600 | 5.70019100 | -1.42181400 |
| H | -8.81398300 | 4.83589500 | -1.83642700 |
| C | -10.96454200 | 0.76029400 | 5.45516900 |
| H | -11.30162700 | -1.14669400 | 4.45531400 |
| H | -12.14454400 | 0.22476700 | 3.71990700 |
| H | -10.51812800 | 2.82206200 | 6.00275100 |
| H | -11.67762900 | 2.65156600 | 4.67653600 |
| H | -7.32819200 | -2.46207800 | -2.09512300 |
| H | -6.18401200 | -1.29914100 | -1.39679300 |
| H | -9.39371500 | 7.07062900 | -0.90917400 |
| H | -8.42873200 | 6.74807000 | 0.53974600 |
| H | -11.81359400 | 0.65247200 | 6.15083900 |
| H | -10.07162200 | 0.38040000 | 5.98479300 |
| C | -1.83315800 | -1.76287200 | 3.68512200 |
| C | -2.42622700 | -3.00795100 | 3.41420700 |
| C | -1.47369300 | -1.45420000 | 5.00278700 |
| C | -2.64933800 | -3.92459500 | 4.44302800 |
| H | -2.71435200 | -3.26210300 | 2.39052300 |
| C | -1.69665200 | -2.37181300 | 6.03622100 |
| H | -1.01779800 | -0.48496200 | 5.22419700 |
| C | -2.28481800 | -3.60836300 | 5.75810500 |
| H | -3.10993000 | -4.89021700 | 4.21952300 |
| H | -1.41238500 | -2.11690800 | 7.06031300 |
| H | -2.46107600 | -4.32610100 | 6.56326100 |
| O | -2.00170300 | -1.58853400 | 0.38978800 |
| C | -0.93048800 | -1.31579700 | 1.30150600 |
| C | -1.61495000 | -0.75508400 | 2.56861900 |
| H | -0.37722400 | -2.24578500 | 1.48650600 |
| H | -0.25636100 | -0.57113800 | 0.84836100 |
| H | -1.04554600 | 0.10472800 | 2.96197600 |
| N | -2.87386500 | -0.28480900 | 1.98312100 |
| C | -3.11846500 | -0.90380000 | 0.76707300 |
| O | -4.13437400 | -0.89929200 | 0.11327000 |
| C | -3.86446900 | 0.42593700 | 2.69780100 |
| H | -4.13565900 | 0.03446300 | 3.68282300 |
| C | -4.47708300 | 1.44778800 | 2.10277900 |
| H | -6.03348400 | 1.87681400 | 4.01517100 |
| C | -4.71054800 | 2.07137500 | 0.92465700 |
| H | -4.45926400 | 3.13351400 | 0.78272400 |
| H | -4.93311500 | 1.47106600 | 0.02737600 |
| Cu | -6.38426500 | 1.97002500 | 2.31411000 |
| P | -8.48086600 | 1.89350100 | 1.55983900 |
| C | -8.52034400 | 0.44782700 | 0.35809900 |
| C | -9.03872200 | 3.39428500 | 0.57825400 |
| C | -9.86201600 | 1.56956100 | 2.79948300 |
| C | -8.03966900 | 0.80429000 | -1.06236600 |
| C | -7.65224400 | -0.71054800 | 0.90378700 |
| H | -9.57382600 | 0.11243900 | 0.28363900 |
| C | -9.83918500 | 4.45033500 | 1.36492800 |
| C | -7.81438900 | 4.06641300 | -0.07928800 |
| H | -9.70194000 | 3.00764700 | -0.21303200 |
| C | -10.05116600 | 0.08928200 | 3.18262700 |
| C | -9.61277100 | 2.40066300 | 4.07579000 |
| H | -10.78835100 | 1.91113300 | 2.31722900 |
| C | -8.07661000 | -0.42079700 | -1.98853200 |
| H | -7.00330000 | 1.17693900 | -0.99871900 |
| H | -8.65003400 | 1.60894800 | -1.49983000 |
| C | -7.70004300 | -1.94004100 | -0.01132700 |
| H | -6.60542900 | -0.36556000 | 0.96405100 |
| H | -7.95042600 | -0.98761000 | 1.92407100 |
| C | -10.26542600 | 5.61017600 | 0.45216100 |
| H | -9.21262900 | 4.85120700 | 2.18116000 |
| H | -10.73117800 | 4.00784100 | 1.83293600 |
| C | -8.22553900 | 5.23116700 | -0.98776000 |
| H | -7.15223100 | 4.43352200 | 0.72614300 |
| H | -7.21454000 | 3.33831700 | -0.64064300 |
| C | -11.19374800 | -0.08038800 | 4.19483400 |
| H | -9.11641100 | -0.29125100 | 3.63125500 |
| H | -10.25553900 | -0.52688700 | 2.29428000 |
| C | -10.74432200 | 2.23380000 | 5.09767800 |

| | | | |
|---|---|---|---|
| H | -8.65455600 | 2.06690300 | 4.51297400 |
| H | -9.47864900 | 3.46529600 | 3.83725100 |
| C | -7.24935100 | -1.58429200 | -1.43148700 |
| H | -7.71420600 | -0.13314100 | -2.98999000 |
| H | -9.12686000 | -0.74403600 | -2.11575700 |
| H | -7.05689700 | -2.73179700 | 0.40724300 |
| H | -8.73000500 | -2.34360900 | -0.03447100 |
| C | -9.06107000 | 6.26804900 | -0.22977100 |
| H | -10.83168400 | 6.35329100 | 1.03836600 |
| H | -10.95735500 | 5.22528800 | -0.31957800 |
| H | -7.32674600 | 5.70019100 | -1.42181400 |
| H | -8.81398300 | 4.83589500 | -1.83642700 |
| C | -10.96454200 | 0.76029400 | 5.45516900 |
| H | -11.30162700 | -1.14669400 | 4.45531400 |
| H | -12.14454400 | 0.22476700 | 3.71990700 |
| H | -10.51812800 | 2.82206200 | 6.00275100 |
| H | -11.67762900 | 2.65156600 | 4.67653600 |
| H | -7.32819200 | -2.46207800 | -2.09512300 |
| H | -6.18401200 | -1.29914100 | -1.39679300 |
| H | -9.39371500 | 7.07062900 | -0.90917400 |
| H | -8.42873200 | 6.74807000 | 0.53974600 |
| H | -11.81359400 | 0.65247200 | 6.15083900 |
| H | -10.07162200 | 0.38040000 | 5.98479300 |
| C | -1.83315800 | -1.76287200 | 3.68512200 |
| C | -2.42622700 | -3.00795100 | 3.41420700 |
| C | -1.47369300 | -1.45420000 | 5.00278700 |
| C | -2.64933800 | -3.92459500 | 4.44302800 |
| H | -2.71435200 | -3.26210300 | 2.39052300 |
| C | -1.69665200 | -2.37181300 | 6.03622100 |
| H | -1.01779800 | -0.48496200 | 5.22419700 |
| C | -2.28481800 | -3.60836300 | 5.75810500 |
| H | -3.10993000 | -4.89021700 | 4.21952300 |
| H | -1.41238500 | -2.11690800 | 7.06031300 |
| H | -2.46107600 | -4.32610100 | 6.56326100 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.825245
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.07617

**iii-3 *cis***

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.703192 (Hartree/Particle)
Thermal correction to Energy= 0.738149
Thermal correction to Enthalpy= 0.739093
Thermal correction to Gibbs Free Energy= 0.634073
Sum of electronic and zero-point Energies= -3355.585243
Sum of electronic and thermal Energies= -3355.550286
Sum of electronic and thermal Enthalpies= -3355.549342
Sum of electronic and thermal Free Energies= -3355.654361

| | | | |
|---|---|---|---|
| O | -2.00170300 | -1.58853400 | 0.38978800 |
| C | -0.93048800 | -1.31579700 | 1.30150600 |
| C | -1.61495000 | -0.75508400 | 2.56861900 |
| H | -0.37722400 | -2.24578500 | 1.48650600 |
| H | -0.25636100 | -0.57113800 | 0.84836100 |
| H | -1.05834600 | 0.10472800 | 2.96197600 |
| N | -2.87386500 | -0.29760900 | 1.97032100 |
| C | -3.11846500 | -0.90380000 | 0.76707300 |
| O | -4.13437400 | -0.89929200 | 0.11327000 |
| C | -3.85166900 | 0.40033700 | 2.71060100 |
| H | -4.07165900 | 0.00886300 | 3.70842300 |
| C | -4.50268300 | 1.48618800 | 2.21797900 |
| H | -5.02228400 | 1.88961400 | 3.28557100 |
| C | -4.71054800 | 2.08417500 | 0.95025700 |
| H | -4.56166400 | 3.15911400 | 0.80832400 |
| H | -4.68991500 | 1.43266600 | 0.06577600 |
| Cu | -6.39706500 | 1.97002500 | 2.30131000 |
| P | -8.48086600 | 1.89350100 | 1.57263900 |
| C | -8.52034400 | 0.44782700 | 0.35809900 |
| C | -9.03872200 | 3.39428500 | 0.57825400 |
| C | -9.86201600 | 1.56956100 | 2.79948300 |
| C | -8.03966900 | 0.80429000 | -1.06236600 |
| C | -7.65224400 | -0.71054800 | 0.90378700 |
| H | -9.57382600 | 0.12523900 | 0.29643900 |
| C | -9.83918500 | 4.45033500 | 1.36492800 |
| C | -7.81438900 | 4.06641300 | -0.07928800 |
| H | -9.70194000 | 2.99484700 | -0.21303200 |
| C | -10.05116600 | 0.08928200 | 3.18262700 |
| C | -9.61277100 | 2.40066300 | 4.07579000 |
| H | -10.80115100 | 1.91113300 | 2.31722900 |
| C | -8.07661000 | -0.42079700 | -1.98853200 |
| H | -7.00330000 | 1.17693900 | -0.99871900 |
| H | -8.65003400 | 1.60894800 | -1.49983000 |
| C | -7.70004300 | -1.94004100 | -0.01132700 |
| H | -6.60542900 | -0.36556000 | 0.96405100 |
| H | -7.95042600 | -0.98761000 | 1.92407100 |
| C | -10.26542600 | 5.61017600 | 0.45216100 |
| H | -9.21262900 | 4.85120700 | 2.18116000 |
| H | -10.73117800 | 4.00784100 | 1.83293600 |
| C | -8.22553900 | 5.23116700 | -0.98776000 |
| H | -7.15223100 | 4.43352200 | 0.72614300 |
| H | -7.21454000 | 3.33831700 | -0.64064300 |
| C | -11.19374800 | -0.08038800 | 4.19483400 |
| H | -9.11641100 | -0.29125100 | 3.63125500 |
| H | -10.25553900 | -0.52688700 | 2.29428000 |
| C | -10.74432200 | 2.23380000 | 5.09767800 |
| H | -8.65455600 | 2.06690300 | 4.51297400 |
| H | -9.47864900 | 3.46529600 | 3.83725100 |
| C | -7.24935100 | -1.58429200 | -1.43148700 |
| H | -7.71420600 | -0.13314100 | -2.98999000 |
| H | -9.12686000 | -0.74403600 | -2.11575700 |
| H | -7.05689700 | -2.73179700 | 0.40724300 |
| H | -8.73000500 | -2.34360900 | -0.03447100 |
| C | -9.06107000 | 6.26804900 | -0.22977100 |
| H | -10.83168400 | 6.35329100 | 1.03836600 |
| H | -10.95735500 | 5.22528800 | -0.31957800 |
| H | -7.32674600 | 5.70019100 | -1.42181400 |
| H | -8.81398300 | 4.83589500 | -1.83642700 |
| C | -10.96454200 | 0.76029400 | 5.45516900 |
| H | -11.30162700 | -1.14669400 | 4.45531400 |
| H | -12.14454400 | 0.22476700 | 3.71990700 |
| H | -10.51812800 | 2.82206200 | 6.00275100 |
| H | -11.67762900 | 2.65156600 | 4.67653600 |
| H | -7.32819200 | -2.46207800 | -2.09512300 |
| H | -6.18401200 | -1.29914100 | -1.39679300 |
| H | -9.39371500 | 7.07062900 | -0.90917400 |
| H | -8.42873200 | 6.74807000 | 0.53974600 |
| H | -11.81359400 | 0.65247200 | 6.15083900 |
| H | -10.07162200 | 0.38040000 | 5.98479300 |
| C | -1.83315800 | -1.76287200 | 3.68512200 |
| C | -2.42622700 | -3.00795100 | 3.41420700 |
| C | -1.47369300 | -1.45420000 | 5.00278700 |
| C | -2.64933800 | -3.92459500 | 4.44302800 |
| H | -2.71435200 | -3.26210300 | 2.39052300 |
| C | -1.69665200 | -2.37181300 | 6.03622100 |
| H | -1.01779800 | -0.48496200 | 5.22419700 |
| C | -2.28481800 | -3.60836300 | 5.75810500 |
| H | -3.10993000 | -4.89021700 | 4.21952300 |
| H | -1.41238500 | -2.11690800 | 7.06031300 |
| H | -2.46107600 | -4.32610100 | 6.56326100 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.893685
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.147305

**TS-i-iii-3 *cis***

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.695919 (Hartree/Particle)
Thermal correction to Energy= 0.731152

Thermal correction to Enthalpy= 0.732096
Thermal correction to Gibbs Free Energy= 0.626031
Sum of electronic and zero-point Energies= -3355.502786
Sum of electronic and thermal Energies= -3355.467553
Sum of electronic and thermal Enthalpies= -3355.466609
Sum of electronic and thermal Free Energies= -3355.572674

| | | | |
|---|---|---|---|
| O | -2.00170300 | -1.58853400 | -0.38978800 |
| C | -0.93048800 | -1.31579700 | -1.30150600 |
| C | -1.61495000 | -0.75508400 | -2.56861900 |
| H | -0.37722400 | -2.24578500 | -1.48650600 |
| H | -0.25636100 | -0.57113800 | -0.84836100 |
| N | -2.87386500 | -0.29210900 | -1.97582100 |
| C | -3.11846500 | -0.90380000 | -0.76707300 |
| O | -4.13437400 | -0.89929200 | -0.11327000 |
| C | -3.85716900 | 0.41133700 | -2.70510100 |
| H | -4.09915900 | 0.01986300 | -3.69742300 |
| C | -4.49168300 | 1.46968800 | -2.16847900 |
| H | -5.45678400 | 1.88411400 | -3.59907100 |
| C | -4.71054800 | 2.07867500 | -0.93925700 |
| H | -4.51766400 | 3.14811400 | -0.79732400 |
| H | -4.79441500 | 1.44916600 | -0.04927600 |
| Cu | -6.39156500 | 1.97002500 | -2.30681000 |
| P | -8.48086600 | 1.89350100 | -1.56713900 |
| C | -8.52034400 | 0.44782700 | -0.35809900 |
| C | -9.03872200 | 3.39428500 | -0.57825400 |
| C | -9.86201600 | 1.56956100 | -2.79948300 |
| C | -8.03966900 | 0.80429000 | 1.06236600 |
| C | -7.65224400 | -0.71054800 | -0.90378700 |
| H | -9.57382600 | 0.11973900 | -0.29093900 |
| C | -9.83918500 | 4.45033500 | -1.36492800 |
| C | -7.81438900 | 4.06641300 | 0.07928800 |
| H | -9.70194000 | 3.00034700 | 0.21303200 |
| C | -10.05116600 | 0.08928200 | -3.18262700 |
| C | -9.61277100 | 2.40066300 | -4.07579000 |
| H | -10.79565100 | 1.91113300 | -2.31722900 |
| C | -8.07661000 | -0.42079700 | 1.98853200 |
| H | -7.00330000 | 1.17693900 | 0.99871900 |
| H | -8.65003400 | 1.60894800 | 1.49983000 |
| C | -7.70004300 | -1.94004100 | 0.01132700 |
| H | -6.60542900 | -0.36556000 | -0.96405100 |
| H | -7.95042600 | -0.98761000 | -1.92407100 |
| C | -10.26542600 | 5.61017600 | -0.45216100 |
| H | -9.21262900 | 4.85120700 | -2.18116000 |
| H | -10.73117800 | 4.00784100 | -1.83293600 |
| C | -8.22553900 | 5.23116700 | 0.98776000 |
| H | -7.15223100 | 4.43352200 | -0.72614300 |
| H | -7.21454000 | 3.33831700 | 0.64064300 |
| C | -11.19374800 | -0.08038800 | -4.19483400 |
| H | -9.11641100 | -0.29125100 | -3.63125500 |
| H | -10.25553900 | -0.52688700 | -2.29428000 |
| C | -10.74432200 | 2.23380000 | -5.09767800 |
| H | -8.65455600 | 2.06690300 | -4.51297400 |
| H | -9.47864900 | 3.46529600 | -3.83725100 |
| C | -7.24935100 | -1.58429200 | 1.43148700 |
| H | -7.71420600 | -0.13314100 | 2.98999000 |
| H | -9.12686000 | -0.74403600 | 2.11575700 |
| H | -7.05689700 | -2.73179700 | -0.40724300 |
| H | -8.73000500 | -2.34360900 | 0.03447100 |
| C | -9.06107000 | 6.26804900 | 0.22977100 |
| H | -10.83168400 | 6.35329100 | -1.03836600 |
| H | -10.95735500 | 5.22528800 | 0.31957800 |
| H | -7.32674600 | 5.70019100 | 1.42181400 |
| H | -8.81398300 | 4.83589500 | 1.83642700 |
| C | -10.96454200 | 0.76029400 | -5.45516900 |
| H | -11.30162700 | -1.14669400 | -4.45531400 |
| H | -12.14454400 | 0.22476700 | -3.71990700 |
| H | -10.51812800 | 2.82206200 | -6.00275100 |
| H | -11.67762900 | 2.65156600 | -4.67653600 |
| H | -7.32819200 | -2.46207800 | 2.09512300 |
| H | -6.18401200 | -1.29914100 | 1.39679300 |
| H | -9.39371500 | 7.07062900 | 0.90917400 |
| H | -8.42873200 | 6.74807000 | -0.53974600 |
| H | -11.81359400 | 0.65247200 | -6.15083900 |
| H | -10.07162200 | 0.38040000 | -5.98479300 |
| H | -1.76857589 | -1.46460119 | -3.35467526 |
| C | -0.82799377 | 0.44866906 | -3.11932624 |
| C | -0.78764598 | 0.68620111 | -4.49318894 |
| C | -0.15492571 | 1.30134547 | -2.24392221 |
| C | -0.07445683 | 1.77666805 | -4.99190181 |
| H | -1.31784018 | 0.01399895 | -5.18324777 |
| C | 0.55772035 | 2.39184315 | -2.74240732 |
| H | -0.18657510 | 1.11357732 | -1.16077141 |
| C | 0.59764462 | 2.62974626 | -4.11682528 |
| H | -0.04347834 | 1.96410325 | -6.07502238 |
| H | 1.08777438 | 3.06456825 | -2.05263924 |
| H | 1.15928970 | 3.48964527 | -4.50979476 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.809753
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.060558

**TS-I-R**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.696896 (Hartree/Particle)
Thermal correction to Energy= 0.732108
Thermal correction to Enthalpy= 0.733052
Thermal correction to Gibbs Free Energy= 0.626203
Sum of electronic and zero-point Energies= -3355.499742
Sum of electronic and thermal Energies= -3355.464530
Sum of electronic and thermal Enthalpies= -3355.463585
Sum of electronic and thermal Free Energies= -3355.570434

| | | | |
|---|---|---|---|
| O | -3.53553800 | 6.61378500 | -3.15011300 |
| C | -3.70420500 | 5.24032600 | -3.50450600 |
| C | -4.67573800 | 4.66198300 | -2.44633500 |
| H | -4.10428600 | 5.18106500 | -4.52582000 |
| H | -2.72551600 | 4.73477200 | -3.46759200 |
| H | -4.30651100 | 3.69002900 | -2.08370400 |
| N | -4.53987500 | 5.67148200 | -1.39724000 |
| C | -3.97133600 | 6.83053500 | -1.87182400 |
| O | -3.86417600 | 7.89964800 | -1.32447200 |
| C | -5.27297000 | 5.55747900 | -0.18020100 |
| H | -6.12572500 | 4.88004800 | -0.30233900 |
| C | -5.02628700 | 6.16762800 | 0.97309900 |
| C | -4.11319500 | 7.09194200 | 1.59214000 |
| H | -3.15531700 | 6.71575800 | 1.97106400 |
| H | -4.07223900 | 8.12450900 | 1.23084600 |
| H | -4.58308900 | 7.64596300 | 3.25758700 |
| Cu | -5.77179000 | 6.63912600 | 2.76641200 |
| P | -7.81263200 | 6.15004300 | 3.47421300 |
| C | -8.13824700 | 5.86519300 | 5.30341600 |
| C | -8.48869000 | 4.63317300 | 2.58684200 |
| C | -8.96516300 | 7.55759400 | 2.98013700 |
| C | -7.97906700 | 4.41094300 | 5.78647900 |
| C | -7.22543800 | 6.78878500 | 6.13698300 |
| H | -9.19213300 | 6.15196400 | 5.47035200 |
| C | -8.94560800 | 4.92982300 | 1.14372400 |
| C | -7.40686300 | 3.53078300 | 2.56028000 |
| H | -9.36383800 | 4.28127100 | 3.16335300 |
| C | -9.20760800 | 8.62926700 | 4.06033700 |
| C | -8.43115300 | 8.24212900 | 1.70180100 |
| H | -9.93902400 | 7.08534700 | 2.75770600 |
| C | -8.28185400 | 4.29167700 | 7.28776700 |
| H | -6.94274000 | 4.07559300 | 5.60367600 |
| H | -8.64049400 | 3.73343800 | 5.22588300 |
| C | -7.51517300 | 6.67184600 | 7.63837000 |
| H | -6.17676200 | 6.51002900 | 5.93024300 |
| H | -7.31963400 | 7.83523700 | 5.81529000 |
| C | -9.42863700 | 3.66288500 | 0.42264000 |
| H | -8.09536500 | 5.35897300 | 0.58761100 |

| | | | |
|---|---|---|---|
| H | -9.75022900 | 5.68005600 | 1.12965700 |
| C | -7.89188200 | 2.26149100 | 1.84848200 |
| H | -6.52575600 | 3.94303600 | 2.03676400 |
| H | -7.06961000 | 3.27930400 | 3.57515900 |
| C | -10.18461100 | 9.70350600 | 3.55809200 |
| H | -8.24732100 | 9.10981200 | 4.31677400 |
| H | -9.60154200 | 8.18314400 | 4.98570500 |
| C | -9.39635800 | 9.31726800 | 1.18902100 |
| H | -7.45817900 | 8.70774800 | 1.94615400 |
| H | -8.22134900 | 7.51001400 | 0.91107900 |
| C | -7.39556400 | 5.22276000 | 8.12179400 |
| H | -8.15339600 | 3.24439800 | 7.60908600 |
| H | -9.34382800 | 4.54564200 | 7.46179800 |
| H | -6.82903600 | 7.32589100 | 8.20193200 |
| H | -8.53779900 | 7.04141700 | 7.83971600 |
| C | -8.36167600 | 2.56466900 | 0.42332300 |
| H | -9.71361300 | 3.91694000 | -0.61200900 |
| H | -10.34085600 | 3.28675000 | 0.92202500 |
| H | -7.08302400 | 1.51154200 | 1.83855800 |
| H | -8.72562600 | 1.81630700 | 2.42292800 |
| C | -9.68952400 | 10.36546900 | 2.26754600 |
| H | -10.33845300 | 10.46009300 | 4.34574600 |
| H | -11.16980900 | 9.23614800 | 3.37478300 |
| H | -8.97640000 | 9.79495700 | 0.28827600 |
| H | -10.34159200 | 8.83490000 | 0.87786200 |
| H | -7.65605900 | 5.14738600 | 9.19083400 |
| H | -6.34296400 | 4.89742400 | 8.02969100 |
| H | -8.74673600 | 1.65319800 | -0.06433100 |
| H | -7.50145400 | 2.90022900 | -0.18205200 |
| H | -10.42683500 | 11.10091600 | 1.90444800 |
| H | -8.76268200 | 10.92788900 | 2.48366000 |
| C | -6.11406200 | 4.49274600 | -2.91153500 |
| C | -6.86962500 | 5.60854900 | -3.30828800 |
| C | -6.71581400 | 3.22865200 | -2.91932900 |
| C | -8.20098900 | 5.45917200 | -3.70048200 |
| H | -6.41596700 | 6.60313800 | -3.29958800 |
| C | -8.05066400 | 3.07556400 | -3.31182700 |
| H | -6.14038500 | 2.35523000 | -2.59946600 |
| C | -8.79678100 | 4.19104100 | -3.70069000 |
| H | -8.77946900 | 6.33583200 | -4.00264900 |
| H | -8.50971900 | 2.08390200 | -3.30105700 |
| H | -9.84126300 | 4.07589900 | -4.00097100 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.808259
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.059313

**TS-i-iii-3 *trans***

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.696640 (Hartree/Particle)
Thermal correction to Energy= 0.731659
Thermal correction to Enthalpy= 0.732603
Thermal correction to Gibbs Free Energy= 0.628013
Sum of electronic and zero-point Energies= -3355.511101
Sum of electronic and thermal Energies= -3355.476083
Sum of electronic and thermal Enthalpies= -3355.475138
Sum of electronic and thermal Free Energies= -3355.579729

| | | | |
|---|---|---|---|
| O | -2.78499300 | -0.26404900 | 5.75948100 |
| C | -3.26673100 | 1.05578500 | 5.49452200 |
| C | -4.26656500 | 0.88110300 | 4.32944700 |
| H | -3.73013500 | 1.45877600 | 6.40385400 |
| H | -2.41870700 | 1.69441900 | 5.19588600 |
| H | -4.18614100 | 1.72111400 | 3.62993600 |
| N | -3.72102000 | -0.33708400 | 3.73430800 |
| C | -2.95106700 | -1.03305100 | 4.65135900 |
| O | -2.49548200 | -2.14374000 | 4.53799300 |
| C | -4.13170600 | -0.96391200 | 2.54653900 |
| H | -3.77116900 | -1.99396800 | 2.48365400 |
| C | -4.89950600 | -0.47905000 | 1.56027400 |
| H | -4.75094900 | 1.25326000 | 1.73754000 |
| C | -5.75732700 | -1.00611700 | 0.58571500 |
| H | -5.57494100 | -0.85818600 | -0.48608000 |
| H | -6.43194900 | -1.82445000 | 0.85696300 |
| Cu | -6.25320500 | 0.94857600 | 1.31386200 |
| P | -8.08220200 | 2.05683700 | 0.72165000 |
| C | -8.02915500 | 2.53510600 | -1.09827100 |
| C | -8.50263100 | 3.65594700 | 1.62265100 |
| C | -9.58372000 | 0.94871300 | 0.93199400 |
| C | -7.42495700 | 3.92654100 | -1.37642600 |
| C | -7.24586000 | 1.47547800 | -1.90358500 |
| H | -9.07976100 | 2.54818600 | -1.44195700 |
| C | -9.42117900 | 3.50808800 | 2.84942300 |
| C | -7.19333900 | 4.35855500 | 2.03718000 |
| H | -9.03552100 | 4.28691900 | 0.88942200 |
| C | -9.78240800 | -0.06342700 | -0.21177800 |
| C | -9.44816400 | 0.18625700 | 2.26800300 |
| H | -10.47201400 | 1.60420900 | 0.96762500 |
| C | -7.43586800 | 4.24604800 | -2.87882000 |
| H | -6.38226300 | 3.94675900 | -1.01263400 |
| H | -7.96785200 | 4.71483100 | -0.83451500 |
| C | -7.24978300 | 1.78480300 | -3.40551000 |
| H | -6.20547200 | 1.46271400 | -1.53009100 |
| H | -7.63808700 | 0.46636100 | -1.72434500 |
| C | -9.69507700 | 4.86944400 | 3.50500200 |
| H | -8.93695700 | 2.85142000 | 3.58837700 |
| H | -10.37583900 | 3.03485600 | 2.57526300 |
| C | -7.45591100 | 5.71549000 | 2.70058000 |
| H | -6.66069000 | 3.69086200 | 2.73704100 |
| H | -6.52080800 | 4.48103100 | 1.17554800 |
| C | -10.99305100 | -0.97142300 | 0.05144100 |
| H | -8.87294800 | -0.68412500 | -0.29437100 |
| H | -9.91516300 | 0.45022600 | -1.17619600 |
| C | -10.65225300 | -0.72095800 | 2.53963100 |
| H | -8.53094200 | -0.42776700 | 2.21368800 |
| H | -9.29707400 | 0.87084500 | 3.11180700 |
| C | -6.69137400 | 3.18219600 | -3.69210600 |
| H | -6.99330800 | 5.24208600 | -3.04746400 |
| H | -8.48385700 | 4.30499000 | -3.22633400 |
| H | -6.66941400 | 1.01733200 | -3.94418200 |
| H | -8.28634800 | 1.71872400 | -3.78497100 |
| C | -8.39607000 | 5.57864600 | 3.90282700 |
| H | -10.34409500 | 4.72995500 | 4.38609300 |
| H | -10.25751400 | 5.50773100 | 2.79870000 |
| H | -6.49965000 | 6.17222700 | 3.00628100 |
| H | -7.90835500 | 6.40068100 | 1.95991800 |
| C | -10.87339700 | -1.70877000 | 1.38975400 |
| H | -11.10183800 | -1.69089400 | -0.77741300 |
| H | -11.91166900 | -0.35588800 | 0.05551500 |
| H | -10.50134900 | -1.25783500 | 3.49128300 |
| H | -11.55689100 | -0.09818800 | 2.66913700 |
| H | -6.74859900 | 3.41019200 | -4.76958400 |
| H | -5.61988600 | 3.20481800 | -3.42085700 |
| H | -8.61470100 | 6.56782100 | 4.33865000 |
| H | -7.89093800 | 4.99140500 | 4.69152500 |
| H | -11.76986600 | -2.32483500 | 1.57190400 |
| H | -10.01530300 | -2.40424500 | 1.34320600 |
| C | -5.71747300 | 0.76760100 | 4.78103000 |
| C | -6.39763200 | -0.45467700 | 4.85923600 |
| C | -6.37734500 | 1.93651700 | 5.19206100 |
| C | -7.70918700 | -0.50701600 | 5.34383900 |
| H | -5.90517300 | -1.37236600 | 4.53434400 |
| C | -7.67908800 | 1.88356400 | 5.69522200 |
| H | -5.86201100 | 2.89938900 | 5.12505800 |
| C | -8.35224800 | 0.65878300 | 5.76872200 |
| H | -8.22958500 | -1.46684100 | 5.38980400 |
| H | -8.17089300 | 2.80156600 | 6.02590200 |
| H | -9.37570000 | 0.61534600 | 6.14907600 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.817728

B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.068883

**TS-I-Q**
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.696846 (Hartree/Particle)
Thermal correction to Energy= 0.731969
Thermal correction to Enthalpy= 0.732913
Thermal correction to Gibbs Free Energy= 0.627419
Sum of electronic and zero-point Energies= -3355.500561
Sum of electronic and thermal Energies= -3355.465438
Sum of electronic and thermal Enthalpies= -3355.464493
Sum of electronic and thermal Free Energies= -3355.569987

| | | | |
|---|---|---|---|
| O | -1.23838900 | 1.23976200 | 0.56691100 |
| C | -0.24991700 | 1.51710400 | 1.57063700 |
| C | -0.97991100 | 1.26108600 | 2.90184200 |
| H | 0.61608900 | 0.86240900 | 1.40969000 |
| H | 0.05951800 | 2.57137000 | 1.48508200 |
| H | -0.64871100 | 1.97314100 | 3.67234500 |
| N | -2.34272000 | 1.59293700 | 2.46832400 |
| C | -2.47733400 | 1.33632700 | 1.13018600 |
| O | -3.49590800 | 1.17403400 | 0.49448500 |
| C | -3.49396900 | 1.52322900 | 3.38738400 |
| H | -3.08519400 | 1.51566600 | 4.41248000 |
| C | -4.52474400 | 2.32626800 | 3.22363600 |
| C | -4.76158000 | 3.58663800 | 2.86874600 |
| H | -3.94347400 | 4.31993000 | 2.74871600 |
| H | -5.77188300 | 3.98265100 | 2.70524400 |
| C | -0.86090600 | -0.15883400 | 3.44291700 |
| C | -0.88809600 | -1.26669700 | 2.57829800 |
| C | -0.79884200 | -0.38053100 | 4.82470700 |
| C | -0.86789900 | -2.56492700 | 3.08912400 |
| H | -0.95489600 | -1.11389500 | 1.49877400 |
| C | -0.78568900 | -1.68167100 | 5.33939800 |
| H | -0.77415400 | 0.47340000 | 5.50785100 |
| C | -0.82237700 | -2.77706000 | 4.47231100 |
| H | -0.90195300 | -3.41607200 | 2.40461800 |
| H | -0.74969700 | -1.83906000 | 6.42026400 |
| H | -0.82056400 | -3.79412600 | 4.87195500 |
| P | -6.12297200 | -1.58111100 | 2.55824000 |
| C | -5.86495200 | -2.83634800 | 3.93648200 |
| C | -5.55624200 | -2.20960700 | 0.87621200 |
| C | -7.99413200 | -1.38266000 | 2.35058100 |
| C | -4.51890100 | -3.57687300 | 3.86326200 |
| C | -5.97426700 | -2.08017400 | 5.27946700 |
| H | -6.67020000 | -3.58594600 | 3.87716800 |
| C | -5.96539400 | -1.14769100 | -0.17761200 |
| C | -4.02360000 | -2.38774500 | 0.81102100 |
| H | -6.05600000 | -3.17141900 | 0.65596200 |
| C | -8.91754100 | -2.41671600 | 3.01528600 |
| C | -8.40350500 | 0.05237800 | 2.73779700 |
| H | -8.14771500 | -1.47886200 | 1.26496400 |
| C | -4.28815400 | -4.47963100 | 5.08346500 |
| H | -3.70401400 | -2.83768500 | 3.80041200 |
| H | -4.47434200 | -4.19089300 | 2.95219300 |
| C | -5.75691600 | -2.99808900 | 6.48757100 |
| H | -5.20399800 | -1.28670000 | 5.28566500 |
| H | -6.94487600 | -1.57039100 | 5.36185800 |
| C | -5.48082800 | -1.50768700 | -1.58857400 |
| H | -5.51603200 | -0.18395100 | 0.12038900 |
| H | -7.05527400 | -1.00019600 | -0.20056600 |
| C | -3.53607200 | -2.75132000 | -0.59681500 |
| H | -3.55964500 | -1.43856600 | 1.12137700 |
| H | -3.67621200 | -3.14552300 | 1.51971700 |
| C | -10.38556700 | -2.13928200 | 2.65534100 |
| H | -8.81667800 | -2.35844800 | 4.11214000 |
| H | -8.64063400 | -3.44153200 | 2.71771400 |
| C | -9.88037800 | 0.32491000 | 2.42725000 |
| H | -8.20790700 | 0.20768400 | 3.81500300 |
| H | -7.75409600 | 0.77252900 | 2.21375400 |
| C | -4.40195800 | -3.70671200 | 6.40046400 |
| H | -3.29722100 | -4.95692400 | 4.99768300 |
| H | -5.03195000 | -5.29797700 | 5.07934900 |
| H | -5.83278400 | -2.40931100 | 7.41700300 |
| H | -6.56356000 | -3.75338600 | 6.52583600 |
| C | -3.96314000 | -1.70525100 | -1.62874800 |
| H | -5.78309500 | -0.71082400 | -2.28872900 |
| H | -5.98645700 | -2.43219600 | -1.92535800 |
| H | -2.43739800 | -2.85578000 | -0.58216000 |
| H | -3.94202200 | -3.74042900 | -0.88125000 |
| C | -10.79758600 | -0.72209600 | 3.06959000 |
| H | -11.03686100 | -2.89000900 | 3.13365200 |
| H | -10.51981300 | -2.25454100 | 1.56389300 |
| H | -10.15395300 | 1.33935500 | 2.76227800 |
| H | -10.02366700 | 0.30742900 | 1.33088200 |
| H | -4.26302700 | -4.38534700 | 7.25881200 |
| H | -3.59320700 | -2.95472700 | 6.45179800 |
| H | -3.63714300 | -2.00021800 | -2.64056900 |
| H | -3.47389500 | -0.74504300 | -1.39137800 |
| H | -11.85085200 | -0.53146100 | 2.80396300 |
| H | -10.72990900 | -0.63620100 | 4.17012200 |
| Cu | -4.84449500 | 0.19444100 | 2.97468000 |
| H | -3.43224500 | -0.12029700 | 3.50702700 |

**TS-i-ii-3**
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.696398 (Hartree/Particle)
Thermal correction to Energy= 0.731661
Thermal correction to Enthalpy= 0.732605
Thermal correction to Gibbs Free Energy= 0.627398
Sum of electronic and zero-point Energies= -3355.515154
Sum of electronic and thermal Energies= -3355.479892
Sum of electronic and thermal Enthalpies= -3355.478948
Sum of electronic and thermal Free Energies= -3355.584155

| | | | |
|---|---|---|---|
| O | -2.24777982 | -1.74149618 | 2.30763239 |
| C | -0.96295259 | -1.11390921 | 2.18934657 |
| C | -1.26889561 | 0.39266057 | 2.01585688 |
| H | -0.39088719 | -1.29720796 | 3.11339781 |
| H | -0.42659724 | -1.55044325 | 1.33671797 |
| H | -1.30223347 | 0.66576687 | 0.94504781 |
| N | -2.62101500 | 0.44000900 | 2.57326400 |
| C | -3.17201525 | -0.80296051 | 2.63006532 |
| O | -4.32640360 | -1.08523077 | 2.90391292 |
| C | -3.40316900 | 1.64508500 | 2.63463600 |
| H | -4.11296900 | 1.68884800 | 3.46496200 |
| C | -2.92218400 | 2.83286800 | 2.03269800 |
| C | -2.25050200 | 3.93111600 | 2.37608500 |
| H | -1.82204500 | 4.00560000 | 3.38329700 |
| H | -2.10794000 | 4.77555500 | 1.69653200 |
| C | -0.28905322 | 1.29917872 | 2.72992298 |
| C | -0.30299499 | 1.39233335 | 4.13072409 |
| C | 0.66051690 | 2.03427243 | 2.00983343 |
| C | 0.61592205 | 2.20446078 | 4.79784066 |
| H | -1.05312260 | 0.83457564 | 4.69551596 |
| C | 1.58782430 | 2.84371457 | 2.67625096 |
| H | 0.67216051 | 1.97763459 | 0.91765300 |
| C | 1.56730538 | 2.93120535 | 4.07126407 |
| H | 0.58516462 | 2.27500621 | 5.88801344 |
| H | 2.32340919 | 3.41267998 | 2.10200173 |
| H | 2.28648525 | 3.56826568 | 4.59220771 |
| P | -6.00239100 | 1.14380200 | -0.21374800 |
| C | -6.58680441 | 1.89931296 | -1.83065086 |
| C | -7.48254115 | 1.31786627 | 0.92994399 |
| C | -5.77720572 | -0.70072142 | -0.34860374 |
| C | -6.15153045 | 3.38223599 | -1.87366294 |
| C | -6.07856288 | 1.18488242 | -3.09703767 |
| H | -7.69108737 | 1.84729885 | -1.82577379 |
| C | -7.18450211 | 0.63975046 | 2.28309853 |
| C | -7.83717136 | 2.80364909 | 1.13707269 |

| | | | |
|---|---|---|---|
| H | -8.34251922 | 0.81548137 | 0.45104419 |
| C | -6.98380737 | -1.53188840 | -0.81315255 |
| C | -4.48172202 | -1.10056991 | -1.08134375 |
| H | -5.58608689 | -0.93874990 | 0.71116088 |
| C | -6.64219765 | 4.08780233 | -3.14349624 |
| H | -5.04790670 | 3.41152125 | -1.82796252 |
| H | -6.50034714 | 3.92385115 | -0.98238779 |
| C | -6.57409785 | 1.88341731 | -4.37169554 |
| H | -4.97420427 | 1.18436397 | -3.09123481 |
| H | -6.39701351 | 0.13306222 | -3.10802863 |
| C | -8.30045355 | 0.85968604 | 3.31275662 |
| H | -6.23593451 | 1.05377784 | 2.66590067 |
| H | -7.02374744 | -0.44063427 | 2.14752578 |
| C | -8.95932722 | 2.99911720 | 2.16482858 |
| H | -6.92782988 | 3.33088453 | 1.47976245 |
| H | -8.13579729 | 3.26364101 | 0.18302507 |
| C | -6.69639217 | -3.03371610 | -0.65805742 |
| H | -7.20956208 | -1.31257862 | -1.87095354 |
| H | -7.88637524 | -1.26677111 | -0.23936493 |
| C | -4.21136299 | -2.60018680 | -0.90362828 |
| H | -4.56082903 | -0.87683994 | -2.15698168 |
| H | -3.64473359 | -0.50679071 | -0.68396648 |
| C | -6.16773601 | 3.36041072 | -4.40587957 |
| H | -6.29430691 | 5.13445037 | -3.14602074 |
| H | -7.74748851 | 4.12392194 | -3.13513390 |
| H | -6.18628717 | 1.35489298 | -5.25880935 |
| H | -7.67632908 | 1.80740247 | -4.41782330 |
| C | -8.61177434 | 2.34669266 | 3.50503908 |
| H | -8.01355825 | 0.39542610 | 4.27200952 |
| H | -9.21602860 | 0.33864607 | 2.97718852 |
| H | -9.15676158 | 4.07633909 | 2.29593918 |
| H | -9.89264235 | 2.55346665 | 1.77352932 |
| C | -5.40343293 | -3.44337031 | -1.37451586 |
| H | -7.55061409 | -3.62182447 | -1.03431283 |
| H | -6.60218746 | -3.26808291 | 0.41832445 |
| H | -3.29781107 | -2.88565097 | -1.45188745 |
| H | -4.01423708 | -2.80123488 | 0.16491367 |
| H | -6.56765363 | 3.85003954 | -5.30972299 |
| H | -5.06626333 | 3.43034575 | -4.46938055 |
| H | -9.43449817 | 2.47964311 | 4.22776377 |
| H | -7.72883055 | 2.85255768 | 3.93464971 |
| H | -5.20395820 | -4.51678548 | -1.21682236 |
| H | -5.53540629 | -3.30550202 | -2.46414570 |
| Cu | -4.19067200 | 2.05452900 | 0.70704600 |
| H | -3.21698800 | 3.25018100 | 0.38071300 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.819825
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.071773

**i-3 *trans***

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.698408 (Hartree/Particle)
Thermal correction to Energy= 0.733631
Thermal correction to Enthalpy= 0.734576
Thermal correction to Gibbs Free Energy= 0.630996
Sum of electronic and zero-point Energies= -3355.529607
Sum of electronic and thermal Energies= -3355.494384
Sum of electronic and thermal Enthalpies= -3355.493440
Sum of electronic and thermal Free Energies= -3355.597019

| | | | |
|---|---|---|---|
| O | 4.08662500 | -1.99792700 | 3.89502900 |
| C | 3.53761700 | -0.67534600 | 3.80721300 |
| C | 2.57149800 | -0.72502700 | 2.60316200 |
| H | 3.03449800 | -0.43676100 | 4.75269400 |
| H | 4.35901800 | 0.03925800 | 3.63442400 |
| H | 2.63247000 | 0.18525900 | 1.99172900 |
| N | 3.15369600 | -1.84974900 | 1.87864200 |
| C | 3.94854200 | -2.62863600 | 2.70314500 |
| O | 4.44391800 | -3.69815100 | 2.44884700 |
| C | 2.78738000 | -2.29736100 | 0.60717100 |
| H | 3.19193500 | -3.29389900 | 0.39690800 |
| C | 2.03732700 | -1.68174800 | -0.30205300 |
| H | 1.61231600 | 1.05367100 | 0.55193300 |
| C | 1.30307600 | -1.78152300 | -1.46022200 |
| H | 1.72260100 | -1.49746700 | -2.43440300 |
| H | 0.39414700 | -2.39448400 | -1.50087900 |
| Cu | 1.01332700 | 0.03193900 | -0.45578100 |
| P | -0.90545900 | 0.92801900 | -1.38772500 |
| C | -1.00967600 | 1.28983300 | -3.23356300 |
| C | -1.44406400 | 2.52377500 | -0.54548900 |
| C | -2.33632500 | -0.25948700 | -1.06257700 |
| C | -0.60241300 | 2.70995300 | -3.67082100 |
| C | -0.17746300 | 0.25259400 | -4.01536600 |
| H | -2.07519800 | 1.16508500 | -3.49765600 |
| C | -2.06449000 | 2.29621800 | 0.84757500 |
| C | -0.24888300 | 3.49206300 | -0.41398300 |
| H | -2.21667300 | 2.97475900 | -1.19601600 |
| C | -2.63859000 | -1.26713000 | -2.18879100 |
| C | -2.08212300 | -1.02958300 | 0.25209900 |
| H | -3.23371400 | 0.37425400 | -0.94042800 |
| C | -0.76580500 | 2.88726300 | -5.18820500 |
| H | 0.45294600 | 2.89049900 | -3.40066100 |
| H | -1.20281300 | 3.47052700 | -3.15029800 |
| C | -0.33099800 | 0.42427700 | -5.53159800 |
| H | 0.88275900 | 0.38185500 | -3.73334300 |
| H | -0.44543300 | -0.77234200 | -3.72428700 |
| C | -2.46609400 | 3.61830900 | 1.51619300 |
| H | -1.32650300 | 1.77974000 | 1.48377700 |
| H | -2.94789300 | 1.64398100 | 0.78778400 |
| C | -0.65225900 | 4.81693200 | 0.24515200 |
| H | 0.52245400 | 2.98840100 | 0.19242600 |
| H | 0.21532700 | 3.69047500 | -1.38932100 |
| C | -3.83447900 | -2.15965400 | -1.82302600 |
| H | -1.75429200 | -1.90612100 | -2.35486600 |
| H | -2.84536100 | -0.75490100 | -3.14022700 |
| C | -3.27008100 | -1.92165800 | 0.62735900 |
| H | -1.18453800 | -1.65826700 | 0.12076500 |
| H | -1.84508900 | -0.35203200 | 1.08148000 |
| C | 0.03617700 | 1.84451600 | -5.97380000 |
| H | -0.46034100 | 3.90723700 | -5.47580100 |
| H | -1.83667200 | 2.79533700 | -5.44771200 |
| H | 0.29250300 | -0.31871300 | -6.05641200 |
| H | -1.37855600 | 0.21154700 | -5.81448100 |
| C | -1.28342900 | 4.58528100 | 1.62116900 |
| H | -2.88827700 | 3.41125200 | 2.51435800 |
| H | -3.27287800 | 4.09175600 | 0.92644100 |
| H | 0.23123100 | 5.47175700 | 0.33014400 |
| H | -1.37469000 | 5.34685600 | -0.40362900 |
| C | -3.60966900 | -2.90093400 | -0.50059000 |
| H | -4.02530900 | -2.87534500 | -2.64031700 |
| H | -4.73956000 | -1.53014700 | -1.73913900 |
| H | -3.04122300 | -2.46289000 | 1.55920100 |
| H | -4.14880700 | -1.28460000 | 0.83988900 |
| H | -0.12758500 | 1.96802900 | -7.05737200 |
| H | 1.11492800 | 2.01004000 | -5.79697600 |
| H | -1.60305100 | 5.54054100 | 2.07058900 |
| H | -0.52331600 | 4.15432200 | 2.29868600 |
| H | -4.49679100 | -3.50256600 | -0.24084400 |
| H | -2.77154000 | -3.61165100 | -0.62347500 |
| C | 1.11499700 | -0.92804900 | 2.99223300 |
| C | 0.54093900 | -2.19941900 | 3.11887100 |
| C | 0.33452700 | 0.20073300 | 3.28532200 |
| C | -0.78446600 | -2.34087100 | 3.54441600 |
| H | 1.12703900 | -3.08836600 | 2.87558400 |
| C | -0.98546900 | 0.06155600 | 3.72069000 |
| H | 0.76442800 | 1.19722500 | 3.15811100 |
| C | -1.54994300 | -1.21211700 | 3.85161700 |
| H | -1.22026900 | -3.33917100 | 3.63431100 |
| H | -1.58054100 | 0.95065700 | 3.94419500 |

| | | | |
|---|---|---|---|
| H | -2.58614900 | -1.32335500 | 4.18026000 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.839431
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.09042

**iii-3 *trans***
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.702950 (Hartree/Particle)
Thermal correction to Energy= 0.738133
Thermal correction to Enthalpy= 0.739078
Thermal correction to Gibbs Free Energy= 0.634159
Sum of electronic and zero-point Energies= -3355.584027
Sum of electronic and thermal Energies= -3355.548843
Sum of electronic and thermal Enthalpies= -3355.547899
Sum of electronic and thermal Free Energies= -3355.652817

| | | | |
|---|---|---|---|
| O | -1.47004100 | -1.54348400 | 2.38416800 |
| C | -0.36830200 | -0.98925700 | 3.11250100 |
| C | -0.52700100 | 0.53841200 | 2.96638500 |
| H | -0.41965700 | -1.33444900 | 4.15340500 |
| H | 0.57284900 | -1.33908200 | 2.65741700 |
| H | 0.44561600 | 1.01757200 | 2.77914700 |
| N | -1.33858900 | 0.58651300 | 1.74574300 |
| C | -1.95224900 | -0.61119000 | 1.50646100 |
| O | -2.79684600 | -0.88114700 | 0.68039900 |
| C | -1.57948000 | 1.78988400 | 1.03163900 |
| H | -1.92980300 | 2.63137700 | 1.63974200 |
| C | -1.49152700 | 1.85454000 | -0.32297700 |
| C | -1.91583500 | 2.93762500 | -1.20984800 |
| H | -1.94336200 | 3.92835400 | -0.72443700 |
| H | -1.34391700 | 2.98023800 | -2.14815700 |
| C | -1.20417700 | 1.22606200 | 4.14193000 |
| C | -2.35332300 | 0.67193800 | 4.73081700 |
| C | -0.70536800 | 2.43713000 | 4.63873900 |
| C | -2.97766100 | 1.31015300 | 5.80424000 |
| H | -2.76570200 | -0.26344000 | 4.34318500 |
| C | -1.33561000 | 3.08367900 | 5.70828200 |
| H | 0.18461200 | 2.88010000 | 4.18290700 |
| C | -2.47118700 | 2.51925900 | 6.29567400 |
| H | -3.86910400 | 0.86719300 | 6.25454400 |
| H | -0.93636700 | 4.02956000 | 6.08317200 |
| H | -2.96362800 | 3.01999500 | 7.13297900 |
| P | -5.70587100 | 1.27139600 | -0.80766000 |
| C | -7.20127400 | 1.75437500 | -1.81529400 |
| C | -6.14207900 | 1.76496800 | 0.95820800 |
| C | -5.59608300 | -0.58649600 | -0.82852000 |
| C | -7.50179000 | 3.26011200 | -1.67961600 |
| C | -6.98173200 | 1.37857100 | -3.29433000 |
| H | -8.06455100 | 1.18703000 | -1.42361400 |
| C | -5.65475000 | 0.76548100 | 2.02595100 |
| C | -5.55102700 | 3.16305300 | 1.25121200 |
| H | -7.24462300 | 1.82124300 | 1.01357800 |
| C | -6.92962900 | -1.34549900 | -0.75534300 |
| C | -4.70081200 | -1.10587000 | -1.97151800 |
| H | -5.02366200 | -0.78972400 | 0.08810100 |
| C | -8.66556300 | 3.69833700 | -2.57889900 |
| H | -6.59154500 | 3.82627300 | -1.95167800 |
| H | -7.73331300 | 3.51507500 | -0.63419800 |
| C | -8.14620300 | 1.82833600 | -4.18609000 |
| H | -6.04404200 | 1.85353900 | -3.63811600 |
| H | -6.83697200 | 0.29316000 | -3.39822500 |
| C | -5.97430700 | 1.25366800 | 3.44651200 |
| H | -4.56567100 | 0.62463700 | 1.91852100 |
| H | -6.11376000 | -0.22283600 | 1.87308900 |
| C | -5.90506900 | 3.65045800 | 2.65993100 |
| H | -4.45140600 | 3.09312000 | 1.15835400 |
| H | -5.87393300 | 3.89582200 | 0.49698500 |
| C | -6.68280700 | -2.85507900 | -0.61301800 |
| H | -7.51709800 | -1.16254100 | -1.67239700 |
| H | -7.54137700 | -0.97920900 | 0.08646100 |
| C | -4.46458500 | -2.61381400 | -1.81826800 |
| H | -5.16390600 | -0.90273400 | -2.95252800 |
| H | -3.74110100 | -0.56502400 | -1.94951200 |
| C | -8.41833700 | 3.32895700 | -4.04473600 |
| H | -8.82654000 | 4.78427500 | -2.47320600 |
| H | -9.59378500 | 3.20763000 | -2.23226600 |
| H | -7.93092300 | 1.56894000 | -5.23614700 |
| H | -9.05510100 | 1.26582200 | -3.90325700 |
| C | -5.41687600 | 2.65449000 | 3.71474400 |
| H | -5.57060600 | 0.53463600 | 4.17927600 |
| H | -7.07115400 | 1.26383700 | 3.58734100 |
| H | -5.46220700 | 4.64579000 | 2.83233600 |
| H | -7.00116500 | 3.77360500 | 2.74090300 |
| C | -5.78786100 | -3.38637200 | -1.74023500 |
| H | -7.64454100 | -3.39538400 | -0.59514800 |
| H | -6.19345200 | -3.04672100 | 0.35930300 |
| H | -3.85260700 | -2.98612800 | -2.65730600 |
| H | -3.87990300 | -2.77747000 | -0.89684400 |
| H | -9.27743500 | 3.62706200 | -4.66870800 |
| H | -7.54436300 | 3.89339400 | -4.41906800 |
| H | -5.68980700 | 2.99032100 | 4.72932500 |
| H | -4.31536900 | 2.61305400 | 3.68617800 |
| H | -5.59647400 | -4.46346600 | -1.59861100 |
| H | -6.32452900 | -3.28715000 | -2.70270000 |
| Cu | -3.76642400 | 2.22776600 | -1.34917400 |
| H | -1.14622300 | 0.93658400 | -0.81880300 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.889435
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.147684

**i-3 int**
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.697749 (Hartree/Particle)
Thermal correction to Energy= 0.733406
Thermal correction to Enthalpy= 0.734350
Thermal correction to Gibbs Free Energy= 0.628858
Sum of electronic and zero-point Energies= -3355.535315
Sum of electronic and thermal Energies= -3355.499658
Sum of electronic and thermal Enthalpies= -3355.498713
Sum of electronic and thermal Free Energies= -3355.604206

| | | | |
|---|---|---|---|
| O | 1.97553400 | -2.39019900 | 1.63782300 |
| C | 3.23930800 | -2.17899500 | 1.00079900 |
| C | 3.43071800 | -0.65067100 | 1.00998300 |
| H | 4.01684900 | -2.72205300 | 1.55355600 |
| H | 3.18684600 | -2.56496200 | -0.03120000 |
| H | 3.87943000 | -0.32431600 | 0.06135200 |
| N | 2.02583900 | -0.22923200 | 1.07341900 |
| C | 1.24121300 | -1.23163200 | 1.55319700 |
| O | 0.07202600 | -1.19794100 | 1.88135400 |
| C | 1.56258000 | 1.15423200 | 0.94600800 |
| H | 1.30694400 | 1.57764300 | 1.93181800 |
| C | 2.39148800 | 2.04188100 | 0.12794700 |
| C | 2.51657200 | 3.38750700 | 0.24846700 |
| H | 2.04079500 | 3.93105100 | 1.07184600 |
| H | 3.07018000 | 3.97292500 | -0.48908300 |
| C | 4.24921500 | -0.08815100 | 2.15750500 |
| C | 4.10735900 | -0.59350400 | 3.46012700 |
| C | 5.11959100 | 0.98631700 | 1.93632300 |
| C | 4.83721300 | -0.04249800 | 4.51564900 |
| H | 3.41947700 | -1.42193200 | 3.64959600 |
| C | 5.84725900 | 1.54352900 | 2.99228400 |
| H | 5.21700700 | 1.40199500 | 0.93063900 |
| C | 5.71044000 | 1.02741800 | 4.28395900 |
| H | 4.72349200 | -0.44770100 | 5.52447600 |
| H | 6.52045700 | 2.38405200 | 2.80491300 |
| H | 6.28004900 | 1.45887500 | 5.11109300 |
| P | -1.73939000 | 0.09498000 | -1.09976300 |

| | | | |
|---|---|---|---|
| C | -2.51006300 | 0.47638400 | -2.74972100 |
| C | -3.08686300 | 0.45078300 | 0.17008100 |
| C | -1.37458900 | -1.73359200 | -1.03257700 |
| C | -2.93603500 | 1.95782600 | -2.79161000 |
| C | -1.51746300 | 0.16221100 | -3.88632400 |
| H | -3.40722200 | -0.15805700 | -2.86649300 |
| C | -3.20871200 | -0.60228300 | 1.28879400 |
| C | -2.81935700 | 1.83963000 | 0.79796300 |
| H | -4.04373900 | 0.48613800 | -0.38203600 |
| C | -2.44004900 | -2.66007500 | -1.63801000 |
| C | 0.03271600 | -2.08349700 | -1.56345200 |
| H | -1.32790300 | -1.90864500 | 0.05350600 |
| C | -3.46585900 | 2.36922200 | -4.17056800 |
| H | -2.05935700 | 2.58139100 | -2.53483800 |
| H | -3.70161800 | 2.16131600 | -2.02680200 |
| C | -2.05501400 | 0.58634300 | -5.25873000 |
| H | -0.56907200 | 0.69301200 | -3.68141100 |
| H | -1.27783300 | -0.91119000 | -3.90099100 |
| C | -4.29058700 | -0.20865900 | 2.30571700 |
| H | -2.23643300 | -0.69904300 | 1.79776200 |
| H | -3.44978100 | -1.59078300 | 0.86917600 |
| C | -3.90078100 | 2.23467600 | 1.80840800 |
| H | -1.84423800 | 1.79673800 | 1.31685200 |
| H | -2.71846300 | 2.61076300 | 0.01813700 |
| C | -2.09984800 | -4.13059400 | -1.35040100 |
| H | -2.48987600 | -2.50688900 | -2.73063100 |
| H | -3.44072800 | -2.41813500 | -1.24375600 |
| C | 0.36884700 | -3.55094900 | -1.26581300 |
| H | 0.08601900 | -1.91222500 | -2.65184900 |
| H | 0.78222200 | -1.41616200 | -1.10857500 |
| C | -2.45041500 | 2.06596800 | -5.27668300 |
| H | -3.72466600 | 3.44120200 | -4.16326600 |
| H | -4.40316600 | 1.82052200 | -4.37692200 |
| H | -1.29948300 | 0.37581900 | -6.03404000 |
| H | -2.93933800 | -0.02931600 | -5.50610300 |
| C | -4.03535600 | 1.17691700 | 2.90874900 |
| H | -4.34151800 | -0.97097900 | 3.10115500 |
| H | -5.27736500 | -0.20988400 | 1.80586400 |
| H | -3.66225300 | 3.22001300 | 2.24275500 |
| H | -4.86821500 | 2.34657400 | 1.28431000 |
| C | -0.69367000 | -4.49373300 | -1.84575300 |
| H | -2.85327400 | -4.78988500 | -1.81348000 |
| H | -2.15638300 | -4.30222300 | -0.26010900 |
| H | 1.36396600 | -3.79757600 | -1.67399800 |
| H | 0.43635500 | -3.68531400 | -0.17205600 |
| H | -2.85815800 | 2.34507200 | -6.26252000 |
| H | -1.54774000 | 2.68534400 | -5.12101300 |
| H | -4.84264900 | 1.44740400 | 3.60993900 |
| H | -3.10002900 | 1.14824500 | 3.49703400 |
| H | -0.45863800 | -5.54090900 | -1.59179400 |
| H | -0.67244300 | -4.42581600 | -2.94961900 |
| Cu | 0.06627400 | 1.11955600 | -0.36973700 |
| H | 2.90184400 | 1.56614900 | -0.72233000 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.839234
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.092678

**ii-3**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.702268 (Hartree/Particle)
Thermal correction to Energy= 0.737930
Thermal correction to Enthalpy= 0.738874
Thermal correction to Gibbs Free Energy= 0.629430
Sum of electronic and zero-point Energies= -3355.582218
Sum of electronic and thermal Energies= -3355.546557
Sum of electronic and thermal Enthalpies= -3355.545613
Sum of electronic and thermal Free Energies= -3355.655056

| | | | |
|---|---|---|---|
| O | 1.98770200 | -2.53169000 | 1.62828400 |
| C | 3.15281400 | -2.12027900 | 0.89572800 |
| C | 3.16076900 | -0.57607900 | 0.98974200 |
| H | 4.03709900 | -2.58214000 | 1.35156300 |
| H | 3.05068500 | -2.46234000 | -0.14610700 |
| H | 3.41898400 | -0.12667300 | 0.01980700 |
| N | 1.74229000 | -0.35307900 | 1.27718500 |
| C | 1.12079900 | -1.48847500 | 1.72592400 |
| O | -0.00533100 | -1.59394200 | 2.15262400 |
| C | 1.10310900 | 0.90494100 | 1.24750600 |
| H | 0.26984200 | 0.99744400 | 1.95026800 |
| C | 1.65704700 | 1.99132500 | 0.61356800 |
| C | 2.49234200 | 3.01844300 | 0.60794500 |
| H | 3.12868900 | 3.22698600 | 1.47714500 |
| H | 2.57208200 | 3.68193700 | -0.25665400 |
| C | 4.06889500 | -0.01360200 | 2.07198900 |
| C | 3.93455000 | -0.44605100 | 3.40180000 |
| C | 5.04866300 | 0.93692300 | 1.76206100 |
| C | 4.76290800 | 0.06756300 | 4.40145700 |
| H | 3.17837400 | -1.19247700 | 3.65897400 |
| C | 5.87993500 | 1.45378500 | 2.76251500 |
| H | 5.15458400 | 1.28566200 | 0.73158800 |
| C | 5.73750500 | 1.02166300 | 4.08411100 |
| H | 4.64782600 | -0.27694400 | 5.43220200 |
| H | 6.63755900 | 2.19901800 | 2.50745500 |
| H | 6.38391800 | 1.42643500 | 4.86686200 |
| P | -1.58869600 | 0.09892100 | -1.00926200 |
| C | -2.39780900 | 0.45966000 | -2.65872000 |
| C | -2.96945500 | 0.45814400 | 0.22184500 |
| C | -1.28073600 | -1.74010900 | -0.95822400 |
| C | -2.85167100 | 1.93259400 | -2.71983100 |
| C | -1.43232400 | 0.14716000 | -3.81810500 |
| H | -3.28812400 | -0.19023700 | -2.73991400 |
| C | -3.13290500 | -0.57858500 | 1.34925600 |
| C | -2.74115500 | 1.86216900 | 0.82470200 |
| H | -3.90788000 | 0.47483300 | -0.36158900 |
| C | -2.35963700 | -2.63834300 | -1.58533900 |
| C | 0.11996800 | -2.09633400 | -1.49920500 |
| H | -1.24882600 | -1.94420300 | 0.12370000 |
| C | -3.43375400 | 2.30259100 | -4.09040100 |
| H | -1.97558300 | 2.57005000 | -2.50413500 |
| H | -3.60210400 | 2.13934200 | -1.94123600 |
| C | -2.02044900 | 0.52881900 | -5.18298600 |
| H | -0.49677700 | 0.70770700 | -3.64303900 |
| H | -1.16917300 | -0.92106800 | -3.82270900 |
| C | -4.25676600 | -0.17573600 | 2.31565000 |
| H | -2.18486800 | -0.67417400 | 1.90236000 |
| H | -3.35345200 | -1.57326900 | 0.93299400 |
| C | -3.86120400 | 2.26196100 | 1.79150900 |
| H | -1.77805500 | 1.85272600 | 1.36484300 |
| H | -2.63232400 | 2.61662100 | 0.03048500 |
| C | -2.03776000 | -4.12018500 | -1.33906500 |
| H | -2.40996800 | -2.45745500 | -2.67297500 |
| H | -3.35566800 | -2.39266800 | -1.18211800 |
| C | 0.43871100 | -3.57723200 | -1.25413200 |
| H | 0.17553300 | -1.88822100 | -2.58034700 |
| H | 0.87493500 | -1.44587500 | -1.02856500 |
| C | -2.44768500 | 1.99886800 | -5.22207800 |
| H | -3.71559700 | 3.36901000 | -4.09632200 |
| H | -4.36530300 | 1.72998600 | -4.25681900 |
| H | -1.28310900 | 0.31725400 | -5.97566700 |
| H | -2.89874100 | -0.11022300 | -5.39188900 |
| C | -4.03146400 | 1.22142200 | 2.90360000 |
| H | -4.33668100 | -0.92484400 | 3.12128400 |
| H | -5.22236000 | -0.18997000 | 1.77646700 |
| H | -3.64991300 | 3.25684900 | 2.21813800 |
| H | -4.80858800 | 2.35540000 | 1.22891000 |
| C | -0.64067700 | -4.48567400 | -1.85769300 |
| H | -2.80280100 | -4.75708400 | -1.81424900 |
| H | -2.08730300 | -4.32237400 | -0.25357800 |
| H | 1.42722400 | -3.82469000 | -1.67782700 |

| | | | |
|---|---|---|---|
| H | 0.50853500 | -3.75577900 | -0.16700200 |
| H | -2.89237400 | 2.24730900 | -6.20051300 |
| H | -1.55438500 | 2.63936900 | -5.10632800 |
| H | -4.86539700 | 1.49941100 | 3.56988200 |
| H | -3.11885400 | 1.20781500 | 3.52772000 |
| H | -0.41649800 | -5.54336600 | -1.64022800 |
| H | -0.62681200 | -4.38107000 | -2.95862600 |
| Cu | 0.28587100 | 1.42239200 | -0.72614200 |
| H | 0.60296400 | 2.35944400 | -1.94520300 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.889845
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.145514

**iii'-3 *cis***

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.937178 (Hartree/Particle)
Thermal correction to Energy= 0.985722
Thermal correction to Enthalpy= 0.986666
Thermal correction to Gibbs Free Energy= 0.852508
Sum of electronic and zero-point Energies= -3951.048741
Sum of electronic and thermal Energies= -3951.000198
Sum of electronic and thermal Enthalpies= -3950.999254
Sum of electronic and thermal Free Energies= -3951.133411

| | | | |
|---|---|---|---|
| O | 1.69054000 | 3.37580600 | 0.82984500 |
| C | 2.25608300 | 3.94189100 | 2.01699700 |
| C | 1.73393100 | 3.04932700 | 3.15860100 |
| H | 3.35475600 | 3.90661500 | 1.94085000 |
| H | 1.93506500 | 4.98804900 | 2.10667000 |
| H | 0.80351300 | 3.46884200 | 3.58188000 |
| N | 1.39040200 | 1.83152200 | 2.41073100 |
| C | 1.30168800 | 2.09158200 | 1.08024200 |
| O | 0.92782700 | 1.36623400 | 0.17420000 |
| C | 0.80684300 | 0.73438800 | 3.10256800 |
| H | 1.38886600 | 0.39816600 | 3.96006900 |
| C | -0.51109200 | 0.35531600 | 2.93353200 |
| H | -0.81357100 | -0.44944600 | 3.61658700 |
| C | -1.42546300 | 0.69102600 | 1.92215900 |
| H | -2.45442400 | 0.34418200 | 2.04510400 |
| H | -1.32576500 | 1.64489700 | 1.39399200 |
| Cu | -0.53946700 | -0.39309400 | -0.00485700 |
| P | -1.57902800 | -0.08579700 | -1.97539500 |
| C | -1.33223300 | 1.63925200 | -2.67324500 |
| C | -3.46285100 | -0.23050600 | -1.86795600 |
| C | -1.06739900 | -1.27473700 | -3.32741800 |
| C | -1.81109400 | 2.68317000 | -1.64236200 |
| C | 0.14314400 | 1.88884800 | -3.04786100 |
| H | -1.95504100 | 1.72474200 | -3.58287200 |
| C | -4.02198700 | -1.59026200 | -2.32639400 |
| C | -3.89638800 | 0.04118800 | -0.41231400 |
| H | -3.88245800 | 0.55606400 | -2.52182500 |
| C | -1.45982000 | -0.89215200 | -4.76439900 |
| C | 0.42666600 | -1.64174400 | -3.22882400 |
| H | -1.61464400 | -2.19327500 | -3.05532100 |
| C | -1.54424100 | 4.12374700 | -2.09730600 |
| H | -1.27803700 | 2.49324200 | -0.69623200 |
| H | -2.88587500 | 2.55729600 | -1.43876800 |
| C | 0.39099100 | 3.33648700 | -3.49513200 |
| H | 0.76867500 | 1.66850400 | -2.16817000 |
| H | 0.45479600 | 1.20542500 | -3.85126700 |
| C | -5.54216700 | -1.68459200 | -2.12725900 |
| H | -3.53740200 | -2.39363300 | -1.74843100 |
| H | -3.78807500 | -1.77544600 | -3.38513500 |
| C | -5.41376500 | -0.04189400 | -0.22315900 |
| H | -3.40361700 | -0.70739800 | 0.23074500 |
| H | -3.52053000 | 1.01523000 | -0.06947800 |
| C | -1.09505000 | -2.01238900 | -5.74999800 |
| H | -0.93001700 | 0.02920700 | -5.06016500 |
| H | -2.53618300 | -0.66335700 | -4.82831600 |
| C | 0.78574200 | -2.75325600 | -4.22276500 |
| H | 1.05382900 | -0.75794700 | -3.43035500 |
| H | 0.65147800 | -1.95212700 | -2.19690100 |
| C | -0.06563500 | 4.34104400 | -2.43275200 |
| H | -1.87191000 | 4.82454700 | -1.31054600 |
| H | -2.15775700 | 4.34505100 | -2.99085400 |
| H | 1.46204800 | 3.47247500 | -3.72249400 |
| H | -0.15702800 | 3.52852700 | -4.43695800 |
| C | -5.95021800 | -1.40204700 | -0.67796500 |
| H | -5.89074600 | -2.68408500 | -2.43891000 |
| H | -6.04139200 | -0.95596900 | -2.79291300 |
| H | -5.66636400 | 0.14213600 | 0.83489700 |
| H | -5.90304000 | 0.75973100 | -0.80754700 |
| C | 0.39224500 | -2.37663500 | -5.65703200 |
| H | -1.35497100 | -1.71120900 | -6.77895600 |
| H | -1.70354400 | -2.90661300 | -5.52004200 |
| H | 1.86380100 | -2.97906100 | -4.16388400 |
| H | 0.25418300 | -3.67846100 | -3.93373300 |
| H | 0.10377500 | 5.37468600 | -2.77991800 |
| H | 0.53837600 | 4.20415400 | -1.51819300 |
| H | -7.04711100 | -1.44714100 | -0.56942200 |
| H | -5.53207400 | -2.19036000 | -0.02606800 |
| H | 0.62993600 | -3.20077800 | -6.35059100 |
| H | 0.99646100 | -1.50885700 | -5.98123600 |
| C | 2.70880000 | 2.79825100 | 4.28886700 |
| C | 3.97495500 | 2.24819700 | 4.03417000 |
| C | 2.34456200 | 3.07847500 | 5.61176300 |
| C | 4.86438400 | 2.00102900 | 5.08163000 |
| H | 4.25783800 | 1.99168700 | 3.01148300 |
| C | 3.23413400 | 2.83355700 | 6.66383900 |
| H | 1.35242500 | 3.48791900 | 5.82092900 |
| C | 4.49768000 | 2.29721000 | 6.40052600 |
| H | 5.84680300 | 1.57128400 | 4.86885000 |
| H | 2.93662000 | 3.05910000 | 7.69105100 |
| H | 5.19431300 | 2.10454800 | 7.22043600 |
| C | 1.52928400 | -1.51707400 | 1.78233000 |
| N | 0.45457700 | -1.77586500 | 1.09343500 |
| C | -1.32999400 | -3.44062800 | 0.70577300 |
| C | -0.74000600 | -3.92951700 | -0.46974900 |
| C | -2.68523700 | -3.70911000 | 0.94178200 |
| C | -1.48609700 | -4.67611500 | -1.38417100 |
| H | 0.31135100 | -3.70936900 | -0.66377900 |
| C | -3.43345300 | -4.46521900 | 0.03336200 |
| H | -3.16203000 | -3.31643800 | 1.84456500 |
| C | -2.83587800 | -4.95115600 | -1.13352700 |
| H | -1.01242100 | -5.04684600 | -2.29684800 |
| H | -4.49055200 | -4.66136600 | 0.23022600 |
| H | -3.42143500 | -5.53237100 | -1.85025400 |
| C | -0.50948000 | -2.67743900 | 1.72107300 |
| H | -1.19133400 | -2.11298800 | 2.37504100 |
| H | 0.01435700 | -3.40622500 | 2.37079200 |
| H | 1.64221100 | -1.95468000 | 2.78671700 |
| C | 2.76020900 | -0.92985600 | 1.23851600 |
| C | 3.84760800 | -0.69213700 | 2.10089300 |
| C | 2.94086000 | -0.71141400 | -0.14117300 |
| C | 5.07963200 | -0.26403400 | 1.60292100 |
| H | 3.71961900 | -0.84370800 | 3.17610300 |
| C | 4.17160300 | -0.28920000 | -0.63925200 |
| H | 2.10061800 | -0.87951300 | -0.81421400 |
| C | 5.24995700 | -0.06491700 | 0.22791300 |
| H | 5.91140200 | -0.08842000 | 2.29050500 |
| H | 4.29374100 | -0.13382400 | -1.71458300 |
| H | 6.21525300 | 0.26309900 | -0.16628000 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3951.484104
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3954.480942

**TS-iii'-iv-3 *cis (S,S,S)***

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.937109 (Hartree/Particle)
Thermal correction to Energy= 0.984712
Thermal correction to Enthalpy= 0.985656
Thermal correction to Gibbs Free Energy= 0.853058
Sum of electronic and zero-point Energies= -3951.035476
Sum of electronic and thermal Energies= -3950.987872
Sum of electronic and thermal Enthalpies= -3950.986928
Sum of electronic and thermal Free Energies= -3951.119527

| | | | |
|---|---|---|---|
| O | -2.39973800 | 5.94181800 | -2.21605300 |
| C | -2.54887100 | 6.55861600 | -0.92869700 |
| C | -2.23079000 | 5.41023800 | 0.04854800 |
| H | -1.86613200 | 7.41363600 | -0.85190200 |
| H | -3.59354700 | 6.89721600 | -0.82201600 |
| H | -2.85125500 | 5.47724400 | 0.95438700 |
| N | -2.66989600 | 4.26879600 | -0.76637700 |
| C | -2.69838700 | 4.61442600 | -2.08304900 |
| O | -2.95581000 | 3.92194700 | -3.04778200 |
| C | -3.32677100 | 3.12947000 | -0.16832300 |
| H | -2.85195300 | 2.85564100 | 0.77567500 |
| C | -4.67552700 | 2.97925900 | -0.32299600 |
| H | -5.11901000 | 2.22051100 | 0.33364300 |
| C | -5.46648700 | 3.36925300 | -1.46103700 |
| H | -6.53957100 | 3.16136700 | -1.38244600 |
| H | -5.25098000 | 4.33717300 | -1.92878200 |
| Cu | -4.64420400 | 2.27544000 | -3.04284700 |
| P | -5.39055100 | 2.65151400 | -5.16933600 |
| C | -5.15909600 | 4.41719600 | -5.78871500 |
| C | -7.25879700 | 2.38281400 | -5.31522500 |
| C | -4.66699700 | 1.55285600 | -6.50212900 |
| C | -5.66856700 | 5.41720700 | -4.72971300 |
| C | -3.69043100 | 4.71286300 | -6.16220300 |
| H | -5.78693400 | 4.51410000 | -6.69404500 |
| C | -7.62842800 | 0.94235100 | -5.72383100 |
| C | -7.93338600 | 2.72430600 | -3.96775500 |
| H | -7.62836900 | 3.07696500 | -6.09194600 |
| C | -4.98616300 | 1.92491000 | -7.95978500 |
| C | -3.16918100 | 1.26898500 | -6.28717300 |
| H | -5.16614500 | 0.59211800 | -6.29042200 |
| C | -5.42438300 | 6.87521600 | -5.13424600 |
| H | -5.14197000 | 5.20787000 | -3.78541100 |
| H | -6.74165900 | 5.26321100 | -4.54144400 |
| C | -3.45098400 | 6.19040600 | -6.50879900 |
| H | -3.04616600 | 4.43039500 | -5.31681500 |
| H | -3.39198800 | 4.09891400 | -7.02320100 |
| C | -9.14496800 | 0.70124200 | -5.71847400 |
| H | -7.14990100 | 0.23750300 | -5.02536600 |
| H | -7.23983200 | 0.70655200 | -6.72499800 |
| C | -9.44911700 | 2.49878000 | -3.99610800 |
| H | -7.48285500 | 2.08027300 | -3.19304900 |
| H | -7.70841000 | 3.75690100 | -3.66577400 |
| C | -4.46832700 | 0.84760300 | -8.92564700 |
| H | -4.51672700 | 2.88898400 | -8.21547300 |
| H | -6.07111000 | 2.06520500 | -8.09506400 |
| C | -2.67762300 | 0.18850800 | -7.25817100 |
| H | -2.57769600 | 2.18454700 | -6.43733000 |
| H | -3.00989100 | 0.96047900 | -5.24236600 |
| C | -3.93688300 | 7.12038900 | -5.39403400 |
| H | -5.81050300 | 7.55163400 | -4.35278200 |
| H | -5.99696200 | 7.09736900 | -6.05447800 |
| H | -2.37878200 | 6.35121200 | -6.71275100 |
| H | -3.98749800 | 6.43542400 | -7.44501300 |
| C | -9.77244400 | 1.04928400 | -4.36659100 |
| H | -9.34967800 | -0.34944300 | -5.98557900 |
| H | -9.61179700 | 1.32386700 | -6.50446800 |
| H | -9.88682500 | 2.76328600 | -3.01852100 |
| H | -9.90621000 | 3.17764300 | -4.74020500 |
| C | -2.97380900 | 0.57106200 | -8.71395500 |
| H | -4.65844400 | 1.15448500 | -9.96813800 |
| H | -5.03759700 | -0.08632400 | -8.76322600 |
| H | -1.59878400 | 0.01027200 | -7.11459400 |
| H | -3.18753400 | -0.76406600 | -7.02513100 |
| H | -3.74691400 | 8.17630000 | -5.65108200 |
| H | -3.37113900 | 6.90375400 | -4.47009800 |
| H | -10.86143500 | 0.87434500 | -4.38057400 |
| H | -9.35035200 | 0.38067900 | -3.59464600 |
| H | -2.62956700 | -0.22169400 | -9.39934500 |
| H | -2.39969000 | 1.48055800 | -8.97197600 |
| C | -0.76218200 | 5.38354600 | 0.44212500 |
| C | 0.17392300 | 4.60385100 | -0.24533500 |
| C | -0.32021300 | 6.23487900 | 1.46823500 |
| C | 1.53087600 | 4.66927800 | 0.09033800 |
| H | -0.15383900 | 3.94438800 | -1.04800600 |
| C | 1.03387600 | 6.30253500 | 1.80268500 |
| H | -1.04405700 | 6.85089700 | 2.01112500 |
| C | 1.96558200 | 5.51683800 | 1.11238800 |
| H | 2.24483800 | 4.04772900 | -0.45489000 |
| H | 1.36373100 | 6.96698100 | 2.60557100 |
| H | 3.02578900 | 5.56622600 | 1.37358000 |
| C | -2.84678700 | 1.19998500 | -1.10997000 |
| N | -3.77126800 | 0.89487100 | -1.96090200 |
| C | -5.43487700 | -0.83174500 | -2.61724900 |
| C | -4.68606800 | -1.23489700 | -3.73443500 |
| C | -6.77629000 | -1.23371700 | -2.53326000 |
| C | -5.26060800 | -2.02582500 | -4.73313000 |
| H | -3.64880100 | -0.90580500 | -3.81430800 |
| C | -7.35350400 | -2.03178500 | -3.52719500 |
| H | -7.38095400 | -0.91384900 | -1.67970100 |
| C | -6.59663800 | -2.43190300 | -4.63247900 |
| H | -4.66179500 | -2.32681900 | -5.59662700 |
| H | -8.40342300 | -2.32504100 | -3.44628700 |
| H | -7.04787500 | -3.04471700 | -5.41695700 |
| C | -4.79583900 | -0.03289200 | -1.49406300 |
| H | -5.59939100 | 0.49439400 | -0.94455600 |
| H | -4.35701900 | -0.74518400 | -0.76764900 |
| H | -2.88149700 | 0.70610500 | -0.12317000 |
| C | -1.43870500 | 1.45323000 | -1.51437900 |
| C | -0.41883100 | 1.25138300 | -0.56582800 |
| C | -1.06842500 | 1.75119400 | -2.83787400 |
| C | 0.92791800 | 1.34820400 | -0.92277400 |
| H | -0.68775100 | 1.00612100 | 0.46625500 |
| C | 0.27616700 | 1.87084900 | -3.19071600 |
| H | -1.85170200 | 1.88460500 | -3.58096200 |
| C | 1.28322000 | 1.67085500 | -2.23647100 |
| H | 1.70214100 | 1.17967100 | -0.17006200 |
| H | 0.54264100 | 2.11264800 | -4.22334900 |
| H | 2.33582100 | 1.75901700 | -2.51774900 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3951.468767
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3954.466648

**iv-3 *(S,S,S)***
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.939137 (Hartree/Particle)
Thermal correction to Energy= 0.986955
Thermal correction to Enthalpy= 0.987899
Thermal correction to Gibbs Free Energy= 0.854840
Sum of electronic and zero-point Energies= -3951.051519
Sum of electronic and thermal Energies= -3951.003702
Sum of electronic and thermal Enthalpies= -3951.002758
Sum of electronic and thermal Free Energies= -3951.135816

| | | | |
|---|---|---|---|
| O | 1.63978000 | 3.35541900 | 0.84746900 |
| C | 2.16855900 | 3.85163400 | 2.08040700 |
| C | 1.68315300 | 2.84605200 | 3.14633200 |
| H | 3.26790200 | 3.87023400 | 2.01452400 |
| H | 1.79827100 | 4.87106400 | 2.25039800 |
| H | 0.71293900 | 3.17025100 | 3.56449700 |
| N | 1.44936700 | 1.66036300 | 2.29142400 |

| | | | |
|---|---|---|---|
| C | 1.28677200 | 2.05380200 | 1.00183200 |
| O | 0.86958000 | 1.40313400 | 0.06313700 |
| C | 0.94107600 | 0.38895300 | 2.83690600 |
| H | 1.45255200 | 0.28509100 | 3.80271200 |
| C | -0.53824800 | 0.36346800 | 3.04959900 |
| H | -0.86736700 | -0.31874400 | 3.84178100 |
| C | -1.46933600 | 0.92197400 | 2.26067400 |
| H | -2.53333600 | 0.74314000 | 2.43568800 |
| H | -1.22302700 | 1.60239600 | 1.44474400 |
| Cu | -0.49415500 | -0.46620500 | -0.13047300 |
| P | -1.59243500 | -0.06710700 | -1.99700300 |
| C | -1.34644100 | 1.65407300 | -2.69399000 |
| C | -3.46749200 | -0.22226600 | -1.86039000 |
| C | -1.07190900 | -1.26815700 | -3.33382600 |
| C | -1.82017600 | 2.69395300 | -1.65646900 |
| C | 0.12851400 | 1.89641700 | -3.07712200 |
| H | -1.97419300 | 1.74497800 | -3.59959700 |
| C | -4.02564200 | -1.58213900 | -2.32020000 |
| C | -3.87977000 | 0.04128500 | -0.39532600 |
| H | -3.90251800 | 0.56617800 | -2.50154600 |
| C | -1.46660500 | -0.89333100 | -4.77180400 |
| C | 0.42424600 | -1.63195200 | -3.23462500 |
| H | -1.61695100 | -2.18526800 | -3.05336600 |
| C | -1.54390600 | 4.13539900 | -2.10154900 |
| H | -1.28708800 | 2.49898800 | -0.71133400 |
| H | -2.89601700 | 2.57241800 | -1.45492600 |
| C | 0.38562000 | 3.34711200 | -3.50730500 |
| H | 0.76058500 | 1.65894400 | -2.20843500 |
| H | 0.42564800 | 1.22089700 | -3.89249900 |
| C | -5.54401500 | -1.67679400 | -2.11295500 |
| H | -3.53660400 | -2.38712000 | -1.74824500 |
| H | -3.79689700 | -1.76116300 | -3.38105700 |
| C | -5.39705100 | -0.04496800 | -0.19620400 |
| H | -3.37620400 | -0.70857700 | 0.24084300 |
| H | -3.50550000 | 1.01901200 | -0.05662700 |
| C | -1.09893700 | -2.01589800 | -5.75318900 |
| H | -0.94025300 | 0.02861300 | -5.07172300 |
| H | -2.54386200 | -0.66857400 | -4.83621100 |
| C | 0.78351700 | -2.74649800 | -4.22509600 |
| H | 1.04951600 | -0.74768100 | -3.43951400 |
| H | 0.65340900 | -1.94227100 | -2.20393500 |
| C | -0.06341000 | 4.34375500 | -2.43418700 |
| H | -1.86776500 | 4.83366800 | -1.31092100 |
| H | -2.15504200 | 4.36604900 | -2.99421400 |
| H | 1.45746800 | 3.47807200 | -3.73357700 |
| H | -0.16125300 | 3.55433400 | -4.44652600 |
| C | -5.94019400 | -1.40058400 | -0.65917100 |
| H | -5.89522700 | -2.67498600 | -2.42532500 |
| H | -6.04736000 | -0.94538800 | -2.77246400 |
| H | -5.64470300 | 0.13045800 | 0.86450800 |
| H | -5.88754300 | 0.76248300 | -0.77134600 |
| C | 0.38933000 | -2.37571600 | -5.66023100 |
| H | -1.36095000 | -1.71866100 | -6.78273900 |
| H | -1.70465300 | -2.91096400 | -5.51949400 |
| H | 1.86182400 | -2.97027700 | -4.16489100 |
| H | 0.25354400 | -3.67109900 | -3.93187900 |
| H | 0.11416800 | 5.37948700 | -2.77065100 |
| H | 0.53875300 | 4.19272800 | -1.52071000 |
| H | -7.03642500 | -1.44113300 | -0.54295500 |
| H | -5.52092600 | -2.19487800 | -0.01563000 |
| H | 0.62832700 | -3.20149700 | -6.35136600 |
| H | 0.99119300 | -1.50746600 | -5.98761500 |
| C | 2.66548000 | 2.66203600 | 4.28371200 |
| C | 3.96252200 | 2.18545900 | 4.03615900 |
| C | 2.30329000 | 2.98945700 | 5.59786700 |
| C | 4.86838500 | 2.01300100 | 5.08413800 |
| H | 4.25587200 | 1.92409000 | 3.01853300 |
| C | 3.21330600 | 2.82754600 | 6.64935400 |
| H | 1.29700700 | 3.36569900 | 5.80262600 |
| C | 4.49508800 | 2.33077300 | 6.39576600 |
| H | 5.86919300 | 1.62587900 | 4.87610700 |
| H | 2.91547000 | 3.08280000 | 7.66942600 |
| H | 5.20304700 | 2.19285200 | 7.21692300 |
| C | 1.37550800 | -1.02920300 | 1.99319900 |
| N | 0.40154800 | -1.59543400 | 1.13683000 |
| C | -1.27753000 | -3.38609400 | 0.74114100 |
| C | -0.70015700 | -3.88165700 | -0.44097800 |
| C | -2.63306800 | -3.66814100 | 0.97605200 |
| C | -1.44680500 | -4.63710800 | -1.34968200 |
| H | 0.34875800 | -3.65194200 | -0.63768000 |
| C | -3.38617900 | -4.43028100 | 0.07244400 |
| H | -3.10977200 | -3.27931200 | 1.88106300 |
| C | -2.79595100 | -4.91870500 | -1.09666000 |
| H | -0.97299500 | -5.01107800 | -2.26145200 |
| H | -4.44117500 | -4.63038200 | 0.27870000 |
| H | -3.38175100 | -5.50571100 | -1.80886100 |
| C | -0.44295100 | -2.60000600 | 1.74709000 |
| H | -1.14797600 | -2.19308800 | 2.50995300 |
| H | 0.17308200 | -3.34172800 | 2.31132600 |
| H | 1.56400600 | -1.70341200 | 2.85305200 |
| C | 2.73593800 | -0.78083900 | 1.34026000 |
| C | 3.86623600 | -0.60875000 | 2.15301600 |
| C | 2.90780600 | -0.69006300 | -0.04991500 |
| C | 5.11585800 | -0.29674900 | 1.60746700 |
| H | 3.76405600 | -0.69628600 | 3.23854500 |
| C | 4.15106400 | -0.36920700 | -0.60256100 |
| H | 2.04683100 | -0.85313800 | -0.69593700 |
| C | 5.26075400 | -0.15573400 | 0.22361800 |
| H | 5.97675400 | -0.15793400 | 2.26778800 |
| H | 4.25202400 | -0.28243900 | -1.68818600 |
| H | 6.23192900 | 0.10149600 | -0.20764200 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3951.483587
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3954.483565

**A-3**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.205249 (Hartree/Particle)
Thermal correction to Energy= 0.218091
Thermal correction to Enthalpy= 0.219035
Thermal correction to Gibbs Free Energy= 0.164339
Sum of electronic and zero-point Energies= -668.394748
Sum of electronic and thermal Energies= -668.381906
Sum of electronic and thermal Enthalpies= -668.380962
Sum of electronic and thermal Free Energies= -668.435658

| | | | |
|---|---|---|---|
| O | 0.03769900 | -0.35934100 | 2.19386000 |
| C | 0.29398200 | 0.92229700 | 2.93270200 |
| C | -1.04031100 | 1.18566900 | 3.66247800 |
| H | 1.16578800 | 0.76629000 | 3.56122500 |
| H | 0.49653000 | 1.69413200 | 2.18495100 |
| H | -1.24911000 | 2.25983700 | 3.70132500 |
| N | -1.97096600 | 0.54986700 | 2.67432100 |
| C | -1.33302000 | -0.41836900 | 1.93111000 |
| O | -1.83137300 | -1.23760100 | 1.13114800 |
| C | -3.31530000 | 0.92391600 | 2.41785700 |
| H | -3.82323700 | 0.27430500 | 1.70743400 |
| C | -3.92508200 | 1.97902100 | 2.93807800 |
| C | -4.57406000 | 2.99226300 | 3.48319900 |
| H | -5.14039000 | 2.87726500 | 4.40955200 |
| H | -4.57276700 | 3.98594100 | 3.03216200 |
| C | -1.18005900 | 0.57823500 | 5.06930700 |
| C | -2.45986300 | 0.50541600 | 5.67056300 |
| C | -0.06783100 | 0.12073300 | 5.80890800 |
| C | -2.62261200 | -0.01577000 | 6.96645300 |
| H | -3.33639500 | 0.84911400 | 5.13293300 |
| C | -0.22855000 | -0.39988000 | 7.10943300 |
| H | 0.93457100 | 0.15974100 | 5.39627700 |
| C | -1.50550900 | -0.47137100 | 7.69554000 |

| | | | |
|---|---|---|---|
| H | -3.61676400 | -0.06299400 | 7.40477300 |
| H | 0.64384900 | -0.74729500 | 7.65799400 |
| H | -1.62895700 | -0.87238600 | 8.69873000 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -668.4895248
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -669.3378016

**[Cu]-H**
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.489971 (Hartree/Particle)
Thermal correction to Energy= 0.511792
Thermal correction to Enthalpy= 0.512736
Thermal correction to Gibbs Free Energy= 0.439237
Sum of electronic and zero-point Energies= -2687.114380
Sum of electronic and thermal Energies= -2687.092558
Sum of electronic and thermal Enthalpies= -2687.091614
Sum of electronic and thermal Free Energies= -2687.165114

| | | | |
|---|---|---|---|
| P | -8.68811700 | 1.44905100 | 1.47485000 |
| C | -9.05026700 | 0.24450000 | 0.09398200 |
| C | -8.75973000 | 3.16459800 | 0.73266200 |
| C | -10.16568000 | 1.39941100 | 2.63963000 |
| C | -10.11560200 | 0.68968300 | -0.92204300 |
| C | -7.76176800 | -0.23128100 | -0.60954200 |
| H | -9.44241300 | -0.63435900 | 0.63380700 |
| C | -8.66310500 | 4.23303700 | 1.84117300 |
| C | -7.62349200 | 3.35138500 | -0.29259100 |
| H | -9.73282900 | 3.27376600 | 0.22147200 |
| C | -10.97132700 | 0.08664000 | 2.61612400 |
| C | -9.67214300 | 1.68387500 | 4.07614000 |
| H | -10.84126100 | 2.21549800 | 2.32553700 |
| C | -10.41286400 | -0.42882600 | -1.93180300 |
| H | -9.75383500 | 1.57677100 | -1.46972700 |
| H | -11.04149300 | 0.99714700 | -0.40825000 |
| C | -8.07103600 | -1.34482900 | -1.61891000 |
| H | -7.28406800 | 0.61104500 | -1.13682500 |
| H | -7.03350600 | -0.57424300 | 0.14405700 |
| C | -8.61563700 | 5.65528100 | 1.26747800 |
| H | -7.74794200 | 4.04213800 | 2.43206500 |
| H | -9.51247800 | 4.14931100 | 2.53626700 |
| C | -7.57654400 | 4.77862600 | -0.85328600 |
| H | -6.66460600 | 3.11353700 | 0.20439400 |
| H | -7.73001000 | 2.63655600 | -1.12166600 |
| C | -12.13016300 | 0.12674900 | 3.62402300 |
| H | -10.30295200 | -0.75777400 | 2.86580100 |
| H | -11.37286000 | -0.11064900 | 1.61071000 |
| C | -10.82906900 | 1.72829400 | 5.08045900 |
| H | -8.96181100 | 0.88566200 | 4.35934800 |
| H | -9.09526700 | 2.62033500 | 4.11405600 |
| C | -9.13451200 | -0.90497900 | -2.63329900 |
| H | -11.15298300 | -0.08040400 | -2.67153000 |
| H | -10.87574600 | -1.28053500 | -1.40017300 |
| H | -7.14629900 | -1.64992600 | -2.13624400 |
| H | -8.43499800 | -2.23519900 | -1.07371500 |
| C | -7.47128000 | 5.82149200 | 0.26335300 |
| H | -8.51961200 | 6.38246900 | 2.09090200 |
| H | -9.57586900 | 5.87395300 | 0.76474500 |
| H | -6.73088500 | 4.87244600 | -1.55474700 |
| H | -8.49466800 | 4.96552900 | -1.44046800 |
| C | -11.64480800 | 0.43151800 | 5.04524300 |
| H | -12.67583000 | -0.83133500 | 3.59838200 |
| H | -12.84921300 | 0.90588900 | 3.31032900 |
| H | -10.43659600 | 1.91250700 | 6.09430000 |
| H | -11.48756700 | 2.58276100 | 4.83742500 |
| H | -9.36421900 | -1.72800900 | -3.33039600 |
| H | -8.72967200 | -0.07810100 | -3.24601000 |
| H | -7.47155300 | 6.84057000 | -0.15800000 |
| H | -6.50649200 | 5.69568900 | 0.78817300 |
| H | -12.50044300 | 0.49247100 | 5.73828900 |
| H | -11.01128400 | -0.40282400 | 5.39838800 |
| Cu | -6.70930400 | 1.11559900 | 2.48473900 |
| H | -5.34066600 | 0.90186300 | 3.16451000 |
| P | -8.68811700 | 1.44905100 | 1.47485000 |
| C | -9.05026700 | 0.24450000 | 0.09398200 |
| C | -8.75973000 | 3.16459800 | 0.73266200 |
| C | -10.16568000 | 1.39941100 | 2.63963000 |
| C | -10.11560200 | 0.68968300 | -0.92204300 |
| C | -7.76176800 | -0.23128100 | -0.60954200 |
| H | -9.44241300 | -0.63435900 | 0.63380700 |
| C | -8.66310500 | 4.23303700 | 1.84117300 |
| C | -7.62349200 | 3.35138500 | -0.29259100 |
| H | -9.73282900 | 3.27376600 | 0.22147200 |
| C | -10.97132700 | 0.08664000 | 2.61612400 |
| C | -9.67214300 | 1.68387500 | 4.07614000 |
| H | -10.84126100 | 2.21549800 | 2.32553700 |
| C | -10.41286400 | -0.42882600 | -1.93180300 |
| H | -9.75383500 | 1.57677100 | -1.46972700 |
| H | -11.04149300 | 0.99714700 | -0.40825000 |
| C | -8.07103600 | -1.34482900 | -1.61891000 |
| H | -7.28406800 | 0.61104500 | -1.13682500 |
| H | -7.03350600 | -0.57424300 | 0.14405700 |
| C | -8.61563700 | 5.65528100 | 1.26747800 |
| H | -7.74794200 | 4.04213800 | 2.43206500 |
| H | -9.51247800 | 4.14931100 | 2.53626700 |
| C | -7.57654400 | 4.77862600 | -0.85328600 |
| H | -6.66460600 | 3.11353700 | 0.20439400 |
| H | -7.73001000 | 2.63655600 | -1.12166600 |
| C | -12.13016300 | 0.12674900 | 3.62402300 |
| H | -10.30295200 | -0.75777400 | 2.86580100 |
| H | -11.37286000 | -0.11064900 | 1.61071000 |
| C | -10.82906900 | 1.72829400 | 5.08045900 |
| H | -8.96181100 | 0.88566200 | 4.35934800 |
| H | -9.09526700 | 2.62033500 | 4.11405600 |
| C | -9.13451200 | -0.90497900 | -2.63329900 |
| H | -11.15298300 | -0.08040400 | -2.67153000 |
| H | -10.87574600 | -1.28053500 | -1.40017300 |
| H | -7.14629900 | -1.64992600 | -2.13624400 |
| H | -8.43499800 | -2.23519900 | -1.07371500 |
| C | -7.47128000 | 5.82149200 | 0.26335300 |
| H | -8.51961200 | 6.38246900 | 2.09090200 |
| H | -9.57586900 | 5.87395300 | 0.76474500 |
| H | -6.73088500 | 4.87244600 | -1.55474700 |
| H | -8.49466800 | 4.96552900 | -1.44046800 |
| C | -11.64480800 | 0.43151800 | 5.04524300 |
| H | -12.67583000 | -0.83133500 | 3.59838200 |
| H | -12.84921300 | 0.90588900 | 3.31032900 |
| H | -10.43659600 | 1.91250700 | 6.09430000 |
| H | -11.48756700 | 2.58276100 | 4.83742500 |
| H | -9.36421900 | -1.72800900 | -3.33039600 |
| H | -8.72967200 | -0.07810100 | -3.24601000 |
| H | -7.47155300 | 6.84057000 | -0.15800000 |
| H | -6.50649200 | 5.69568900 | 0.78817300 |
| H | -12.50044300 | 0.49247100 | 5.73828900 |
| H | -11.01128400 | -0.40282400 | 5.39838800 |
| Cu | -6.70930400 | 1.11559900 | 2.48473900 |
| H | -5.34066600 | 0.90186300 | 3.16451000 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -2687.313561
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -2688.733196

**B-3**
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.231324 (Hartree/Particle)
Thermal correction to Energy= 0.242723
Thermal correction to Enthalpy= 0.243667
Thermal correction to Gibbs Free Energy= 0.192235
Sum of electronic and zero-point Energies= -595.424997

Sum of electronic and thermal Energies= -595.413598
Sum of electronic and thermal Enthalpies= -595.412654
Sum of electronic and thermal Free Energies= -595.464087

| | | | |
|---|---|---|---|
| C | 0.20822402 | -3.08812667 | -0.01752813 |
| C | 1.60338402 | -3.08812667 | -0.01752813 |
| C | 2.30092202 | -1.88037567 | -0.01752813 |
| C | 1.60326802 | -0.67186667 | -0.01872713 |
| C | 0.20844302 | -0.67194467 | -0.01920613 |
| C | -0.48915798 | -1.88015067 | -0.01821013 |
| H | -0.34153498 | -4.04044367 | -0.01707813 |
| H | 2.15289202 | -4.04063967 | -0.01621313 |
| H | 3.40060202 | -1.88029567 | -0.01689413 |
| H | -0.34167898 | 0.28033633 | -0.02015913 |
| H | -1.58876198 | -1.87996767 | -0.01839013 |
| C | 2.37377210 | 0.66152130 | -0.01880975 |
| H | 3.44376877 | 0.65899798 | -0.01794682 |
| N | 1.73183948 | 1.78460733 | -0.01991884 |
| C | 2.40570589 | 2.94017658 | -0.01766960 |
| H | 3.02317442 | 2.99468043 | -0.88982896 |
| H | 3.01903207 | 2.99369561 | 0.85746851 |
| C | 1.41005648 | 4.11502950 | -0.01936733 |
| C | 0.95655099 | 4.64683637 | 1.18772105 |
| C | 0.96208438 | 4.64779385 | -1.22845502 |
| C | 0.05471900 | 5.71133970 | 1.18595111 |
| H | 1.30983997 | 4.22719683 | 2.14073332 |
| C | 0.06010360 | 5.71173195 | -1.23030316 |
| H | 1.32014265 | 4.22855228 | -2.18003528 |
| C | -0.39397314 | 6.24341223 | -0.02268280 |
| H | -0.30321900 | 6.12987883 | 2.13776369 |
| H | -0.29376909 | 6.13145524 | -2.18314250 |
| H | -1.10529034 | 7.08205529 | -0.02415871 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -595.5515182
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -596.3014042

**[Si]-H**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.129476 (Hartree/Particle)
Thermal correction to Energy= 0.139432
Thermal correction to Enthalpy= 0.140376
Thermal correction to Gibbs Free Energy= 0.093337
Sum of electronic and zero-point Energies= -559.959068
Sum of electronic and thermal Energies= -559.949112
Sum of electronic and thermal Enthalpies= -559.948168
Sum of electronic and thermal Free Energies= -559.995207

| | | | |
|---|---|---|---|
| Si | -7.72559635 | 7.37652277 | 1.77112694 |
| H | -7.23558787 | 8.06948103 | 2.97137713 |
| O | -9.55559635 | 7.37654531 | 1.77112694 |
| O | -7.11561729 | 5.65117482 | 1.77112694 |
| C | -10.03295191 | 8.72451849 | 1.77112639 |
| H | -11.10294998 | 8.72397200 | 1.76916999 |
| H | -9.67814067 | 9.22853777 | 2.64575405 |
| H | -9.67494703 | 9.22966856 | 0.89845468 |
| C | -5.68561987 | 5.65043834 | 1.76851313 |
| H | -5.32947197 | 4.64144944 | 1.76881714 |
| H | -5.33029258 | 6.15383042 | 0.89373377 |
| H | -5.32709743 | 6.15548409 | 2.64103273 |
| C | -7.07891849 | 8.29103911 | 0.18712327 |
| H | -6.00891864 | 8.29152008 | 0.18740885 |
| H | -7.43512569 | 7.78631091 | -0.68652762 |
| H | -7.43603848 | 9.29968436 | 0.18683746 |
| Si | -7.72559635 | 7.37652277 | 1.77112694 |
| H | -7.23558787 | 8.06948103 | 2.97137713 |
| O | -9.55559635 | 7.37654531 | 1.77112694 |
| O | -7.11561729 | 5.65117482 | 1.77112694 |
| C | -10.03295191 | 8.72451849 | 1.77112639 |
| H | -11.10294998 | 8.72397200 | 1.76916999 |
| H | -9.67814067 | 9.22853777 | 2.64575405 |
| H | -9.67494703 | 9.22966856 | 0.89845468 |
| C | -5.68561987 | 5.65043834 | 1.76851313 |
| H | -5.32947197 | 4.64144944 | 1.76881714 |
| H | -5.33029258 | 6.15383042 | 0.89373377 |
| H | -5.32709743 | 6.15548409 | 2.64103273 |
| C | -7.07891849 | 8.29103911 | 0.18712327 |
| H | -6.00891864 | 8.29152008 | 0.18740885 |
| H | -7.43512569 | 7.78631091 | -0.68652762 |
| H | -7.43603848 | 9.29968436 | 0.18683746 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -560.0115474
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -560.524137

**[Si]-OR**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.247875 (Hartree/Particle)
Thermal correction to Energy= 0.264332
Thermal correction to Enthalpy= 0.265276
Thermal correction to Gibbs Free Energy= 0.202064
Sum of electronic and zero-point Energies= -792.217774
Sum of electronic and thermal Energies= -792.201317
Sum of electronic and thermal Enthalpies= -792.200373
Sum of electronic and thermal Free Energies= -792.263585

| | | | |
|---|---|---|---|
| Si | -7.72559635 | 7.37652277 | 1.77112694 |
| O | -9.55559635 | 7.37654531 | 1.77112694 |
| O | -7.11561729 | 5.65117482 | 1.77112694 |
| C | -10.03295191 | 8.72451849 | 1.77112639 |
| H | -11.10294998 | 8.72397200 | 1.76916999 |
| H | -9.67814067 | 9.22853777 | 2.64575405 |
| H | -9.67494703 | 9.22966856 | 0.89845468 |
| C | -5.68561987 | 5.65043834 | 1.76851313 |
| H | -5.32947197 | 4.64144944 | 1.76881714 |
| H | -5.33029258 | 6.15383042 | 0.89373377 |
| H | -5.32709743 | 6.15548409 | 2.64103273 |
| C | -7.07891849 | 8.29103911 | 0.18712327 |
| H | -6.00891864 | 8.29152008 | 0.18740885 |
| H | -7.43512569 | 7.78631091 | -0.68652762 |
| H | -7.43603848 | 9.29968436 | 0.18683746 |
| O | -7.11558579 | 8.23918510 | 3.26531596 |
| C | -7.50200826 | 7.50628511 | 4.43083528 |
| C | -6.98852162 | 8.23289485 | 5.68780376 |
| H | -7.40927062 | 9.21585905 | 5.72844424 |
| H | -7.27797380 | 7.68469184 | 6.55992239 |
| H | -5.92154738 | 8.30298564 | 5.64839250 |
| C | -9.03761387 | 7.40494621 | 4.48780750 |
| H | -9.46794099 | 8.14443174 | 3.84525033 |
| H | -9.34299698 | 6.43132798 | 4.16576913 |
| H | -9.36884995 | 7.56866814 | 5.49198765 |
| C | -6.89603635 | 6.09173765 | 4.37206868 |
| H | -7.63115357 | 5.40355720 | 4.01025333 |
| H | -6.05288863 | 6.09200091 | 3.71328051 |
| H | -6.58303458 | 5.79682032 | 5.35184093 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -792.339444
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -793.1682918

**[Cu]-OR**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.608685 (Hartree/Particle)
Thermal correction to Energy= 0.637351
Thermal correction to Enthalpy= 0.638296
Thermal correction to Gibbs Free Energy= 0.547703
Sum of electronic and zero-point Energies= -2919.356235
Sum of electronic and thermal Energies= -2919.327569
Sum of electronic and thermal Enthalpies= -2919.326624
Sum of electronic and thermal Free Energies= -2919.417217

| | | | |
|---|---|---|---|
| P | -8.68811700 | 1.44905100 | 1.47485000 |
| C | -9.05026700 | 0.24450000 | 0.09398200 |
| C | -8.75973000 | 3.16459800 | 0.73266200 |
| C | -10.16568000 | 1.39941100 | 2.63963000 |
| C | -10.11560200 | 0.68968300 | -0.92204300 |
| C | -7.76176800 | -0.23128100 | -0.60954200 |
| H | -9.44241300 | -0.63435900 | 0.63380700 |
| C | -8.66310500 | 4.23303700 | 1.84117300 |
| C | -7.62349200 | 3.35138500 | -0.29259100 |
| H | -9.73282900 | 3.27376600 | 0.22147200 |
| C | -10.97132700 | 0.08664000 | 2.61612400 |
| C | -9.67214300 | 1.68387500 | 4.07614000 |
| H | -10.84126100 | 2.21549800 | 2.32553700 |
| C | -10.41286400 | -0.42882600 | -1.93180300 |
| H | -9.75383500 | 1.57677100 | -1.46972700 |
| H | -11.04149300 | 0.99714700 | -0.40825000 |
| C | -8.07103600 | -1.34482900 | -1.61891000 |
| H | -7.28406800 | 0.61104500 | -1.13682500 |
| H | -7.03350600 | -0.57424300 | 0.14405700 |
| C | -8.61563700 | 5.65528100 | 1.26747800 |
| H | -7.74794200 | 4.04213800 | 2.43206500 |
| H | -9.51247800 | 4.14931100 | 2.53626700 |
| C | -7.57654400 | 4.77862600 | -0.85328600 |
| H | -6.66460600 | 3.11353700 | 0.20439400 |
| H | -7.73001000 | 2.63655600 | -1.12166600 |
| C | -12.13016300 | 0.12674900 | 3.62402300 |
| H | -10.30295200 | -0.75777400 | 2.86580100 |
| H | -11.37286000 | -0.11064900 | 1.61071000 |
| C | -10.82906900 | 1.72829400 | 5.08045900 |
| H | -8.96181100 | 0.88566200 | 4.35934800 |
| H | -9.09526700 | 2.62033500 | 4.11405600 |
| C | -9.13451200 | -0.90497900 | -2.63329900 |
| H | -11.15298300 | -0.08040400 | -2.67153000 |
| H | -10.87574600 | -1.28053500 | -1.40017300 |
| H | -7.14629900 | -1.64992600 | -2.13624400 |
| H | -8.43499800 | -2.23519900 | -1.07371500 |
| C | -7.47128000 | 5.82149200 | 0.26335300 |
| H | -8.51961200 | 6.38246900 | 2.09090200 |
| H | -9.57586900 | 5.87395300 | 0.76474500 |
| H | -6.73088500 | 4.87244600 | -1.55474700 |
| H | -8.49466800 | 4.96552900 | -1.44046800 |
| C | -11.64480800 | 0.43151800 | 5.04524300 |
| H | -12.67583000 | -0.83133500 | 3.59838200 |
| H | -12.84921300 | 0.90588900 | 3.31032900 |
| H | -10.43659600 | 1.91250700 | 6.09430000 |
| H | -11.48756700 | 2.58276100 | 4.83742500 |
| H | -9.36421900 | -1.72800900 | -3.33039600 |
| H | -8.72967200 | -0.07810100 | -3.24601000 |
| H | -7.47155300 | 6.84057000 | -0.15800000 |
| H | -6.50649200 | 5.69568900 | 0.78817300 |
| H | -12.50044300 | 0.49247100 | 5.73828900 |
| H | -11.01128400 | -0.40282400 | 5.39838800 |
| Cu | -6.70930400 | 1.11559900 | 2.48473900 |
| O | -5.08612915 | 0.86211276 | 3.29093260 |
| C | -4.96527355 | -0.50213138 | 3.70218902 |
| C | -6.09249694 | -0.81032632 | 4.66488586 |
| C | -5.05959324 | -1.37995344 | 2.47222864 |
| C | -3.62283933 | -0.67732586 | 4.38005160 |
| H | -6.03359671 | -0.14353278 | 5.55840414 |
| H | -7.08054428 | -0.65479854 | 4.16888148 |
| H | -6.03372026 | -1.87045617 | 5.01066968 |
| H | -4.24189704 | -1.13151417 | 1.75380999 |
| H | -4.96906620 | -2.45724760 | 2.75182429 |
| H | -6.04064813 | -1.22887953 | 1.96117674 |
| H | -3.48929488 | -1.73327057 | 4.71785613 |
| H | -2.79533216 | -0.42472473 | 3.67444514 |
| H | -3.54743542 | -0.00912278 | 5.27128455 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -2919.63165

B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -2921.356927

**tBuOH**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.135049 (Hartree/Particle)
Thermal correction to Energy= 0.141632
Thermal correction to Enthalpy= 0.142576
Thermal correction to Gibbs Free Energy= 0.106228
Sum of electronic and zero-point Energies= -233.381645
Sum of electronic and thermal Energies= -233.375061
Sum of electronic and thermal Enthalpies= -233.374117
Sum of electronic and thermal Free Energies= -233.410465

| | | | |
|---|---|---|---|
| C | -4.96527355 | -0.50213138 | 3.70218902 |
| C | -6.09249694 | -0.81032632 | 4.66488586 |
| C | -5.05959324 | -1.37995344 | 2.47222864 |
| C | -3.62283933 | -0.67732586 | 4.38005160 |
| H | -6.03359671 | -0.14353278 | 5.55840414 |
| H | -7.08054428 | -0.65479854 | 4.16888148 |
| H | -6.03372026 | -1.87045617 | 5.01066968 |
| H | -4.24189704 | -1.13151417 | 1.75380999 |
| H | -4.96906620 | -2.45724760 | 2.75182429 |
| H | -6.04064813 | -1.22887953 | 1.96117674 |
| H | -3.48929488 | -1.73327057 | 4.71785613 |
| H | -2.79533216 | -0.42472473 | 3.67444514 |
| H | -3.54743542 | -0.00912278 | 5.27128455 |
| O | -5.08612915 | 0.86211276 | 3.29093260 |
| H | -5.93285487 | 0.99240792 | 2.85771357 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -233.4673658
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -233.7890572

**v-3**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.940807 (Hartree/Particle)
Thermal correction to Energy= 0.988672
Thermal correction to Enthalpy= 0.989616
Thermal correction to Gibbs Free Energy= 0.854147
Sum of electronic and zero-point Energies= -3951.060126
Sum of electronic and thermal Energies= -3951.012261
Sum of electronic and thermal Enthalpies= -3951.011317
Sum of electronic and thermal Free Energies= -3951.146786

| | | | |
|---|---|---|---|
| C | 0.20822402 | -3.08812667 | -0.01752813 |
| C | 1.60338402 | -3.08812667 | -0.01752813 |
| C | 2.30092202 | -1.88037567 | -0.01752813 |
| C | 1.60326802 | -0.67186667 | -0.01872713 |
| C | 0.20844302 | -0.67194467 | -0.01920613 |
| C | -0.48915798 | -1.88015067 | -0.01821013 |
| H | -0.34153498 | -4.04044367 | -0.01707813 |
| H | 2.15289202 | -4.04063967 | -0.01621313 |
| H | 3.40060202 | -1.88029567 | -0.01689413 |
| H | -0.34167898 | 0.28033633 | -0.02015913 |
| H | -1.58876198 | -1.87996767 | -0.01839013 |
| C | 2.37377210 | 0.66152130 | -0.01880975 |
| H | 3.44376877 | 0.65899798 | -0.01794682 |
| N | 1.73183948 | 1.78460733 | -0.01991884 |
| C | 2.40570589 | 2.94017658 | -0.01766960 |
| H | 3.02317442 | 2.99468043 | -0.88982896 |
| H | 3.01903207 | 2.99369561 | 0.85746851 |
| C | 1.41005648 | 4.11502950 | -0.01936733 |
| C | 0.95655099 | 4.64683637 | 1.18772105 |
| C | 0.96208438 | 4.64779385 | -1.22845502 |
| C | 0.05471900 | 5.71133970 | 1.18595111 |
| H | 1.30983997 | 4.22719683 | 2.14073332 |
| C | 0.06010360 | 5.71173195 | -1.23030316 |
| H | 1.32014265 | 4.22855228 | -2.18003528 |
| C | -0.39397314 | 6.24341223 | -0.02268280 |

| | | | |
|---|---|---|---|
| H | -0.30321900 | 6.12987883 | 2.13776369 |
| H | -0.29376909 | 6.13145524 | -2.18314250 |
| H | -1.10529034 | 7.08205529 | -0.02415871 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3951.487773
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3954.495183

**TS-iii'-iv-3** ***cis (R,R,S)***
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.937494 (Hartree/Particle)
Thermal correction to Energy= 0.985041
Thermal correction to Enthalpy= 0.985985
Thermal correction to Gibbs Free Energy= 0.853692
Sum of electronic and zero-point Energies= -3951.036531
Sum of electronic and thermal Energies= -3950.988984
Sum of electronic and thermal Enthalpies= -3950.988040
Sum of electronic and thermal Free Energies= -3951.120333

| | | | |
|---|---|---|---|
| O | -1.94214900 | 5.68924800 | 2.43525700 |
| C | -1.13003200 | 5.86515500 | 1.26458800 |
| C | -2.00824900 | 5.32261400 | 0.12812900 |
| H | -0.22065300 | 5.25350500 | 1.37290000 |
| H | -0.85176800 | 6.92000500 | 1.18653900 |
| N | -2.77525000 | 4.31822200 | 0.89198700 |
| C | -2.76142400 | 4.62780900 | 2.21367400 |
| O | -3.36411400 | 4.09577300 | 3.13237200 |
| C | -3.35353100 | 3.14351800 | 0.29760800 |
| H | -2.86151400 | 2.92188800 | -0.65222100 |
| C | -4.75801200 | 2.88787400 | 0.36178900 |
| H | -5.07580100 | 2.08832700 | -0.31943600 |
| C | -5.67286000 | 3.32627500 | 1.27732800 |
| H | -6.69948900 | 2.95729000 | 1.24266900 |
| H | -5.47249400 | 4.16859700 | 1.93874600 |
| Cu | -4.52591500 | 2.14423900 | 3.43323600 |
| P | -5.52410400 | 2.46763800 | 5.39791000 |
| C | -5.35166800 | 4.21286000 | 6.06008400 |
| C | -7.39070300 | 2.18863500 | 5.38312300 |
| C | -4.84737900 | 1.32864400 | 6.71941200 |
| C | -5.96084900 | 5.20219100 | 5.04352300 |
| C | -3.87388900 | 4.55390600 | 6.34475100 |
| H | -5.92412400 | 4.27404100 | 7.00401100 |
| C | -7.82685000 | 0.80044200 | 5.88715000 |
| C | -7.91071600 | 2.40666200 | 3.94589300 |
| H | -7.83494400 | 2.95446900 | 6.04495200 |
| C | -5.18435100 | 1.69698600 | 8.17405200 |
| C | -3.33770800 | 1.06908800 | 6.53813000 |
| H | -5.34184800 | 0.37124500 | 6.48314800 |
| C | -5.73594700 | 6.66749500 | 5.43711900 |
| H | -5.49276400 | 5.01474500 | 4.06374200 |
| H | -7.04032800 | 5.01596200 | 4.92947700 |
| C | -3.67804800 | 6.02703400 | 6.72774500 |
| H | -3.28306600 | 4.33480400 | 5.44204700 |
| H | -3.48665100 | 3.91678600 | 7.15311400 |
| C | -9.34502000 | 0.60044000 | 5.77227500 |
| H | -7.31882400 | 0.02382800 | 5.29306000 |
| H | -7.52370700 | 0.64903500 | 6.93366000 |
| C | -9.42744400 | 2.21689000 | 3.83992500 |
| H | -7.39979800 | 1.68365700 | 3.28586700 |
| H | -7.62254000 | 3.40095800 | 3.57481200 |
| C | -4.68363100 | 0.61638400 | 9.14392400 |
| H | -4.70708200 | 2.65721100 | 8.43332000 |
| H | -6.26914600 | 1.84783800 | 8.29835600 |
| C | -2.84384600 | -0.00320700 | 7.51724200 |
| H | -2.76610700 | 1.99765900 | 6.69843200 |
| H | -3.14736800 | 0.76345300 | 5.49799600 |
| C | -4.25056300 | 6.96559600 | 5.66168200 |
| H | -6.15220000 | 7.32566500 | 4.65561100 |
| H | -6.29508200 | 6.88884700 | 6.36558300 |
| H | -2.60409400 | 6.22556600 | 6.88385000 |
| H | -4.17867300 | 6.22670900 | 7.69398900 |
| C | -9.84693400 | 0.83243900 | 4.34361000 |
| H | -9.60752700 | -0.41558800 | 6.11319200 |
| H | -9.85665000 | 1.30352800 | 6.45570300 |
| H | -9.74892000 | 2.36417800 | 2.79493400 |
| H | -9.93687900 | 2.99515000 | 4.43832600 |
| C | -3.18139600 | 0.35963700 | 8.96894700 |
| H | -4.90673300 | 0.90894200 | 10.18390700 |
| H | -5.23732600 | -0.32182600 | 8.95457200 |
| H | -1.75742500 | -0.15117800 | 7.39756500 |
| H | -3.32233600 | -0.96711400 | 7.26516200 |
| H | -4.10786800 | 8.01934300 | 5.95577300 |
| H | -3.69975500 | 6.81719400 | 4.71549000 |
| H | -10.94270400 | 0.71490900 | 4.29523100 |
| H | -9.41355200 | 0.06177500 | 3.68072000 |
| H | -2.84595400 | -0.43766500 | 9.65339400 |
| H | -2.62449100 | 1.27221400 | 9.25228700 |
| C | -2.64096300 | 1.34309400 | 1.38544600 |
| N | -3.58484300 | 0.90409100 | 2.22601700 |
| C | -5.18078700 | -0.91531900 | 2.76476700 |
| C | -4.49029200 | -1.34015900 | 3.91135600 |
| C | -6.52440600 | -1.28892700 | 2.61821200 |
| C | -5.12328400 | -2.12368800 | 4.87924100 |
| H | -3.44863900 | -1.03810100 | 4.03553700 |
| C | -7.16102600 | -2.08068800 | 3.58112800 |
| H | -7.08202100 | -0.95108900 | 1.73967200 |
| C | -6.46217600 | -2.50140700 | 4.71637500 |
| H | -4.56920800 | -2.44436400 | 5.76535900 |
| H | -8.21065900 | -2.35663800 | 3.45017800 |
| H | -6.95915300 | -3.11151600 | 5.47491300 |
| C | -4.47393600 | -0.11541200 | 1.68837900 |
| H | -5.23884300 | 0.32002900 | 1.01758200 |
| H | -3.90094200 | -0.82958600 | 1.05865100 |
| H | -2.51712100 | 0.78301300 | 0.44400100 |
| C | -1.35239600 | 1.90365900 | 1.87093100 |
| C | -0.32660900 | 2.17913500 | 0.94597400 |
| C | -1.10024800 | 2.15772900 | 3.23007800 |
| C | 0.89886500 | 2.70466000 | 1.35864700 |
| H | -0.50075200 | 1.98215500 | -0.11614600 |
| C | 0.12129700 | 2.69198400 | 3.64579700 |
| H | -1.88208100 | 1.94746500 | 3.95920800 |
| C | 1.12745700 | 2.97263000 | 2.71479800 |
| H | 1.67904400 | 2.90869700 | 0.62020900 |
| H | 0.28774500 | 2.89100000 | 4.70794200 |
| H | 2.08270100 | 3.39129200 | 3.04170100 |
| C | -2.89997700 | 6.34100000 | -0.59197600 |
| C | -2.66179900 | 7.72265400 | -0.53723300 |
| C | -3.98226400 | 5.88952600 | -1.36961300 |
| C | -3.48105800 | 8.62604900 | -1.22480500 |
| H | -1.82961500 | 8.12302700 | 0.04276700 |
| C | -4.80204300 | 6.78839300 | -2.05455200 |
| H | -4.19787800 | 4.82329100 | -1.42988900 |
| C | -4.55643900 | 8.16402100 | -1.98542200 |
| H | -3.27312200 | 9.69719400 | -1.15988100 |
| H | -5.63980000 | 6.40950800 | -2.64570600 |
| H | -5.19803000 | 8.86826500 | -2.52103900 |
| H | -1.38403000 | 4.79992800 | -0.61495800 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3951.470792
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3954.466648

**TS-iii'-iv-3** ***cis (S,R,S)***
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.937558 (Hartree/Particle)
Thermal correction to Energy= 0.985153
Thermal correction to Enthalpy= 0.986098
Thermal correction to Gibbs Free Energy= 0.853680
Sum of electronic and zero-point Energies= -3951.027701

Sum of electronic and thermal Energies= -3950.980106
Sum of electronic and thermal Enthalpies= -3950.979162
Sum of electronic and thermal Free Energies= -3951.111579

| | | | |
|---|---|---|---|
| O | -4.65723700 | 3.92176800 | -3.30627200 |
| C | -3.61531000 | 2.94783000 | -3.31054400 |
| C | -4.34299600 | 1.58765300 | -3.36355000 |
| H | -3.02550600 | 3.04457600 | -2.38360600 |
| H | -2.96180000 | 3.11999400 | -4.17647800 |
| N | -5.64424100 | 1.96911300 | -2.81202500 |
| C | -5.84285800 | 3.33192600 | -2.97026300 |
| O | -6.86197900 | 3.96328900 | -2.85662100 |
| C | -6.76254000 | 1.05317700 | -2.75661000 |
| H | -7.11143700 | 0.76074300 | -3.75444900 |
| C | -7.79315600 | 1.31238800 | -1.80916300 |
| H | -8.77192900 | 0.89799800 | -2.07533500 |
| C | -7.64813000 | 1.83323100 | -0.54326700 |
| H | -8.53590600 | 2.08716400 | 0.03915700 |
| H | -6.72557300 | 2.35354500 | -0.26571300 |
| Cu | -7.30035500 | -0.20414300 | 0.47739300 |
| P | -8.76016800 | -0.61245400 | 2.11705200 |
| C | -9.06365700 | 0.86042100 | 3.24788200 |
| C | -10.46322400 | -1.07648000 | 1.45700400 |
| C | -8.29206500 | -2.02106300 | 3.27271000 |
| C | -10.15213800 | 1.84486700 | 2.77914900 |
| C | -7.73329600 | 1.61703300 | 3.44304500 |
| H | -9.39089600 | 0.44518800 | 4.21805100 |
| C | -10.67390700 | -2.57882900 | 1.18724700 |
| C | -10.74408800 | -0.28009600 | 0.16432700 |
| H | -11.18917500 | -0.77603000 | 2.23384000 |
| C | -7.41782000 | -1.61564000 | 4.47406400 |
| C | -7.56553400 | -3.11920500 | 2.46697000 |
| H | -9.24051700 | -2.42612400 | 3.66976900 |
| C | -10.30570000 | 3.00959800 | 3.76875500 |
| H | -9.87745700 | 2.25490400 | 1.79245300 |
| H | -11.12087700 | 1.33800700 | 2.65598900 |
| C | -7.87595200 | 2.79039800 | 4.41880000 |
| H | -7.40605500 | 1.98843100 | 2.45545300 |
| H | -6.93926100 | 0.93905100 | 3.78156400 |
| C | -12.08367600 | -2.85552900 | 0.64348300 |
| H | -9.93339700 | -2.92336700 | 0.44675500 |
| H | -10.51209200 | -3.17225300 | 2.09923200 |
| C | -12.15027200 | -0.55076800 | -0.38285600 |
| H | -9.99155400 | -0.57439800 | -0.58791700 |
| H | -10.60651200 | 0.79787600 | 0.32419800 |
| C | -7.09757300 | -2.83013700 | 5.35853100 |
| H | -6.47324700 | -1.18261200 | 4.10614600 |
| H | -7.91234600 | -0.84458200 | 5.08378200 |
| C | -7.24466200 | -4.34084400 | 3.33658600 |
| H | -6.63201300 | -2.68528700 | 2.06745500 |
| H | -8.15340500 | -3.42797300 | 1.59107700 |
| C | -8.98234300 | 3.75410900 | 3.97749800 |
| H | -11.08526700 | 3.70110200 | 3.40777000 |
| H | -10.66001500 | 2.61455100 | 4.73882400 |
| H | -6.91233000 | 3.31986000 | 4.50776000 |
| H | -8.11237000 | 2.39694500 | 5.42488000 |
| C | -12.37554000 | -2.04637200 | -0.62494000 |
| H | -12.19729700 | -3.93519500 | 0.44806300 |
| H | -12.82629600 | -2.59717900 | 1.42083800 |
| H | -12.30173600 | 0.01957700 | -1.31436800 |
| H | -12.89892900 | -0.17779300 | 0.34054300 |
| C | -6.41626100 | -3.95024700 | 4.56493400 |
| H | -6.45952200 | -2.51383900 | 6.20114200 |
| H | -8.03609200 | -3.21260600 | 5.80108000 |
| H | -6.71057400 | -5.09574200 | 2.73537800 |
| H | -8.19042600 | -4.81140000 | 3.66403000 |
| H | -9.10821700 | 4.56478000 | 4.71451900 |
| H | -8.68493300 | 4.23425600 | 3.02716800 |
| H | -13.40553300 | -2.23312700 | -0.97189400 |
| H | -11.70259000 | -2.38382600 | -1.43342500 |
| H | -6.24124000 | -4.82777900 | 5.20991100 |
| H | -5.42576000 | -3.59798300 | 4.22970000 |
| C | -6.01189600 | -0.79814300 | -2.02702600 |
| N | -5.81589200 | -0.71793000 | -0.69771100 |
| C | -7.04119700 | -1.71866300 | -2.59333900 |
| C | -7.07822300 | -1.93352100 | -3.98611100 |
| C | -7.97557900 | -2.39890200 | -1.79555300 |
| C | -8.02865600 | -2.77878700 | -4.55955300 |
| H | -6.34982300 | -1.42516500 | -4.62424500 |
| C | -8.92697100 | -3.24908900 | -2.36831700 |
| H | -7.93942100 | -2.27402800 | -0.71137500 |
| C | -8.96461000 | -3.43916000 | -3.75289600 |
| H | -8.03798400 | -2.92593200 | -5.64288400 |
| H | -9.63976600 | -3.77391800 | -1.72698300 |
| H | -9.71038700 | -4.10154400 | -4.19971700 |
| H | -5.11588000 | -0.76948000 | -2.66103500 |
| C | -4.54717400 | -0.12268200 | -0.28916300 |
| H | -4.53518200 | 0.96704000 | -0.48541600 |
| H | -3.71132100 | -0.55749300 | -0.87403600 |
| C | -4.26880100 | -0.34923500 | 1.18012400 |
| C | -3.85270300 | -1.60967300 | 1.63786000 |
| C | -4.44414800 | 0.68024900 | 2.11505100 |
| C | -3.59361200 | -1.82812500 | 2.99267900 |
| H | -3.72785800 | -2.42285300 | 0.91749300 |
| C | -4.19314000 | 0.46487300 | 3.47546500 |
| H | -4.78441700 | 1.66108900 | 1.77185000 |
| C | -3.76278500 | -0.78930800 | 3.91718500 |
| H | -3.25525600 | -2.81078500 | 3.33105000 |
| H | -4.33536500 | 1.27935400 | 4.19040800 |
| H | -3.56434000 | -0.96123000 | 4.97813200 |
| C | -4.43287100 | 0.95827000 | -4.74552500 |
| C | -3.69428400 | -0.19592400 | -5.03920500 |
| C | -5.25935200 | 1.50435400 | -5.74023400 |
| C | -3.77800000 | -0.79890400 | -6.29878500 |
| H | -3.05519800 | -0.63705200 | -4.26871000 |
| C | -5.34746300 | 0.90351900 | -6.99830400 |
| H | -5.85417900 | 2.39612100 | -5.52795400 |
| C | -4.60848200 | -0.25161900 | -7.28104000 |
| H | -3.20064300 | -1.70282900 | -6.50858200 |
| H | -6.00098400 | 1.33544100 | -7.76038200 |
| H | -4.68367800 | -0.72455800 | -8.26339200 |
| H | -3.82996300 | 0.88487600 | -2.69652000 |

**TS-iii'-iv-3** ***trans (R,R,S)***
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.936337 (Hartree/Particle)
Thermal correction to Energy= 0.984301
Thermal correction to Enthalpy= 0.985245
Thermal correction to Gibbs Free Energy= 0.850080
Sum of electronic and zero-point Energies= -3951.035706
Sum of electronic and thermal Energies= -3950.987742
Sum of electronic and thermal Enthalpies= -3950.986798
Sum of electronic and thermal Free Energies= -3951.121963

| | | | |
|---|---|---|---|
| O | -0.00147600 | 6.73280500 | 0.15896400 |
| C | -0.00018700 | 5.97968700 | -1.05236400 |
| C | -1.31715400 | 5.18387000 | -1.01762800 |
| H | 0.88070300 | 5.31736900 | -1.06584300 |
| H | 0.05840300 | 6.66504500 | -1.90872500 |
| N | -1.56635200 | 5.16618100 | 0.42863900 |
| C | -0.88126600 | 6.17675800 | 1.05222900 |
| O | -0.99458600 | 6.59109400 | 2.18109100 |
| C | -2.68714300 | 4.44895900 | 0.96702300 |
| H | -3.17273000 | 3.88223400 | 0.16848600 |
| C | -3.57941100 | 5.05175200 | 1.90417200 |
| H | -3.17776900 | 5.85564100 | 2.52640000 |
| C | -4.82955500 | 4.54340300 | 2.19785300 |
| H | -5.33603900 | 3.87734400 | 1.48737900 |
| H | -5.48249000 | 5.09560900 | 2.87786500 |
| Cu | -4.32672100 | 2.79355300 | 3.58406500 |
| P | -5.44442800 | 2.54641600 | 5.49058000 |
| C | -5.38831300 | 4.01892100 | 6.64529100 |

| | | | |
|---|---|---|---|
| C | -7.28703200 | 2.24121200 | 5.24207000 |
| C | -4.79586000 | 1.08575300 | 6.46327100 |
| C | -6.13752100 | 5.22767700 | 6.05018000 |
| C | -3.93061700 | 4.40478900 | 6.96382100 |
| H | -5.89545700 | 3.72169500 | 7.58067500 |
| C | -7.69607500 | 0.75717600 | 5.27049100 |
| C | -7.71310300 | 2.87723500 | 3.90010400 |
| H | -7.81130200 | 2.75785500 | 6.06623900 |
| C | -5.21317700 | 1.01101000 | 7.94050500 |
| C | -3.27268300 | 0.90205000 | 6.30513700 |
| H | -5.25332300 | 0.23476600 | 5.93055900 |
| C | -6.04559800 | 6.46096400 | 6.95916900 |
| H | -5.69604500 | 5.46583400 | 5.06662500 |
| H | -7.19598300 | 4.98277800 | 5.87334900 |
| C | -3.84389300 | 5.63876000 | 7.87067200 |
| H | -3.40966200 | 4.61804900 | 6.01420200 |
| H | -3.39831900 | 3.56354700 | 7.43146100 |
| C | -9.19453800 | 0.57646500 | 4.98735400 |
| H | -7.11905000 | 0.20596800 | 4.51023400 |
| H | -7.45634600 | 0.30400900 | 6.24408700 |
| C | -9.21045300 | 2.70034000 | 3.62665100 |
| H | -7.12989600 | 2.39668300 | 3.09359700 |
| H | -7.44376200 | 3.94337800 | 3.87127600 |
| C | -4.75468900 | -0.31348700 | 8.56959200 |
| H | -4.75367800 | 1.84865000 | 8.49400900 |
| H | -6.30433800 | 1.12726400 | 8.04842600 |
| C | -2.82285300 | -0.42403900 | 6.93036000 |
| H | -2.73419000 | 1.73116800 | 6.79395300 |
| H | -3.00207500 | 0.94763700 | 5.23908200 |
| C | -4.59078500 | 6.83089800 | 7.26493300 |
| H | -6.57058700 | 7.30818900 | 6.48704500 |
| H | -6.57509900 | 6.25113500 | 7.90691200 |
| H | -2.78555300 | 5.89306600 | 8.04791900 |
| H | -4.28012300 | 5.39599400 | 8.85723300 |
| C | -9.60806600 | 1.22136100 | 3.66056600 |
| H | -9.43992700 | -0.49911400 | 4.98634800 |
| H | -9.77678700 | 1.03104000 | 5.81037100 |
| H | -9.46649900 | 3.14939100 | 2.65227900 |
| H | -9.78839400 | 3.25404400 | 4.38984100 |
| C | -3.24402900 | -0.52266400 | 8.40245900 |
| H | -5.03221100 | -0.34088300 | 9.63680400 |
| H | -5.29394300 | -1.14672300 | 8.08235000 |
| H | -1.73003000 | -0.53478500 | 6.83276400 |
| H | -3.27582200 | -1.25922200 | 6.36424500 |
| H | -4.54710100 | 7.70025700 | 7.94199700 |
| H | -4.08855300 | 7.13367800 | 6.32778500 |
| H | -10.69277300 | 1.10618900 | 3.49728400 |
| H | -9.10228200 | 0.69402700 | 2.83205600 |
| H | -2.94342700 | -1.49581600 | 8.82562700 |
| H | -2.70722900 | 0.25108600 | 8.98227600 |
| C | -1.98657500 | 2.74205000 | 1.89818800 |
| N | -3.05107900 | 2.01919100 | 2.31664500 |
| C | -4.66211800 | 0.21548900 | 1.84638700 |
| C | -4.25479300 | -0.60642400 | 2.91147600 |
| C | -5.95073100 | 0.04008100 | 1.32346800 |
| C | -5.10644200 | -1.58484800 | 3.42820700 |
| H | -3.25946900 | -0.45929800 | 3.33506900 |
| C | -6.80677600 | -0.94387000 | 1.83408200 |
| H | -6.29003600 | 0.68381500 | 0.50653100 |
| C | -6.38669400 | -1.76137200 | 2.88701200 |
| H | -4.77133200 | -2.21301600 | 4.25816200 |
| H | -7.80785500 | -1.06544500 | 1.41221700 |
| H | -7.05631400 | -2.52408600 | 3.29257400 |
| C | -3.71046800 | 1.24894200 | 1.27638800 |
| H | -4.27499400 | 1.89665200 | 0.57055800 |
| H | -2.96001700 | 0.72555900 | 0.64591900 |
| H | -1.49064900 | 2.39114600 | 0.98054900 |
| C | -1.01955000 | 3.28908100 | 2.88522800 |
| C | 0.29815100 | 3.57842800 | 2.48481600 |
| C | -1.36949800 | 3.55874400 | 4.21997600 |
| C | 1.21433900 | 4.15198300 | 3.36871600 |
| H | 0.60430400 | 3.35593800 | 1.46164900 |
| C | -0.45805000 | 4.12810200 | 5.10867200 |
| H | -2.37265300 | 3.30964200 | 4.57173800 |
| C | 0.83972000 | 4.43776100 | 4.68523400 |
| H | 2.22780000 | 4.37813500 | 3.02654600 |
| H | -0.76468300 | 4.33207200 | 6.13850500 |
| H | 1.55392000 | 4.89132000 | 5.37723000 |
| H | -1.29394667 | 4.21324422 | -1.46734682 |
| C | -2.43460867 | 5.99423241 | -1.70042212 |
| C | -2.42437243 | 7.38757513 | -1.63686562 |
| C | -3.45756227 | 5.33453118 | -2.38216262 |
| C | -3.43695067 | 8.12151613 | -2.25532122 |
| H | -1.61832261 | 7.90759502 | -1.09927299 |
| C | -4.46967241 | 6.06824640 | -3.00089687 |
| H | -3.46559709 | 4.23591846 | -2.43175848 |
| C | -4.45912711 | 7.46220316 | -2.93773126 |
| H | -3.42817593 | 9.22001563 | -2.20568609 |
| H | -5.27575713 | 5.54862000 | -3.53896022 |
| H | -5.25694440 | 8.04065744 | -3.42576275 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3951.468797
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3954.465382

**TS-iii'-iv-3** ***trans (S,S,S)***

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.937435 (Hartree/Particle)
Thermal correction to Energy= 0.985177
Thermal correction to Enthalpy= 0.986121
Thermal correction to Gibbs Free Energy= 0.852879
Sum of electronic and zero-point Energies= -3951.041933
Sum of electronic and thermal Energies= -3950.994191
Sum of electronic and thermal Enthalpies= -3950.993247
Sum of electronic and thermal Free Energies= -3951.126489

| | | | |
|---|---|---|---|
| O | 0.48942800 | 5.81398900 | -0.14737200 |
| C | 0.37704400 | 6.61785200 | -1.32104400 |
| C | -0.94905800 | 6.18968600 | -2.01087900 |
| H | 0.35299000 | 7.67814000 | -1.02564200 |
| H | 1.24910600 | 6.43858700 | -1.96527000 |
| H | -0.73156800 | 5.59166300 | -2.90943900 |
| N | -1.52865100 | 5.33764800 | -0.97850000 |
| C | -0.64375900 | 5.08291500 | 0.03578700 |
| O | -0.78867800 | 4.32149300 | 0.96570100 |
| C | -2.68393500 | 4.50214600 | -1.14596000 |
| H | -3.04194700 | 4.16739300 | -0.16891600 |
| C | -3.68660900 | 4.87690000 | -2.09039300 |
| H | -3.40230500 | 5.55285300 | -2.90114600 |
| C | -4.93316000 | 4.28767400 | -2.17071800 |
| H | -5.33672300 | 3.72810600 | -1.31937700 |
| H | -5.67142500 | 4.69720700 | -2.86249200 |
| Cu | -4.37974100 | 2.47702000 | -3.45588700 |
| P | -5.38968000 | 2.39892900 | -5.44248600 |
| C | -5.25538100 | 4.02047800 | -6.38531900 |
| C | -7.23252600 | 2.03320900 | -5.35575700 |
| C | -4.67362200 | 1.08942700 | -6.57270400 |
| C | -6.26219900 | 5.08844800 | -5.91598900 |
| C | -3.81838000 | 4.56785500 | -6.26934500 |
| H | -5.47161300 | 3.79848300 | -7.44462600 |
| C | -7.57317000 | 0.53375700 | -5.45175000 |
| C | -7.79467600 | 2.61106500 | -4.03761000 |
| H | -7.70915900 | 2.54818300 | -6.20903700 |
| C | -5.09424000 | 1.16482100 | -8.04938800 |
| C | -3.14417800 | 0.95948800 | -6.43914000 |
| H | -5.09213800 | 0.16384600 | -6.14136200 |
| C | -6.08169300 | 6.40686500 | -6.68135300 |
| H | -6.11069200 | 5.28119200 | -4.84044000 |
| H | -7.29655700 | 4.73257600 | -6.03525000 |
| C | -3.63422300 | 5.89616100 | -7.01250100 |

| | | | |
|---|---|---|---|
| H | -3.59227100 | 4.71618600 | -5.19945000 |
| H | -3.09096100 | 3.83063000 | -6.63979500 |
| C | -9.08225400 | 0.28722500 | -5.30676000 |
| H | -7.03806700 | -0.00952800 | -4.65496800 |
| H | -7.23414200 | 0.11440900 | -6.41068000 |
| C | -9.30263800 | 2.37087800 | -3.90174100 |
| H | -7.26386200 | 2.12836100 | -3.19710900 |
| H | -7.57805300 | 3.68567600 | -3.95627100 |
| C | -4.57621700 | -0.05252500 | -8.83019800 |
| H | -4.67573800 | 2.08136900 | -8.50141500 |
| H | -6.19012100 | 1.24126000 | -8.14414300 |
| C | -2.63000600 | -0.25667700 | -7.22003800 |
| H | -2.65163700 | 1.86724400 | -6.82753000 |
| H | -2.86829900 | 0.88562100 | -5.37541200 |
| C | -4.65255100 | 6.94175100 | -6.54862700 |
| H | -6.80863800 | 7.14980600 | -6.31278100 |
| H | -6.31450600 | 6.24109500 | -7.74947600 |
| H | -2.60521900 | 6.26287900 | -6.85916900 |
| H | -3.75095800 | 5.72586800 | -8.09862800 |
| C | -9.64034900 | 0.88104400 | -4.00972900 |
| H | -9.28232900 | -0.79667000 | -5.35212200 |
| H | -9.60536600 | 0.73951400 | -6.16980400 |
| H | -9.65806100 | 2.78031400 | -2.94125500 |
| H | -9.83269600 | 2.92781300 | -4.69674700 |
| C | -3.05573600 | -0.20122000 | -8.69272000 |
| H | -4.86169500 | 0.03184300 | -9.89222200 |
| H | -5.06868600 | -0.96355700 | -8.44321500 |
| H | -1.53222400 | -0.31883800 | -7.13653300 |
| H | -3.03340200 | -1.17666900 | -6.75805400 |
| H | -4.53415800 | 7.87716100 | -7.12098600 |
| H | -4.45458400 | 7.19416900 | -5.49174900 |
| H | -10.73064400 | 0.72447500 | -3.95257900 |
| H | -9.19485600 | 0.35023600 | -3.15086800 |
| H | -2.70847100 | -1.10051500 | -9.22832200 |
| H | -2.56416800 | 0.66259900 | -9.17782300 |
| C | -1.79729200 | 7.37632700 | -2.42799500 |
| C | -2.55503400 | 8.09525500 | -1.49279400 |
| C | -1.80543400 | 7.78135600 | -3.76913800 |
| C | -3.31101600 | 9.19894500 | -1.89448100 |
| H | -2.56430300 | 7.77058900 | -0.44924400 |
| C | -2.55542400 | 8.89137700 | -4.17263000 |
| H | -1.22967200 | 7.21357500 | -4.50596800 |
| C | -3.31248300 | 9.60152700 | -3.23590100 |
| H | -3.90632700 | 9.74613900 | -1.15895500 |
| H | -2.55606800 | 9.19383800 | -5.22264000 |
| H | -3.90648600 | 10.46361800 | -3.54970000 |
| C | -2.06049200 | 2.61589500 | -1.71585100 |
| N | -3.12873100 | 1.86864000 | -2.07817200 |
| C | -4.90779000 | 0.28636100 | -1.45161900 |
| C | -4.63512500 | -0.64933500 | -2.46566900 |
| C | -6.19543700 | 0.31536000 | -0.89862600 |
| C | -5.61758500 | -1.54209400 | -2.89880600 |
| H | -3.63994500 | -0.66037800 | -2.91558700 |
| C | -7.18318100 | -0.57918700 | -1.32876300 |
| H | -6.42818700 | 1.04837600 | -0.12079200 |
| C | -6.89649200 | -1.51314100 | -2.32795500 |
| H | -5.38690800 | -2.26376700 | -3.68715500 |
| H | -8.18118200 | -0.54103400 | -0.88451000 |
| H | -7.66803000 | -2.20803300 | -2.66924800 |
| C | -3.81952700 | 1.22445900 | -0.97020400 |
| H | -4.26896700 | 1.96205400 | -0.27186700 |
| H | -3.10103300 | 0.64231900 | -0.35558600 |
| H | -1.63340800 | 2.40359200 | -0.72467100 |
| C | -1.00701000 | 2.95412400 | -2.70824200 |
| C | 0.31841500 | 3.14957100 | -2.27322700 |
| C | -1.28676600 | 3.15652800 | -4.07109500 |
| C | 1.31230300 | 3.57761400 | -3.15847100 |
| H | 0.56869300 | 2.97369800 | -1.22422000 |
| C | -0.29793900 | 3.57925600 | -4.95934300 |
| H | -2.30173200 | 2.99460000 | -4.43300600 |
| C | 1.00811700 | 3.80685100 | -4.50510700 |
| H | 2.33006600 | 3.73504300 | -2.79147200 |
| H | -0.54962500 | 3.74082000 | -6.01131700 |
| H | 1.78241400 | 4.14849900 | -5.19660800 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3951.475837
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3954.472808

**iii'-3 *trans***

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.937256 (Hartree/Particle)
Thermal correction to Energy= 0.985784
Thermal correction to Enthalpy= 0.986728
Thermal correction to Gibbs Free Energy= 0.852690
Sum of electronic and zero-point Energies= -3951.053687
Sum of electronic and thermal Energies= -3951.005159
Sum of electronic and thermal Enthalpies= -3951.004215
Sum of electronic and thermal Free Energies= -3951.138254

| | | | |
|---|---|---|---|
| O | 4.33438000 | 2.50194100 | 3.57672200 |
| C | 4.22497100 | 3.29491400 | 2.39660700 |
| C | 2.90128100 | 2.85886500 | 1.70421000 |
| H | 4.19825800 | 4.35737600 | 2.68320400 |
| H | 5.10018500 | 3.11260700 | 1.75721000 |
| H | 3.12913000 | 2.28037900 | 0.79702500 |
| N | 2.33138400 | 1.98324800 | 2.72830100 |
| C | 3.21140000 | 1.75595100 | 3.75454700 |
| O | 3.07260700 | 1.00272000 | 4.69073600 |
| C | 1.21387400 | 1.05381700 | 2.53038800 |
| H | 0.79403700 | 0.86026000 | 3.52652500 |
| C | 0.16064300 | 1.57505200 | 1.63176800 |
| H | 0.45035800 | 2.24873500 | 0.82292700 |
| C | -1.11127200 | 1.11674600 | 1.65767600 |
| H | -1.47549400 | 0.48158300 | 2.47072400 |
| H | -1.86016700 | 1.50074200 | 0.96359600 |
| Cu | -0.53468200 | -0.86362900 | 0.28298500 |
| P | -1.56567600 | -0.90864300 | -1.67885500 |
| C | -1.46459800 | 0.71409100 | -2.61746600 |
| C | -3.40486000 | -1.29433100 | -1.60924300 |
| C | -0.81027600 | -2.20529000 | -2.80114900 |
| C | -2.42912900 | 1.78339200 | -2.06911600 |
| C | -0.01718800 | 1.24361600 | -2.58554400 |
| H | -1.75196000 | 0.50537300 | -3.66242900 |
| C | -3.75757600 | -2.78021100 | -1.80835800 |
| C | -3.95696700 | -0.80069400 | -0.25339100 |
| H | -3.88352000 | -0.72095400 | -2.42318600 |
| C | -1.14020800 | -2.07333300 | -4.29681500 |
| C | 0.70534600 | -2.38273800 | -2.58197500 |
| H | -1.27656300 | -3.13194700 | -2.42551100 |
| C | -2.27881600 | 3.11523000 | -2.81713500 |
| H | -2.21288500 | 1.95001800 | -1.00044200 |
| H | -3.47298700 | 1.44148500 | -2.13427800 |
| C | 0.13550500 | 2.58403200 | -3.31361400 |
| H | 0.27687900 | 1.37274200 | -1.53000700 |
| H | 0.67605700 | 0.50433600 | -3.01385000 |
| C | -5.27009300 | -3.01704000 | -1.68122000 |
| H | -3.23050500 | -3.38276600 | -1.04942700 |
| H | -3.42088400 | -3.13394800 | -2.79444200 |
| C | -5.46699900 | -1.03409500 | -0.13032400 |
| H | -3.42894000 | -1.34345500 | 0.55132300 |
| H | -3.72697000 | 0.26466600 | -0.10337800 |
| C | -0.60996200 | -3.28003600 | -5.08560500 |
| H | -0.67021900 | -1.15595300 | -4.69315300 |
| H | -2.22625400 | -1.96153500 | -4.45257700 |
| C | 1.23099200 | -3.58837900 | -3.37192900 |
| H | 1.24555300 | -1.47803100 | -2.90844700 |
| H | 0.91734700 | -2.49724400 | -1.50727100 |
| C | -0.83747400 | 3.63030700 | -2.76238300 |
| H | -2.97231300 | 3.85879800 | -2.39008900 |

| | | | |
|---|---|---|---|
| H | -2.57862700 | 2.97384500 | -3.87192600 |
| H | 1.17684200 | 2.93595400 | -3.22040500 |
| H | -0.05378000 | 2.43756900 | -4.39289200 |
| C | -5.82126700 | -2.50900100 | -0.34491600 |
| H | -5.48504700 | -4.09214000 | -1.80291600 |
| H | -5.78644700 | -2.49810800 | -2.51016400 |
| H | -5.81624900 | -0.69212300 | 0.85840000 |
| H | -5.99292900 | -0.41568600 | -0.88142900 |
| C | 0.89525000 | -3.47553300 | -4.86449600 |
| H | -0.83001000 | -3.15407400 | -6.15901600 |
| H | -1.14834000 | -4.18838700 | -4.75809800 |
| H | 2.31973600 | -3.68481500 | -3.22636100 |
| H | 0.77623500 | -4.51028200 | -2.96466800 |
| H | -0.74286600 | 4.57801100 | -3.31857700 |
| H | -0.57032200 | 3.85464300 | -1.71441900 |
| H | -6.91343300 | -2.65579000 | -0.29913100 |
| H | -5.38313700 | -3.10457100 | 0.47432300 |
| H | 1.24985900 | -4.36730700 | -5.40779400 |
| H | 1.43724700 | -2.61132500 | -5.29173800 |
| C | 2.05314000 | 4.05225100 | 1.30090100 |
| C | 1.31890200 | 4.78215700 | 2.24673600 |
| C | 2.03440300 | 4.46187400 | -0.03918300 |
| C | 0.57595000 | 5.89910900 | 1.85676600 |
| H | 1.31822000 | 4.45638700 | 3.29006100 |
| C | 1.29639300 | 5.58429800 | -0.43135100 |
| H | 2.59250600 | 3.88779900 | -0.78476400 |
| C | 0.56279900 | 6.30447900 | 0.51605400 |
| H | 0.00029300 | 6.45511700 | 2.60128200 |
| H | 1.28693200 | 5.88850600 | -1.48083800 |
| H | -0.02110800 | 7.17681700 | 0.21182000 |
| C | 1.74287800 | -0.48313400 | 2.06110500 |
| N | 0.69560200 | -1.35800100 | 1.68558100 |
| C | -1.05314000 | -2.95584400 | 2.33263400 |
| C | -0.81222800 | -3.90319500 | 1.32012900 |
| C | -2.34257900 | -2.88744400 | 2.88062600 |
| C | -1.82254100 | -4.76553200 | 0.88727600 |
| H | 0.18253200 | -3.94557500 | 0.87096500 |
| C | -3.35976700 | -3.74861600 | 2.44925800 |
| H | -2.55401600 | -2.14586600 | 3.65662700 |
| C | -3.10232300 | -4.69409100 | 1.45321800 |
| H | -1.61287500 | -5.49697500 | 0.10185200 |
| H | -4.35761700 | -3.67418700 | 2.88968700 |
| H | -3.89501200 | -5.36447700 | 1.11112500 |
| C | 0.05792400 | -2.03020200 | 2.79958300 |
| H | -0.38183600 | -1.32993500 | 3.54955200 |
| H | 0.79357000 | -2.63339700 | 3.38068900 |
| H | 2.23467400 | -0.81852400 | 2.99119700 |
| C | 2.82913700 | -0.28655500 | 1.02193200 |
| C | 4.17061400 | -0.16172600 | 1.42332300 |
| C | 2.53200200 | -0.09101800 | -0.33450800 |
| C | 5.16551000 | 0.21319300 | 0.51409600 |
| H | 4.43453400 | -0.33190700 | 2.47020600 |
| C | 3.51971600 | 0.27424500 | -1.25173000 |
| H | 1.50303900 | -0.21061000 | -0.67315000 |
| C | 4.84231500 | 0.44879100 | -0.82688600 |
| H | 6.19719200 | 0.32665300 | 0.85781500 |
| H | 3.25222100 | 0.43547700 | -2.29987100 |
| H | 5.61591300 | 0.75234400 | -1.53685900 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3951.490381
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3954.486666

**4**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.578558 (Hartree/Particle)
Thermal correction to Energy= 0.614834
Thermal correction to Enthalpy= 0.615778
Thermal correction to Gibbs Free Energy= 0.502194
Sum of electronic and zero-point Energies= -1823.915293
Sum of electronic and thermal Energies= -1823.879018
Sum of electronic and thermal Enthalpies= -1823.878074
Sum of electronic and thermal Free Energies= -1823.991658

| | | | |
|---|---|---|---|
| C | 0.51669000 | 0.10030600 | -1.75597000 |
| H | 0.41936900 | 0.08123900 | -0.65366300 |
| C | 1.39440200 | -1.12279100 | -2.18142000 |
| H | 1.30972400 | -1.90496300 | -1.41115600 |
| N | 1.35994000 | 1.23897400 | -2.14877200 |
| N | 2.71963800 | -0.53036100 | -2.15436700 |
| C | 2.69232000 | 0.84275900 | -2.19099100 |
| C | 1.59983900 | 3.67794800 | -2.57236400 |
| H | 2.68815700 | 3.66845900 | -2.43665100 |
| H | 1.39385600 | 3.45750300 | -3.63374100 |
| O | 1.03585400 | 4.93008100 | -2.23700300 |
| O | 3.67572600 | 1.56860000 | -2.25898600 |
| C | -0.85318900 | 0.15220300 | -2.36762800 |
| C | 1.04232400 | -1.73367600 | -3.52983500 |
| C | 0.27763200 | -2.90635000 | -3.58769200 |
| C | 1.44091300 | -1.12331800 | -4.72903400 |
| C | -0.09154500 | -3.45815100 | -4.81859200 |
| H | -0.03313800 | -3.39237900 | -2.65848300 |
| C | 1.07478000 | -1.67307700 | -5.96058200 |
| H | 2.04313300 | -0.21251300 | -4.69919800 |
| C | 0.30567600 | -2.84154400 | -6.00908500 |
| H | -0.68662400 | -4.37454800 | -4.84735400 |
| H | 1.39244300 | -1.18796500 | -6.88711300 |
| H | 0.02160900 | -3.27232400 | -6.97254600 |
| C | 4.16410500 | -2.19187400 | -1.05232000 |
| C | 4.01383500 | -1.66682500 | 0.24145700 |
| C | 4.53409900 | -3.53491700 | -1.19903800 |
| C | 4.23732200 | -2.46768400 | 1.36370000 |
| H | 3.71364100 | -0.62243700 | 0.36421000 |
| C | 4.76268600 | -4.33906900 | -0.07623400 |
| H | 4.64110300 | -3.95788500 | -2.20226400 |
| C | 4.61472000 | -3.80745700 | 1.20806000 |
| H | 4.11749300 | -2.04550700 | 2.36496200 |
| H | 5.04988300 | -5.38571300 | -0.20686000 |
| H | 4.78836600 | -4.43480800 | 2.08611800 |
| C | -1.98491000 | 0.10272600 | -1.66022700 |
| H | -2.96431800 | 0.13458900 | -2.14520100 |
| H | -1.97086900 | 0.02557400 | -0.56773300 |
| H | -0.88187500 | 0.23907200 | -3.45858400 |
| C | 0.94614000 | 2.57940400 | -1.71847000 |
| H | -0.13053000 | 2.63787200 | -1.93829200 |
| C | 1.11006000 | 2.79197500 | -0.21733200 |
| C | -0.02504600 | 2.85789800 | 0.60368100 |
| C | 2.37942900 | 2.91150000 | 0.37437600 |
| C | 0.09557400 | 3.04596500 | 1.98463200 |
| H | -1.01738800 | 2.76767600 | 0.15280600 |
| C | 2.50199700 | 3.10141600 | 1.75326300 |
| H | 3.27068200 | 2.86464200 | -0.25125100 |
| C | 1.36217100 | 3.17101000 | 2.56298000 |
| H | -0.80099600 | 3.10027500 | 2.60758300 |
| H | 3.49531900 | 3.20487700 | 2.19747500 |
| H | 1.46196500 | 3.32457300 | 3.64058600 |
| C | 3.93234200 | -1.30762900 | -2.26426500 |
| H | 4.75308900 | -0.58130100 | -2.37240300 |
| H | 3.91042300 | -1.92125700 | -3.18177100 |
| Si | 1.76975900 | 6.15134600 | -1.36317500 |
| O | 1.83594500 | 7.48379800 | -2.35752800 |
| O | 3.33402900 | 5.76871500 | -0.97921800 |
| C | 0.83669700 | 6.46985700 | 0.20526100 |
| C | 0.88471800 | 7.85433100 | -3.33228300 |
| C | 4.45326000 | 5.79041200 | -1.84486100 |
| H | 0.96739000 | 5.62821200 | 0.90241200 |
| H | 1.19106100 | 7.39306600 | 0.68963100 |
| H | -0.23957800 | 6.57624200 | -0.00420200 |
| H | 1.35804800 | 8.54105200 | -4.05304600 |
| H | 0.50062900 | 6.97868600 | -3.88533800 |

| | | | |
|---|---|---|---|
| H | 0.02242300 | 8.37903700 | -2.87928800 |
| H | 4.28955600 | 6.45066800 | -2.71419200 |
| H | 5.33129200 | 6.16085700 | -1.29051400 |
| H | 4.68361100 | 4.77432900 | -2.21196900 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1824.188146
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1826.303241

**3**
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.467196 (Hartree/Particle)
Thermal correction to Energy= 0.492718
Thermal correction to Enthalpy= 0.493662
Thermal correction to Gibbs Free Energy= 0.408055
Sum of electronic and zero-point Energies= -1265.063319
Sum of electronic and thermal Energies= -1265.037797
Sum of electronic and thermal Enthalpies= -1265.036853
Sum of electronic and thermal Free Energies= -1265.122460

| | | | |
|---|---|---|---|
| C | 0.88173700 | 1.51702900 | -1.07466400 |
| O | 2.07100700 | 2.18438000 | -1.51826200 |
| C | 0.03727100 | 2.62503000 | -0.41415800 |
| H | 0.39050200 | 1.05608500 | -1.94045700 |
| H | 1.15885900 | 0.73819300 | -0.34522200 |
| H | -0.46379200 | 2.24016400 | 0.47854200 |
| C | 2.25767600 | 3.30315800 | -0.76552200 |
| O | 3.28075800 | 3.94717800 | -0.79436800 |
| C | -1.01120900 | 3.21220400 | -1.34399900 |
| C | -2.34813000 | 3.28389700 | -0.93495700 |
| C | -0.66256100 | 3.68239900 | -2.62048300 |
| C | -3.32283100 | 3.82935800 | -1.77737800 |
| H | -2.62458700 | 2.92490300 | 0.06050500 |
| C | -1.63274600 | 4.23089000 | -3.46221300 |
| H | 0.37635000 | 3.62431700 | -2.95527700 |
| C | -2.96629500 | 4.30892200 | -3.04114600 |
| H | -4.36178600 | 3.88559700 | -1.44244400 |
| H | -1.34861200 | 4.59849700 | -4.45155900 |
| H | -3.72475300 | 4.74031400 | -3.69932300 |
| N | 1.11908900 | 3.55417100 | -0.03852600 |
| C | 1.17684000 | 4.44324300 | 1.11401400 |
| H | 2.09355200 | 5.03024000 | 0.94859900 |
| C | 0.06728800 | 5.46803200 | 1.20873100 |
| H | -0.10578100 | 5.85059200 | 2.21981400 |
| C | 1.41925400 | 3.69320600 | 2.47338300 |
| C | -0.61306200 | 6.00848100 | 0.19631600 |
| H | -1.35029400 | 6.79521400 | 0.37771900 |
| H | -0.46603300 | 5.69334600 | -0.83752600 |
| N | 0.21323957 | 2.98675295 | 2.88770834 |
| H | -0.55786949 | 3.65034793 | 2.92277826 |
| C | 0.26745868 | 2.23026165 | 4.14388398 |
| H | 1.08064328 | 1.49538283 | 4.02832205 |
| H | 0.57688341 | 2.90282548 | 4.95686590 |
| C | -1.01701166 | 1.51270767 | 4.52879087 |
| C | -1.71869201 | 1.86305435 | 5.69098529 |
| C | -1.55484088 | 0.51689332 | 3.69652645 |
| C | -2.92498458 | 1.23307156 | 6.01994905 |
| H | -1.31396648 | 2.63820471 | 6.34856198 |
| C | -2.75871850 | -0.11411502 | 4.01820379 |
| H | -1.02289920 | 0.23494722 | 2.78230176 |
| C | -3.44889498 | 0.24343752 | 5.18355023 |
| H | -3.45708351 | 1.51934163 | 6.93099550 |
| H | -3.16091689 | -0.88936226 | 3.36049364 |
| H | -4.39141530 | -0.24888386 | 5.43659378 |
| H | 1.75799864 | 4.33929580 | 3.25614736 |
| C | 2.56677060 | 2.71348550 | 2.16523789 |
| C | 3.89043063 | 3.14978914 | 2.22101753 |
| C | 2.28228450 | 1.38924421 | 1.83077932 |
| C | 4.92987622 | 2.26198612 | 1.94203708 |
| H | 4.11474994 | 4.19342030 | 2.48494497 |
| C | 3.32140824 | 0.50171918 | 1.55139036 |
| H | 1.23855866 | 1.04541527 | 1.78727931 |
| C | 4.64560378 | 0.93836926 | 1.60670247 |
| H | 5.97328368 | 2.60646669 | 1.98534769 |
| H | 3.09751672 | -0.54196658 | 1.28702513 |
| H | 5.46482571 | 0.23869616 | 1.38618151 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1265.303506
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -1266.906722

**TS-ii-iii-3 *cis***
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.701987 (Hartree/Particle)
Thermal correction to Energy= 0.736617
Thermal correction to Enthalpy= 0.737561
Thermal correction to Gibbs Free Energy= 0.632092
Sum of electronic and zero-point Energies= -3355.574160
Sum of electronic and thermal Energies= -3355.539530
Sum of electronic and thermal Enthalpies= -3355.538586
Sum of electronic and thermal Free Energies= -3355.644055

| | | | |
|---|---|---|---|
| C | 1.55026500 | 0.14110700 | 3.46816300 |
| C | 3.39986000 | -1.37856100 | 2.61109600 |
| Cu | 1.86252100 | 0.06687300 | 1.32954700 |
| H | 1.35801700 | 1.06513100 | 4.01539900 |
| H | 4.46314600 | -1.47943600 | 2.38880500 |
| H | 2.77863400 | -2.27168100 | 2.50330200 |
| C | 0.44522700 | -1.49238700 | 5.09747800 |
| C | -0.66259100 | -2.52785100 | 4.79894000 |
| H | 1.38387700 | -1.99715200 | 5.39129700 |
| H | -1.65913700 | -2.11983400 | 5.03461900 |
| H | -0.52529200 | -3.48182400 | 5.32471000 |
| N | 0.60884200 | -0.90577400 | 3.76405700 |
| C | 0.10236200 | -1.73324300 | 2.81367000 |
| O | 0.23503300 | -1.63324800 | 1.60084100 |
| O | -0.57726000 | -2.75689400 | 3.38332300 |
| C | 2.91160700 | -0.20688900 | 3.16743300 |
| H | 3.62933100 | 0.61827000 | 3.28095100 |
| P | 1.33097500 | 0.74073300 | -0.68996300 |
| C | -0.53860500 | 0.93988000 | -0.83338800 |
| C | 1.78358800 | -0.49107000 | -2.03720900 |
| C | 2.05993900 | 2.38158300 | -1.23826000 |
| C | -1.29054400 | -0.36795900 | -1.15480100 |
| C | -1.10455900 | 1.53519400 | 0.47515900 |
| H | -0.71631500 | 1.65098800 | -1.66154700 |
| C | 3.17636800 | -0.29846000 | -2.66616000 |
| C | 1.68490600 | -1.91975400 | -1.45784500 |
| H | 1.03686800 | -0.36759600 | -2.84245100 |
| C | 1.26661000 | 3.62186400 | -0.78482900 |
| C | 3.50883700 | 2.48498200 | -0.71374300 |
| H | 2.07113900 | 2.37486000 | -2.34320900 |
| C | -2.80454500 | -0.12912200 | -1.25404600 |
| H | -1.09074200 | -1.09290200 | -0.34825800 |
| H | -0.93325600 | -0.81107400 | -2.09621500 |
| C | -2.61607900 | 1.77758400 | 0.38510000 |
| H | -0.88744700 | 0.82203800 | 1.28763700 |
| H | -0.59064700 | 2.46755800 | 0.74591200 |
| C | 3.44222600 | -1.35435100 | -3.75003100 |
| H | 3.94547000 | -0.39256400 | -1.87885500 |
| H | 3.28290700 | 0.70693400 | -3.10163200 |
| C | 1.94399900 | -2.98458700 | -2.52940900 |
| H | 2.43509200 | -2.00668900 | -0.65098000 |
| H | 0.71656200 | -2.09134500 | -0.97004300 |
| C | 1.94330500 | 4.91965200 | -1.25015900 |
| H | 1.20412200 | 3.62505900 | 0.31795400 |
| H | 0.23443800 | 3.59147600 | -1.16494200 |
| C | 4.19420800 | 3.77860400 | -1.17018100 |
| H | 3.46860900 | 2.44877000 | 0.39078700 |
| H | 4.10581800 | 1.61516500 | -1.02133100 |

| | | | |
|---|---|---|---|
| C | -3.36559700 | 0.48937400 | 0.03055500 |
| H | -3.31404300 | -1.08157700 | -1.47815200 |
| H | -3.01228500 | 0.54638400 | -2.10493600 |
| H | -2.98384300 | 2.18941300 | 1.34030500 |
| H | -2.81912800 | 2.54403200 | -0.38617600 |
| C | 3.30540300 | -2.77993100 | -3.20319000 |
| H | 4.44709200 | -1.20064500 | -4.17856300 |
| H | 2.72276400 | -1.20968200 | -4.57714400 |
| H | 1.88299700 | -3.98971300 | -2.07951200 |
| H | 1.14559300 | -2.93337500 | -3.29304200 |
| C | 3.39059300 | 5.01542800 | -0.75559900 |
| H | 1.35817700 | 5.78713700 | -0.90116400 |
| H | 1.93143300 | 4.95685200 | -2.35517700 |
| H | 5.21667500 | 3.82495200 | -0.75925800 |
| H | 4.29852700 | 3.76235000 | -2.27092600 |
| H | -4.44673100 | 0.68317400 | -0.07243700 |
| H | -3.24894000 | -0.23374300 | 0.85846500 |
| H | 3.45453500 | -3.51682700 | -4.01036800 |
| H | 4.10465000 | -2.95890500 | -2.46058200 |
| H | 3.86844900 | 5.93386100 | -1.13592100 |
| H | 3.39059900 | 5.09288500 | 0.34732300 |
| C | 0.06531500 | -0.49240400 | 6.16744800 |
| C | -0.83868200 | 0.54444900 | 5.88648900 |
| C | 0.58065200 | -0.61179800 | 7.46440600 |
| C | -1.22160600 | 1.44128100 | 6.88611400 |
| H | -1.22878500 | 0.65176800 | 4.87097000 |
| C | 0.19357100 | 0.28171700 | 8.46932500 |
| H | 1.29474300 | -1.40911700 | 7.68951600 |
| C | -0.70845400 | 1.31045600 | 8.18246200 |
| H | -1.92084400 | 2.24848800 | 6.65302400 |
| H | 0.60344600 | 0.17671900 | 9.47713000 |
| H | -1.00722900 | 2.01299900 | 8.96461500 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.888342
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.135889

**TS-i-iii-3 *trans***
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.701895 (Hartree/Particle)
Thermal correction to Energy= 0.736512
Thermal correction to Enthalpy= 0.737456
Thermal correction to Gibbs Free Energy= 0.632980
Sum of electronic and zero-point Energies= -3355.570311
Sum of electronic and thermal Energies= -3355.535694
Sum of electronic and thermal Enthalpies= -3355.534750
Sum of electronic and thermal Free Energies= -3355.639226

| | | | |
|---|---|---|---|
| C | 1.31661600 | -0.29458900 | 3.42918700 |
| C | 3.08362900 | -1.79419200 | 2.38305700 |
| Cu | 1.73509800 | -0.06020800 | 1.36320800 |
| H | 4.14652500 | -1.95942100 | 2.20149800 |
| H | 2.39601200 | -2.60044700 | 2.10401900 |
| C | 2.66448200 | -0.71528400 | 3.14598200 |
| H | 3.44101200 | -0.00191900 | 3.45872500 |
| P | 1.25455900 | 0.63961000 | -0.66254900 |
| C | -0.56588000 | 1.00096900 | -0.96293300 |
| C | 1.78540800 | -0.51675500 | -2.04462200 |
| C | 2.13959200 | 2.26900400 | -0.99708000 |
| C | -1.39957900 | -0.17066400 | -1.51361700 |
| C | -1.20155000 | 1.51352800 | 0.34717700 |
| H | -0.59426800 | 1.80650600 | -1.71811200 |
| C | 3.27809600 | -0.39827700 | -2.40956700 |
| C | 1.48095500 | -1.97351400 | -1.63179400 |
| H | 1.19096800 | -0.25351700 | -2.93845900 |
| C | 1.35074200 | 3.53741300 | -0.61358600 |
| C | 3.49461400 | 2.27252800 | -0.25392800 |
| H | 2.31986500 | 2.30049400 | -2.08731300 |
| C | -2.86070800 | 0.25134700 | -1.73242000 |
| H | -1.37344600 | -1.00827600 | -0.79391400 |
| H | -0.98194200 | -0.54621900 | -2.46019100 |
| C | -2.66015100 | 1.93683400 | 0.14045000 |
| H | -1.14691500 | 0.69862200 | 1.09165800 |
| H | -0.61607100 | 2.33560100 | 0.77994900 |
| C | 3.66659300 | -1.39152900 | -3.51424700 |
| H | 3.88111400 | -0.60792000 | -1.50772600 |
| H | 3.52809700 | 0.62329600 | -2.73285900 |
| C | 1.86745500 | -2.97582200 | -2.72643700 |
| H | 2.05317100 | -2.18462300 | -0.70960700 |
| H | 0.42192500 | -2.10032500 | -1.36779000 |
| C | 2.15944800 | 4.80341000 | -0.93493800 |
| H | 1.14000400 | 3.51218300 | 0.46660500 |
| H | 0.38613100 | 3.57983600 | -1.14166800 |
| C | 4.30871500 | 3.53501200 | -0.56218000 |
| H | 3.27920300 | 2.22953600 | 0.82783000 |
| H | 4.08271700 | 1.37530300 | -0.49457100 |
| C | -3.49562300 | 0.79405600 | -0.44720000 |
| H | -3.44029800 | -0.60419800 | -2.11834400 |
| H | -2.89546300 | 1.03232700 | -2.51436500 |
| H | -3.08955200 | 2.27707900 | 1.09771300 |
| H | -2.69298400 | 2.80482200 | -0.54399700 |
| C | 3.34159900 | -2.83566200 | -3.11886500 |
| H | 4.73982600 | -1.28616800 | -3.74596500 |
| H | 3.11868600 | -1.13393600 | -4.43952000 |
| H | 1.65413300 | -4.00210100 | -2.38325300 |
| H | 1.23347400 | -2.80396200 | -3.61607400 |
| C | 3.51667600 | 4.80213500 | -0.22323100 |
| H | 1.57594500 | 5.69492900 | -0.64928700 |
| H | 2.31941900 | 4.86883100 | -2.02759500 |
| H | 5.25874800 | 3.51078100 | -0.00213900 |
| H | 4.57631500 | 3.54423500 | -1.63549300 |
| H | -4.52954500 | 1.12657600 | -0.63980300 |
| H | -3.56006300 | -0.02283500 | 0.29518400 |
| H | 3.59232500 | -3.52711500 | -3.94078200 |
| H | 3.97262800 | -3.12485900 | -2.25844000 |
| H | 4.09392300 | 5.70384600 | -0.48908000 |
| H | 3.34929200 | 4.83920000 | 0.86829000 |
| N | 1.11846900 | 0.87580800 | 4.22499200 |
| C | 1.04948300 | 0.85928600 | 5.69557800 |
| C | 1.25408800 | 2.15014000 | 3.75843500 |
| C | 0.65852700 | 2.32728300 | 5.95686200 |
| H | 0.24693300 | 0.17724000 | 6.01613500 |
| C | 2.36015200 | 0.41367200 | 6.31908600 |
| O | 1.49902400 | 2.52434200 | 2.62786900 |
| O | 1.09516300 | 3.03390400 | 4.78755400 |
| H | 1.15086000 | 2.76155200 | 6.83685000 |
| H | -0.43357600 | 2.44047600 | 6.05663600 |
| C | 3.50335400 | 1.22643100 | 6.23059700 |
| C | 2.46749100 | -0.83984400 | 6.93280600 |
| C | 4.72431500 | 0.79341500 | 6.75077700 |
| H | 3.43726200 | 2.20358000 | 5.74435600 |
| C | 3.69063600 | -1.27803400 | 7.45394100 |
| H | 1.58637800 | -1.48452200 | 6.99730100 |
| C | 4.82153400 | -0.46242800 | 7.36387400 |
| H | 5.60544800 | 1.43588600 | 6.67589700 |
| H | 3.75936300 | -2.26089300 | 7.92724800 |
| H | 5.77819000 | -0.80271100 | 7.76837000 |
| H | 0.52654200 | -1.04759900 | 3.54257000 |

M06-L/def2-SVP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3355.882164
B3LYP-D3/def2-TZVPP-gas//B3LYP-D3/def2-SVP-CPCM(toluene)
HF = -3358.131786

**TS-i-ii-3 conf2**
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.696120 (Hartree/Particle)
Thermal correction to Energy= 0.731446
Thermal correction to Enthalpy= 0.732390
Thermal correction to Gibbs Free Energy= 0.627176

Sum of electronic and zero-point Energies= -3355.513471
Sum of electronic and thermal Energies= -3355.478146
Sum of electronic and thermal Enthalpies= -3355.477201
Sum of electronic and thermal Free Energies= -3355.582416

| | | | |
|---|---|---|---|
| O | -1.40146700 | -1.15654500 | 1.60757900 |
| C | -1.14513200 | -1.27417000 | 3.01438200 |
| C | -1.69552100 | 0.03349000 | 3.63126900 |
| H | -1.68602400 | -2.15253900 | 3.40249500 |
| H | -0.06753000 | -1.41092900 | 3.17339600 |
| H | -0.89418400 | 0.78878800 | 3.72983100 |
| N | -2.62101500 | 0.44000900 | 2.57326400 |
| C | -2.34639000 | -0.20479100 | 1.40681000 |
| O | -2.83356900 | 0.01575600 | 0.31077300 |
| C | -3.40316900 | 1.64508500 | 2.63463600 |
| H | -4.11296900 | 1.68884800 | 3.46496200 |
| C | -2.92218400 | 2.83286800 | 2.03269800 |
| C | -2.25050200 | 3.93111600 | 2.37608500 |
| H | -1.82204500 | 4.00560000 | 3.38329700 |
| H | -2.10794000 | 4.77555500 | 1.69653200 |
| C | -2.36319200 | -0.16142200 | 4.97588100 |
| C | -3.60993900 | -0.80139300 | 5.06058600 |
| C | -1.73805800 | 0.26645200 | 6.15346600 |
| C | -4.21868200 | -1.00991400 | 6.29951900 |
| H | -4.10946800 | -1.12103000 | 4.14348300 |
| C | -2.34247500 | 0.05230400 | 7.39766400 |
| H | -0.77214800 | 0.77641800 | 6.09730500 |
| C | -3.58405300 | -0.58555300 | 7.47355700 |
| H | -5.19446800 | -1.49969200 | 6.34808400 |
| H | -1.84388900 | 0.39178200 | 8.30911100 |
| H | -4.06005800 | -0.74711900 | 8.44400200 |
| P | -6.00239100 | 1.14380200 | -0.21374800 |
| C | -7.26038300 | 2.33583400 | -0.93709200 |
| C | -6.97813100 | 0.17589100 | 1.06697600 |
| C | -5.49272800 | -0.16055500 | -1.44259200 |
| C | -7.16124600 | 3.68236600 | -0.18383400 |
| C | -7.11355200 | 2.58892300 | -2.44932300 |
| H | -8.25777500 | 1.89422700 | -0.75719600 |
| C | -6.09116100 | -0.92669800 | 1.68120500 |
| C | -7.51166000 | 1.11489200 | 2.16690300 |
| H | -7.83971900 | -0.29072400 | 0.55586500 |
| C | -6.60312300 | -1.01830900 | -2.07013700 |
| C | -4.49528200 | 0.35764300 | -2.49693400 |
| H | -4.89268700 | -0.80849400 | -0.78197800 |
| C | -8.19960600 | 4.69549700 | -0.68025000 |
| H | -6.14198300 | 4.08056800 | -0.33703200 |
| H | -7.26388000 | 3.53801100 | 0.90153200 |
| C | -8.15674700 | 3.59717000 | -2.95275200 |
| H | -6.10223000 | 2.98384300 | -2.65158000 |
| H | -7.20762500 | 1.65106900 | -3.01451100 |
| C | -6.78374600 | -1.67018700 | 2.83075500 |
| H | -5.16620100 | -0.44973500 | 2.04820900 |
| H | -5.78655500 | -1.65202300 | 0.91141800 |
| C | -8.20592400 | 0.35084300 | 3.30178200 |
| H | -6.65854400 | 1.68692000 | 2.57591700 |
| H | -8.21442500 | 1.84609700 | 1.73977600 |
| C | -5.99808600 | -2.17512000 | -2.88122700 |
| H | -7.23053500 | -0.39858500 | -2.73368900 |
| H | -7.27278800 | -1.42155200 | -1.29354700 |
| C | -3.89814300 | -0.81487600 | -3.28570000 |
| H | -4.99592900 | 1.04263900 | -3.19938900 |
| H | -3.70138200 | 0.92868000 | -1.99228400 |
| C | -8.07973200 | 4.92419600 | -2.19059800 |
| H | -8.08248900 | 5.64664400 | -0.13425600 |
| H | -9.21350000 | 4.32120800 | -0.44579500 |
| H | -8.01948900 | 3.76381900 | -4.03446100 |
| H | -9.16596700 | 3.16287500 | -2.82752200 |
| C | -7.28325600 | -0.70718900 | 3.91159100 |
| H | -6.08901900 | -2.41158400 | 3.26168100 |
| H | -7.64118800 | -2.24314000 | 2.43215200 |
| H | -8.54504300 | 1.06267900 | 4.07305700 |
| H | -9.11395400 | -0.14128500 | 2.90670200 |
| C | -4.99523700 | -1.67368900 | -3.92800000 |
| H | -6.80124400 | -2.75845500 | -3.36267500 |
| H | -5.48134500 | -2.86342200 | -2.18723900 |
| H | -3.20540300 | -0.43645100 | -4.05612900 |
| H | -3.29652800 | -1.43590400 | -2.59762700 |
| H | -8.86271600 | 5.61714300 | -2.54183000 |
| H | -7.10934800 | 5.40818900 | -2.40570500 |
| H | -7.80132500 | -1.26014300 | 4.71329400 |
| H | -6.41901800 | -0.20493100 | 4.38157400 |
| H | -4.55143900 | -2.52605100 | -4.46966400 |
| H | -5.53281200 | -1.06840000 | -4.68189400 |
| Cu | -4.19067200 | 2.05452900 | 0.70704600 |
| H | -3.21698800 | 3.25018100 | 0.38071300 |

**TS-i-ii-3 conf3**

B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.696353 (Hartree/Particle)
Thermal correction to Energy= 0.731609
Thermal correction to Enthalpy= 0.732553
Thermal correction to Gibbs Free Energy= 0.627790
Sum of electronic and zero-point Energies= -3355.512882
Sum of electronic and thermal Energies= -3355.477626
Sum of electronic and thermal Enthalpies= -3355.476682
Sum of electronic and thermal Free Energies= -3355.581445

| | | | |
|---|---|---|---|
| O | -3.04499100 | -2.02106400 | 2.43349200 |
| C | -1.82256500 | -1.36352600 | 2.07028100 |
| C | -1.92048400 | 0.03866800 | 2.70669200 |
| H | -0.97652500 | -1.95363000 | 2.44486500 |
| H | -1.76749800 | -1.29929900 | 0.97110800 |
| H | -1.54800500 | 0.80685000 | 2.01458300 |
| N | -3.38175600 | 0.14549300 | 2.81617700 |
| C | -3.97969000 | -1.07998100 | 2.76513700 |
| O | -5.14139900 | -1.35403600 | 2.97190600 |
| C | -4.06765600 | 1.33447600 | 3.20044100 |
| H | -4.71032200 | 1.26575700 | 4.08171500 |
| C | -3.62627500 | 2.57850900 | 2.73356800 |
| C | -3.11082800 | 3.71071100 | 3.22574400 |
| H | -2.69506600 | 3.71805100 | 4.23871700 |
| H | -3.09245900 | 4.63982900 | 2.65094600 |
| C | -1.23165600 | 0.19946400 | 4.05094000 |
| C | -1.37535800 | -0.77745300 | 5.05027800 |
| C | -0.47946000 | 1.34783600 | 4.32717500 |
| C | -0.77102900 | -0.60910200 | 6.29788200 |
| H | -1.96584600 | -1.67591300 | 4.85093400 |
| C | 0.12694600 | 1.51916200 | 5.57676100 |
| H | -0.37887900 | 2.12119600 | 3.56114800 |
| C | -0.01729400 | 0.54077300 | 6.56450600 |
| H | -0.88855200 | -1.37737700 | 7.06640000 |
| H | 0.71038700 | 2.42116000 | 5.77879100 |
| H | 0.45463000 | 0.67259500 | 7.54151400 |
| P | -6.50703300 | 1.09953200 | 0.06719700 |
| C | -7.41614500 | 2.36938600 | -0.95279000 |
| C | -7.88121200 | 0.21189100 | 0.99789700 |
| C | -5.71566300 | -0.07005300 | -1.15968300 |
| C | -8.43591900 | 1.81240900 | -1.96080100 |
| C | -8.05741700 | 3.43371000 | -0.04141800 |
| H | -6.60759900 | 2.87001300 | -1.51309400 |
| C | -7.85861600 | -1.32660900 | 0.95073600 |
| C | -7.88908500 | 0.70267200 | 2.46094900 |
| H | -8.81759800 | 0.54245800 | 0.51537600 |
| C | -4.98544500 | 0.71167600 | -2.27189800 |
| C | -4.71443000 | -0.98359700 | -0.42248300 |
| H | -6.50702800 | -0.68820700 | -1.61749300 |
| C | -9.07451000 | 2.94402400 | -2.78056100 |
| H | -9.23146600 | 1.26952900 | -1.42077700 |
| H | -7.96117200 | 1.08084000 | -2.63416100 |
| C | -8.69445300 | 4.55905600 | -0.86729600 |
| H | -8.83699400 | 2.96477300 | 0.58514500 |
| H | -7.29729600 | 3.83807300 | 0.64900100 |

| | | | |
|---|---|---|---|
| C | -9.04877100 | -1.91020600 | 1.72663100 |
| H | -6.92961900 | -1.68831600 | 1.41621600 |
| H | -7.87648600 | -1.68659000 | -0.09050600 |
| C | -9.06566700 | 0.11017400 | 3.24524700 |
| H | -6.93590000 | 0.40016500 | 2.92346200 |
| H | -7.91802900 | 1.80478400 | 2.49672400 |
| C | -4.22798100 | -0.22597600 | -3.22325300 |
| H | -4.27388400 | 1.41307500 | -1.79844300 |
| H | -5.69157900 | 1.32285400 | -2.85385800 |
| C | -3.96383500 | -1.91884100 | -1.37520500 |
| H | -3.98522500 | -0.33328300 | 0.09408300 |
| H | -5.21371400 | -1.56523000 | 0.36109200 |
| C | -9.71000300 | 4.00643500 | -1.87541900 |
| H | -9.82471300 | 2.52796500 | -3.47370400 |
| H | -8.29614800 | 3.41770400 | -3.40661600 |
| H | -9.17429400 | 5.29185400 | -0.19733700 |
| H | -7.89921100 | 5.10143800 | -1.41063900 |
| C | -9.06027300 | -1.42174500 | 3.18024500 |
| H | -9.00909600 | -3.01204200 | 1.69111700 |
| H | -9.99272900 | -1.61274000 | 1.23224000 |
| H | -9.02508000 | 0.45206000 | 4.29326300 |
| H | -10.01636800 | 0.49089800 | 2.82650000 |
| C | -3.24484800 | -1.13202000 | -2.47466800 |
| H | -3.70110400 | 0.37100000 | -3.98642800 |
| H | -4.95850000 | -0.85426400 | -3.76562500 |
| H | -3.25064500 | -2.53106600 | -0.79801700 |
| H | -4.68077900 | -2.62352300 | -1.83513000 |
| H | -10.13300800 | 4.82428100 | -2.48233600 |
| H | -10.55567000 | 3.55338000 | -1.32530600 |
| H | -9.93037800 | -1.83453400 | 3.71832800 |
| H | -8.15679300 | -1.79882300 | 3.69153800 |
| H | -2.73895300 | -1.81545300 | -3.17698700 |
| H | -2.45553500 | -0.50843400 | -2.01518500 |
| Cu | -4.93216000 | 2.03333400 | 1.33010000 |
| H | -3.65915100 | 2.93337300 | 1.01789900 |

**TS-i-ii-3 conf4**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.696371 (Hartree/Particle)
Thermal correction to Energy= 0.731687
Thermal correction to Enthalpy= 0.732631
Thermal correction to Gibbs Free Energy= 0.627460
Sum of electronic and zero-point Energies= -3355.508103
Sum of electronic and thermal Energies= -3355.472788
Sum of electronic and thermal Enthalpies= -3355.471844
Sum of electronic and thermal Free Energies= -3355.577015

| | | | |
|---|---|---|---|
| O | -2.83358900 | -1.33212400 | 3.77300900 |
| C | -1.90154700 | -1.23063100 | 2.69637400 |
| C | -2.23908000 | 0.10873900 | 2.00768400 |
| H | -0.87592600 | -1.21559700 | 3.10103500 |
| H | -2.01720700 | -2.09495600 | 2.02898600 |
| H | -2.98036200 | -0.05230000 | 1.20039100 |
| N | -2.88890300 | 0.80341000 | 3.11257900 |
| C | -3.33670000 | -0.09016700 | 4.05023300 |
| O | -4.08733300 | 0.11835600 | 4.97682800 |
| C | -3.55027500 | 2.07808600 | 2.97396400 |
| H | -4.23380000 | 2.26887400 | 3.80356600 |
| C | -3.00944800 | 3.17430800 | 2.27557600 |
| C | -2.45838000 | 4.35716000 | 2.55801700 |
| H | -2.09282800 | 4.55402200 | 3.57264000 |
| H | -2.34934600 | 5.14732200 | 1.81014500 |
| C | -1.03652600 | 0.80799100 | 1.41430500 |
| C | -0.08379500 | 1.42242500 | 2.23878100 |
| C | -0.85172700 | 0.82520800 | 0.02692300 |
| C | 1.03292600 | 2.04852800 | 1.68239400 |
| H | -0.23825300 | 1.42928000 | 3.32056100 |
| C | 0.26825500 | 1.44703700 | -0.53387500 |
| H | -1.59706900 | 0.35922600 | -0.62187500 |
| C | 1.21220200 | 2.06251600 | 0.29337800 |
| H | 1.76409800 | 2.53459300 | 2.33334200 |
| H | 0.39690700 | 1.45852900 | -1.61911500 |
| H | 2.08421600 | 2.55712900 | -0.14197500 |
| P | -5.85945500 | 1.24765000 | -0.10657400 |
| C | -7.16462700 | 2.35478100 | -0.87624000 |
| C | -6.82035600 | 0.10592800 | 1.03107300 |
| C | -5.10532600 | 0.08606500 | -1.35947500 |
| C | -7.26600500 | 3.65268000 | -0.04087700 |
| C | -6.92328100 | 2.72053700 | -2.35269400 |
| H | -8.12089900 | 1.80514500 | -0.80743900 |
| C | -5.85694400 | -0.91333400 | 1.66973400 |
| C | -7.54425900 | 0.91551700 | 2.12533400 |
| H | -7.57460500 | -0.42547300 | 0.42338400 |
| C | -6.06772400 | -0.83080200 | -2.13305400 |
| C | -4.09049900 | 0.77458800 | -2.29272000 |
| H | -4.50604800 | -0.56195000 | -0.69428500 |
| C | -8.36531800 | 4.58470900 | -0.56384700 |
| H | -6.28765000 | 4.16573000 | -0.09406300 |
| H | -7.43349900 | 3.42882200 | 1.02245200 |
| C | -8.02554300 | 3.64873800 | -2.88408300 |
| H | -5.94699100 | 3.22893900 | -2.44213900 |
| H | -6.87251400 | 1.81824000 | -2.97801000 |
| C | -6.52739300 | -1.79879400 | 2.72682900 |
| H | -5.04657100 | -0.33962500 | 2.14512500 |
| H | -5.39314600 | -1.55152200 | 0.90135900 |
| C | -8.21955700 | 0.01205000 | 3.16587800 |
| H | -6.79801400 | 1.55984900 | 2.62608800 |
| H | -8.29791100 | 1.58029100 | 1.67580100 |
| C | -5.28587500 | -1.85466400 | -2.97115500 |
| H | -6.70609800 | -0.22611800 | -2.79918800 |
| H | -6.74528100 | -1.35657200 | -1.44195800 |
| C | -3.31440300 | -0.26808000 | -3.10757700 |
| H | -4.61001000 | 1.45139700 | -2.98822100 |
| H | -3.41025100 | 1.40435200 | -1.69644800 |
| C | -8.15245500 | 4.92317200 | -2.04297900 |
| H | -8.39335400 | 5.50410500 | 0.04428600 |
| H | -9.34750400 | 4.09315000 | -0.43666500 |
| H | -7.82078400 | 3.89973500 | -3.93832800 |
| H | -8.98859800 | 3.10578400 | -2.87178400 |
| C | -7.22211400 | -0.95940400 | 3.80262500 |
| H | -5.76386600 | -2.45149100 | 3.18141000 |
| H | -7.26549200 | -2.45933000 | 2.23503100 |
| H | -8.69849100 | 0.63826500 | 3.93716900 |
| H | -9.03047300 | -0.55977500 | 2.67701100 |
| C | -4.26622600 | -1.17761900 | -3.89565000 |
| H | -5.98662900 | -2.47353200 | -3.55605300 |
| H | -4.75435500 | -2.54299800 | -2.28834200 |
| H | -2.60829500 | 0.23626000 | -3.78803400 |
| H | -2.70373700 | -0.88665300 | -2.42344300 |
| H | -8.97603500 | 5.55272100 | -2.41914300 |
| H | -7.22669800 | 5.51839400 | -2.14692600 |
| H | -7.73177900 | -1.61351800 | 4.52976800 |
| H | -6.45585400 | -0.39474900 | 4.36077900 |
| H | -3.69700400 | -1.93692700 | -4.45729900 |
| H | -4.80507600 | -0.57012400 | -4.64625900 |
| Cu | -4.30546100 | 2.38452000 | 0.98867800 |
| H | -3.08357300 | 3.31725200 | 0.58171700 |

**TS-i-iii-3 *cis* conf2**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.696136 (Hartree/Particle)
Thermal correction to Energy= 0.731322
Thermal correction to Enthalpy= 0.732266
Thermal correction to Gibbs Free Energy= 0.626001
Sum of electronic and zero-point Energies= -3355.501275
Sum of electronic and thermal Energies= -3355.466089
Sum of electronic and thermal Enthalpies= -3355.465145
Sum of electronic and thermal Free Energies= -3355.571410

| | | | |
|---|---|---|---|
| O | -2.00170300 | -1.58853400 | 0.38978800 |
| C | -0.93048800 | -1.31579700 | 1.30150600 |
| C | -1.61495000 | -0.75508400 | 2.56861900 |

| | | | |
|---|---|---|---|
| H | -0.37722400 | -2.24578500 | 1.48650600 |
| H | -0.25636100 | -0.57113800 | 0.84836100 |
| H | -1.05284600 | 0.10472800 | 2.96197600 |
| N | -2.87386500 | -0.29210900 | 1.97582100 |
| C | -3.11846500 | -0.90380000 | 0.76707300 |
| O | -4.13437400 | -0.89929200 | 0.11327000 |
| C | -3.85716900 | 0.41133700 | 2.70510100 |
| H | -4.09915900 | 0.01986300 | 3.69742300 |
| C | -4.49168300 | 1.46968800 | 2.16847900 |
| H | -5.45678400 | 1.88411400 | 3.59907100 |
| C | -4.71054800 | 2.07867500 | 0.93925700 |
| H | -4.51766400 | 3.14811400 | 0.79732400 |
| H | -4.79441500 | 1.44916600 | 0.04927600 |
| Cu | -6.39156500 | 1.97002500 | 2.30681000 |
| P | -8.48086600 | 1.89350100 | 1.56713900 |
| C | -8.52034400 | 0.44782700 | 0.35809900 |
| C | -9.03872200 | 3.39428500 | 0.57825400 |
| C | -9.86201600 | 1.56956100 | 2.79948300 |
| C | -8.03966900 | 0.80429000 | -1.06236600 |
| C | -7.65224400 | -0.71054800 | 0.90378700 |
| H | -9.57382600 | 0.11973900 | 0.29093900 |
| C | -9.83918500 | 4.45033500 | 1.36492800 |
| C | -7.81438900 | 4.06641300 | -0.07928800 |
| H | -9.70194000 | 3.00034700 | -0.21303200 |
| C | -10.05116600 | 0.08928200 | 3.18262700 |
| C | -9.61277100 | 2.40066300 | 4.07579000 |
| H | -10.79565100 | 1.91113300 | 2.31722900 |
| C | -8.07661000 | -0.42079700 | -1.98853200 |
| H | -7.00330000 | 1.17693900 | -0.99871900 |
| H | -8.65003400 | 1.60894800 | -1.49983000 |
| C | -7.70004300 | -1.94004100 | -0.01132700 |
| H | -6.60542900 | -0.36556000 | 0.96405100 |
| H | -7.95042600 | -0.98761000 | 1.92407100 |
| C | -10.26542600 | 5.61017600 | 0.45216100 |
| H | -9.21262900 | 4.85120700 | 2.18116000 |
| H | -10.73117800 | 4.00784100 | 1.83293600 |
| C | -8.22553900 | 5.23116700 | -0.98776000 |
| H | -7.15223100 | 4.43352200 | 0.72614300 |
| H | -7.21454000 | 3.33831700 | -0.64064300 |
| C | -11.19374800 | -0.08038800 | 4.19483400 |
| H | -9.11641100 | -0.29125100 | 3.63125500 |
| H | -10.25553900 | -0.52688700 | 2.29428000 |
| C | -10.74432200 | 2.23380000 | 5.09767800 |
| H | -8.65455600 | 2.06690300 | 4.51297400 |
| H | -9.47864900 | 3.46529600 | 3.83725100 |
| C | -7.24935100 | -1.58429200 | -1.43148700 |
| H | -7.71420600 | -0.13314100 | -2.98999000 |
| H | -9.12686000 | -0.74403600 | -2.11575700 |
| H | -7.05689700 | -2.73179700 | 0.40724300 |
| H | -8.73000500 | -2.34360900 | -0.03447100 |
| C | -9.06107000 | 6.26804900 | -0.22977100 |
| H | -10.83168400 | 6.35329100 | 1.03836600 |
| H | -10.95735500 | 5.22528800 | -0.31957800 |
| H | -7.32674600 | 5.70019100 | -1.42181400 |
| H | -8.81398300 | 4.83589500 | -1.83642700 |
| C | -10.96454200 | 0.76029400 | 5.45516900 |
| H | -11.30162700 | -1.14669400 | 4.45531400 |
| H | -12.14454400 | 0.22476700 | 3.71990700 |
| H | -10.51812800 | 2.82206200 | 6.00275100 |
| H | -11.67762900 | 2.65156600 | 4.67653600 |
| H | -7.32819200 | -2.46207800 | -2.09512300 |
| H | -6.18401200 | -1.29914100 | -1.39679300 |
| H | -9.39371500 | 7.07062900 | -0.90917400 |
| H | -8.42873200 | 6.74807000 | 0.53974600 |
| H | -11.81359400 | 0.65247200 | 6.15083900 |
| H | -10.07162200 | 0.38040000 | 5.98479300 |
| C | -1.83315800 | -1.76287200 | 3.68512200 |
| C | -2.42622700 | -3.00795100 | 3.41420700 |
| C | -1.47369300 | -1.45420000 | 5.00278700 |
| C | -2.64933800 | -3.92459500 | 4.44302800 |
| H | -2.71435200 | -3.26210300 | 2.39052300 |
| C | -1.69665200 | -2.37181300 | 6.03622100 |
| H | -1.01779800 | -0.48496200 | 5.22419700 |
| C | -2.28481800 | -3.60836300 | 5.75810500 |
| H | -3.10993000 | -4.89021700 | 4.21952300 |
| H | -1.41238500 | -2.11690800 | 7.06031300 |
| H | -2.46107600 | -4.32610100 | 6.56326100 |

**TS-i-iii-3 *trans* conf2**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.696282 (Hartree/Particle)
Thermal correction to Energy= 0.731442
Thermal correction to Enthalpy= 0.732386
Thermal correction to Gibbs Free Energy= 0.626547
Sum of electronic and zero-point Energies= -3355.505837
Sum of electronic and thermal Energies= -3355.470677
Sum of electronic and thermal Enthalpies= -3355.469733
Sum of electronic and thermal Free Energies= -3355.575572

| | | | |
|---|---|---|---|
| O | -3.07037400 | -0.31440800 | -5.85630700 |
| C | -4.23032500 | 0.52430800 | -5.87239000 |
| H | -5.08104400 | -0.04875600 | -6.27730800 |
| H | -4.03332300 | 1.39312100 | -6.51289600 |
| N | -3.77892300 | -0.20757700 | -3.74316900 |
| C | -2.90596100 | -0.83920200 | -4.61479900 |
| O | -2.11955700 | -1.71634200 | -4.36137100 |
| C | -3.93894100 | -0.67939000 | -2.43334500 |
| H | -3.35041000 | -1.58569500 | -2.26398300 |
| C | -4.70157800 | -0.21006000 | -1.43521700 |
| H | -5.07774100 | 1.42642300 | -2.01782500 |
| C | -5.25818900 | -0.70674600 | -0.23964400 |
| H | -4.87983700 | -0.38376000 | 0.73953000 |
| H | -5.77909200 | -1.67068300 | -0.25441700 |
| Cu | -6.22376600 | 0.97293800 | -1.06387000 |
| P | -8.08506500 | 2.04229000 | -0.53096500 |
| C | -8.27253100 | 2.48154000 | 1.29064800 |
| C | -8.37997000 | 3.65424000 | -1.45569500 |
| C | -9.56327400 | 0.95146400 | -0.93590100 |
| C | -7.75397100 | 3.87622200 | 1.69257100 |
| C | -7.58212700 | 1.41001200 | 2.16115200 |
| H | -9.35939900 | 2.46496700 | 1.49043200 |
| C | -9.00028700 | 3.48632000 | -2.85572700 |
| C | -7.04822600 | 4.42435200 | -1.58184300 |
| H | -9.08969200 | 4.23919900 | -0.84312600 |
| C | -9.94969200 | -0.03639600 | 0.18172700 |
| C | -9.27631600 | 0.15764200 | -2.23058600 |
| H | -10.42083300 | 1.62785000 | -1.10400000 |
| C | -7.98408500 | 4.13993400 | 3.18837500 |
| H | -6.67185900 | 3.93846500 | 1.48164200 |
| H | -8.24187600 | 4.66757900 | 1.10444300 |
| C | -7.80061000 | 1.66603900 | 3.65718200 |
| H | -6.50210400 | 1.42427200 | 1.92985100 |
| H | -7.92318300 | 0.40036700 | 1.89641700 |
| C | -9.20582100 | 4.84672300 | -3.53811800 |
| H | -8.32420300 | 2.87175200 | -3.47713700 |
| H | -9.96321100 | 2.95624700 | -2.80457300 |
| C | -7.23084700 | 5.78177600 | -2.27127700 |
| H | -6.34967600 | 3.79790000 | -2.16252100 |
| H | -6.57447000 | 4.56712500 | -0.60060400 |
| C | -11.15440300 | -0.89680500 | -0.22749800 |
| H | -9.08691200 | -0.69458400 | 0.38689100 |
| H | -10.18261800 | 0.49255500 | 1.11784700 |
| C | -10.47391300 | -0.70329900 | -2.65069500 |
| H | -8.40357900 | -0.49484000 | -2.03990700 |
| H | -8.98546700 | 0.82444000 | -3.05367700 |
| C | -7.32782600 | 3.06592900 | 4.06222700 |
| H | -7.60001500 | 5.14005000 | 3.45036800 |
| H | -9.07157300 | 4.15895100 | 3.38731800 |
| H | -7.27736100 | 0.89476400 | 4.24662400 |
| H | -8.87694100 | 1.56162300 | 3.88859700 |
| C | -7.89451600 | 5.63156100 | -3.64384400 |

| | | | |
|---|---|---|---|
| H | -9.64886400 | 4.69717700 | -4.53710000 |
| H | -9.93820600 | 5.43451500 | -2.95458000 |
| H | -6.25111700 | 6.27816800 | -2.36938600 |
| H | -7.85384500 | 6.43620700 | -1.63380700 |
| C | -10.89314000 | -1.66008500 | -1.53010400 |
| H | -11.40149500 | -1.59722900 | 0.58774300 |
| H | -12.03631600 | -0.24272000 | -0.35772900 |
| H | -10.22580300 | -1.26448900 | -3.56701400 |
| H | -11.32226500 | -0.04190300 | -2.90671800 |
| H | -7.53909400 | 3.25399600 | 5.12818100 |
| H | -6.23030600 | 3.12454800 | 3.94279700 |
| H | -8.07127900 | 6.61977800 | -4.10042900 |
| H | -7.20741200 | 5.09108400 | -4.31911600 |
| H | -11.78572300 | -2.23640300 | -1.82553500 |
| H | -10.08395200 | -2.39431000 | -1.36227300 |
| C | -3.89670600 | 2.27775300 | -4.04324200 |
| C | -4.63893200 | 3.41655500 | -4.39076700 |
| C | -2.64646600 | 2.44071200 | -3.43587600 |
| C | -4.14580200 | 4.69598000 | -4.12968100 |
| H | -5.62135800 | 3.29743200 | -4.85725300 |
| C | -2.15241100 | 3.72217300 | -3.16793900 |
| H | -2.06522200 | 1.56165900 | -3.15009500 |
| C | -2.89888400 | 4.85299900 | -3.51245600 |
| H | -4.73875000 | 5.57308600 | -4.40025100 |
| H | -1.17898400 | 3.83546100 | -2.68392100 |
| H | -2.51287900 | 5.85316900 | -3.30027400 |
| C | -4.45769200 | 0.90655000 | -4.39025700 |
| H | -5.52752600 | 0.89164900 | -4.12915400 |

**TS-I-Q conf2**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.696939 (Hartree/Particle)
Thermal correction to Energy= 0.731975
Thermal correction to Enthalpy= 0.732919
Thermal correction to Gibbs Free Energy= 0.628386
Sum of electronic and zero-point Energies= -3355.499887
Sum of electronic and thermal Energies= -3355.464851
Sum of electronic and thermal Enthalpies= -3355.463906
Sum of electronic and thermal Free Energies= -3355.568439

| | | | |
|---|---|---|---|
| O | -0.40682400 | -1.53007200 | 4.15219100 |
| C | -0.61182700 | -0.25026500 | 4.75786800 |
| C | -1.17153000 | 0.62579600 | 3.62323000 |
| H | -1.34239900 | -0.34899000 | 5.57790400 |
| H | 0.34058500 | 0.12088100 | 5.15816100 |
| H | -0.34404000 | 1.06417000 | 3.03095500 |
| N | -1.79223600 | -0.41141500 | 2.80060100 |
| C | -1.15019100 | -1.62089400 | 3.01886900 |
| O | -1.21070500 | -2.61563600 | 2.34240300 |
| C | -2.34726800 | -0.14898600 | 1.50532700 |
| H | -2.21613400 | -1.02173600 | 0.85421600 |
| C | -3.54641600 | 0.62051300 | 1.33623300 |
| C | -4.82049400 | 0.39905000 | 1.65926800 |
| H | -5.16008900 | -0.51093600 | 2.18255000 |
| H | -5.60892000 | 1.12990100 | 1.43204300 |
| C | -2.06219600 | 1.74923900 | 4.09851100 |
| C | -3.35931100 | 1.50442300 | 4.57163600 |
| C | -1.56478700 | 3.05891900 | 4.11888900 |
| C | -4.14696900 | 2.55373200 | 5.04690300 |
| H | -3.75903700 | 0.48948800 | 4.53459800 |
| C | -2.34733200 | 4.11024500 | 4.60833900 |
| H | -0.55756000 | 3.25834000 | 3.74325200 |
| C | -3.64267000 | 3.86041000 | 5.06838800 |
| H | -5.16274600 | 2.35384300 | 5.39687800 |
| H | -1.94712900 | 5.12701000 | 4.61935500 |
| H | -4.26177600 | 4.68139600 | 5.43846500 |
| P | -1.99320800 | 3.73067500 | -0.33133800 |
| C | -1.79532300 | 3.54846300 | -2.19379600 |
| C | -0.63561400 | 4.92291800 | 0.19672600 |
| C | -3.61533100 | 4.64896500 | -0.07766200 |
| C | -0.33794200 | 3.56799100 | -2.69487400 |
| C | -2.47063600 | 2.23913400 | -2.66025600 |
| H | -2.31959800 | 4.40956400 | -2.64668100 |
| C | -0.99627400 | 5.86847300 | 1.35783900 |
| C | 0.63258700 | 4.11983400 | 0.55416000 |
| H | -0.42623000 | 5.55363500 | -0.68548400 |
| C | -4.74282200 | 4.16963900 | -1.01259400 |
| C | -4.06821500 | 4.48006000 | 1.38870000 |
| H | -3.42123900 | 5.71625900 | -0.28940400 |
| C | -0.27625000 | 3.42326300 | -4.22290600 |
| H | 0.21289600 | 2.73010500 | -2.23226700 |
| H | 0.17553800 | 4.49398000 | -2.39607100 |
| C | -2.41549600 | 2.08165700 | -4.18464900 |
| H | -1.93872700 | 1.39485400 | -2.18278400 |
| H | -3.50986900 | 2.17745500 | -2.31115500 |
| C | 0.17910400 | 6.79241300 | 1.70814800 |
| H | -1.25460800 | 5.27135900 | 2.24694800 |
| H | -1.88051200 | 6.47534900 | 1.11254300 |
| C | 1.80809100 | 5.03387300 | 0.91919900 |
| H | 0.38831500 | 3.45911800 | 1.40504300 |
| H | 0.91729700 | 3.44590700 | -0.26607600 |
| C | -6.06043400 | 4.90605100 | -0.72906200 |
| H | -4.89489700 | 3.08712700 | -0.85514500 |
| H | -4.46956100 | 4.30956000 | -2.06948100 |
| C | -5.38238800 | 5.21231100 | 1.67884700 |
| H | -4.19424500 | 3.39979300 | 1.57794800 |
| H | -3.29494400 | 4.81527600 | 2.09009200 |
| C | -0.97485800 | 2.14629200 | -4.70198100 |
| H | 0.77608900 | 3.43507200 | -4.55282200 |
| H | -0.76105300 | 4.30174300 | -4.68737700 |
| H | -2.89031800 | 1.13057900 | -4.47770800 |
| H | -3.01082100 | 2.88761900 | -4.65232600 |
| C | 1.44050400 | 5.99458500 | 2.05462700 |
| H | -0.10556500 | 7.45010000 | 2.54666700 |
| H | 0.39027500 | 7.45387000 | 0.84773200 |
| H | 2.68314400 | 4.42240400 | 1.19599700 |
| H | 2.10271300 | 5.61818100 | 0.02793700 |
| C | -6.49493600 | 4.75265900 | 0.73214600 |
| H | -6.84486200 | 4.53151200 | -1.40802400 |
| H | -5.93115300 | 5.97973400 | -0.96020800 |
| H | -5.66997200 | 5.04183800 | 2.72994400 |
| H | -5.23119100 | 6.30221600 | 1.56528600 |
| H | -0.95463400 | 2.08565100 | -5.80295100 |
| H | -0.41788200 | 1.26805800 | -4.32704600 |
| H | 2.28006600 | 6.67492100 | 2.27466400 |
| H | 1.25739200 | 5.41204000 | 2.97677400 |
| H | -7.42547600 | 5.31448500 | 0.91936100 |
| H | -6.72022700 | 3.68883900 | 0.93192500 |
| Cu | -2.07108500 | 1.73605100 | 0.62544600 |
| H | -0.94464600 | 0.60240100 | 0.85854200 |

**TS-I-Q conf3**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.696953 (Hartree/Particle)
Thermal correction to Energy= 0.731973
Thermal correction to Enthalpy= 0.732917
Thermal correction to Gibbs Free Energy= 0.628666
Sum of electronic and zero-point Energies= -3355.499854
Sum of electronic and thermal Energies= -3355.464834
Sum of electronic and thermal Enthalpies= -3355.463890
Sum of electronic and thermal Free Energies= -3355.568141

| | | | |
|---|---|---|---|
| O | -3.43595300 | -2.54796000 | 3.55770900 |
| C | -2.11615400 | -2.10898100 | 3.22239600 |
| C | -2.32994200 | -0.76409000 | 2.50595000 |
| H | -1.53151800 | -1.97533700 | 4.14772800 |
| H | -1.63124800 | -2.86216100 | 2.58790100 |
| H | -2.52479500 | -0.92844300 | 1.42762700 |
| N | -3.59504400 | -0.36184000 | 3.11910400 |
| C | -4.28704100 | -1.48946100 | 3.53410100 |
| O | -5.45096700 | -1.56646500 | 3.83431100 |
| C | -4.33821200 | 0.78438900 | 2.68557900 |

| | | | |
|---|---|---|---|
| H | -5.41345600 | 0.60598400 | 2.80716400 |
| C | -3.86589700 | 2.12143300 | 2.90607100 |
| C | -3.68846100 | 2.85123000 | 4.00721800 |
| H | -3.88950200 | 2.46907100 | 5.02246500 |
| H | -3.31158300 | 3.88238100 | 3.96150700 |
| C | -1.16995000 | 0.19406900 | 2.63797600 |
| C | -0.89647200 | 0.84850900 | 3.84765900 |
| C | -0.31772200 | 0.39727900 | 1.54470100 |
| C | 0.20526800 | 1.69779700 | 3.95715100 |
| H | -1.57261100 | 0.71249700 | 4.69366900 |
| C | 0.79532700 | 1.23745300 | 1.65628400 |
| H | -0.53091400 | -0.10200400 | 0.59575100 |
| C | 1.05615200 | 1.89374800 | 2.86170600 |
| H | 0.39906700 | 2.21598800 | 4.89957700 |
| H | 1.45256400 | 1.38706000 | 0.79619800 |
| H | 1.91701900 | 2.56135200 | 2.94827000 |
| P | -3.12265000 | 3.07544300 | -0.75276800 |
| C | -2.02108300 | 2.32551500 | -2.08196200 |
| C | -2.22533800 | 4.61094600 | -0.13996700 |
| C | -4.64339800 | 3.70395500 | -1.66709900 |
| C | -0.50539000 | 2.48544000 | -1.85970400 |
| C | -2.36778400 | 0.83077400 | -2.24481900 |
| H | -2.27139200 | 2.85711700 | -3.01715400 |
| C | -3.17588300 | 5.68330700 | 0.42749600 |
| C | -1.21190100 | 4.20410200 | 0.95160200 |
| H | -1.69103200 | 5.04406500 | -1.00521300 |
| C | -5.08853300 | 2.83307000 | -2.85808500 |
| C | -5.82195000 | 3.84240500 | -0.67717700 |
| H | -4.37844200 | 4.70260800 | -2.05945500 |
| C | 0.29393900 | 1.84106300 | -3.00157900 |
| H | -0.22286700 | 2.00080000 | -0.91126600 |
| H | -0.22944500 | 3.54670900 | -1.77113500 |
| C | -1.56497700 | 0.17505200 | -3.37445100 |
| H | -2.15426200 | 0.32514000 | -1.28614300 |
| H | -3.44459900 | 0.69125400 | -2.41507300 |
| C | -2.40145500 | 6.89138300 | 0.97459100 |
| H | -3.76493500 | 5.23306500 | 1.24610400 |
| H | -3.88964600 | 6.02624600 | -0.33681500 |
| C | -0.43655000 | 5.40522100 | 1.50281300 |
| H | -1.77479100 | 3.71854500 | 1.76770500 |
| H | -0.50870300 | 3.44690300 | 0.58532800 |
| C | -6.32678300 | 3.42729400 | -3.54613400 |
| H | -5.33280900 | 1.82044400 | -2.49155700 |
| H | -4.28080700 | 2.72127700 | -3.59665300 |
| C | -7.06595900 | 4.43390000 | -1.35138900 |
| H | -6.05754600 | 2.83388000 | -0.28841800 |
| H | -5.54270000 | 4.44533900 | 0.19701600 |
| C | -0.05753000 | 0.35938900 | -3.17172900 |
| H | 1.37355200 | 1.96344400 | -2.81144400 |
| H | 0.07809400 | 2.37805500 | -3.94363900 |
| H | -1.81984600 | -0.89594400 | -3.43943500 |
| H | -1.86150200 | 0.62739100 | -4.33883600 |
| C | -1.38552100 | 6.47830400 | 2.04425100 |
| H | -3.11216800 | 7.63107600 | 1.37998500 |
| H | -1.87151200 | 7.38877400 | 0.14109800 |
| H | 0.25397500 | 5.06180500 | 2.29138300 |
| H | 0.18986400 | 5.84025200 | 0.70155600 |
| C | -7.49185300 | 3.60391800 | -2.56664700 |
| H | -6.62545000 | 2.78271500 | -4.38976200 |
| H | -6.06114600 | 4.40917700 | -3.97954000 |
| H | -7.88860700 | 4.50107200 | -0.62020100 |
| H | -6.84483600 | 5.46883500 | -1.67190300 |
| H | 0.50374000 | -0.07656400 | -4.01497600 |
| H | 0.25597900 | -0.19249400 | -2.26602400 |
| H | -0.82116400 | 7.35634800 | 2.40081300 |
| H | -1.92677300 | 6.07177600 | 2.91842600 |
| H | -8.35361700 | 4.07040900 | -3.07258800 |
| H | -7.82831600 | 2.60854900 | -2.22295200 |
| Cu | -3.73848800 | 1.80755300 | 0.95384100 |
| H | -4.40510200 | 0.33840400 | 1.02955600 |

**TS-I-Q conf4**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.697362 (Hartree/Particle)
Thermal correction to Energy= 0.732247
Thermal correction to Enthalpy= 0.733191
Thermal correction to Gibbs Free Energy= 0.629548
Sum of electronic and zero-point Energies= -3355.497499
Sum of electronic and thermal Energies= -3355.462614
Sum of electronic and thermal Enthalpies= -3355.461670
Sum of electronic and thermal Free Energies= -3355.565313

| | | | |
|---|---|---|---|
| O | -0.09962500 | -1.21052400 | 4.29924400 |
| C | 0.04067800 | 0.01520900 | 5.02940100 |
| C | -1.16827300 | 0.85959800 | 4.58879800 |
| H | 0.04492200 | -0.21005200 | 6.10341000 |
| H | 0.99155900 | 0.49564300 | 4.74720300 |
| H | -0.89295100 | 1.92060300 | 4.49603700 |
| N | -1.37168600 | 0.28667800 | 3.24974200 |
| C | -0.89455700 | -1.00952400 | 3.20939600 |
| O | -1.12051300 | -1.87668700 | 2.40319000 |
| C | -2.31007500 | 0.84125200 | 2.33537500 |
| H | -2.42804100 | 1.91597200 | 2.51767000 |
| C | -2.41815300 | 0.40026100 | 0.96846400 |
| C | -1.57941900 | 0.48952000 | -0.06411800 |
| H | -0.57110500 | 0.92909400 | 0.01870700 |
| H | -1.84610400 | 0.11205600 | -1.05961800 |
| C | -2.39755900 | 0.73266600 | 5.47794200 |
| C | -2.81394200 | -0.52256700 | 5.95161900 |
| C | -3.16192100 | 1.86301300 | 5.79256900 |
| C | -3.98055700 | -0.64244000 | 6.70778000 |
| H | -2.23725800 | -1.41773800 | 5.70832700 |
| C | -4.33362800 | 1.74514900 | 6.54765000 |
| H | -2.84825100 | 2.84501800 | 5.42698400 |
| C | -4.74862200 | 0.49040300 | 7.00272900 |
| H | -4.29822900 | -1.62684200 | 7.06015600 |
| H | -4.92680200 | 2.63449100 | 6.77483100 |
| H | -5.66843200 | 0.39341100 | 7.58474600 |
| P | -5.75934600 | -1.59963100 | 1.85163900 |
| C | -5.09349300 | -3.22692700 | 2.52937000 |
| C | -6.51048900 | -2.04804500 | 0.18192900 |
| C | -7.20639900 | -1.08575600 | 2.93666400 |
| C | -4.31509000 | -4.02922400 | 1.46471900 |
| C | -4.16215200 | -2.95931900 | 3.73264500 |
| H | -5.96422800 | -3.82508900 | 2.85711200 |
| C | -7.78521900 | -1.27673500 | -0.21163600 |
| C | -5.44971800 | -1.87297900 | -0.92593100 |
| H | -6.78277700 | -3.11679400 | 0.25581300 |
| C | -7.01001700 | -1.38481000 | 4.43390300 |
| C | -7.44777800 | 0.42759400 | 2.74070100 |
| H | -8.09189100 | -1.64702500 | 2.59009900 |
| C | -3.72080600 | -5.32069700 | 2.04557400 |
| H | -3.49322300 | -3.39803800 | 1.08384200 |
| H | -4.95845800 | -4.28175900 | 0.60868600 |
| C | -3.57546700 | -4.24948800 | 4.31533400 |
| H | -3.33443700 | -2.32289600 | 3.38372100 |
| H | -4.67091100 | -2.39178300 | 4.51803600 |
| C | -8.32044500 | -1.75522100 | -1.56994900 |
| H | -7.55393500 | -0.19927800 | -0.28132800 |
| H | -8.57114100 | -1.38688600 | 0.55060100 |
| C | -5.97081600 | -2.34425800 | -2.28883400 |
| H | -5.17932800 | -0.80319000 | -0.97291200 |
| H | -4.51752300 | -2.39619600 | -0.67289300 |
| C | -8.18554400 | -0.87191200 | 5.27731600 |
| H | -6.08645200 | -0.89059900 | 4.77834700 |
| H | -6.88452900 | -2.46518700 | 4.60192800 |
| C | -8.61851300 | 0.94434200 | 3.58543600 |
| H | -6.51873000 | 0.95139200 | 3.03177000 |
| H | -7.61720500 | 0.66630800 | 1.68081800 |
| C | -2.81361400 | -5.03861400 | 3.24718500 |
| H | -3.16384000 | -5.85257600 | 1.25592900 |

| | | | |
|---|---|---|---|
| H | -4.54404600 | -5.99113500 | 2.35608000 |
| H | -2.91071700 | -3.99875800 | 5.15985800 |
| H | -4.39043500 | -4.87214700 | 4.73018700 |
| C | -7.26614300 | -1.62188000 | -2.67434100 |
| H | -9.22852900 | -1.18634500 | -1.83180100 |
| H | -8.62717500 | -2.81398400 | -1.48300700 |
| H | -5.19671100 | -2.18682800 | -3.05837500 |
| H | -6.15675000 | -3.43367200 | -2.24882900 |
| C | -8.41615900 | 0.62811700 | 5.07049200 |
| H | -7.99447100 | -1.09042500 | 6.34180600 |
| H | -9.10301100 | -1.42460500 | 5.00242300 |
| H | -8.73572700 | 2.03031600 | 3.43208200 |
| H | -9.55648200 | 0.47446300 | 3.23559200 |
| H | -2.41927400 | -5.98103700 | 3.66327100 |
| H | -1.94780000 | -4.43845700 | 2.91647800 |
| H | -7.65811500 | -2.00953700 | -3.62968400 |
| H | -7.04652900 | -0.55028000 | -2.83496300 |
| H | -9.28042600 | 0.97276000 | 5.66285200 |
| H | -7.53394800 | 1.18164100 | 5.44129500 |
| Cu | -4.07252400 | -0.16346500 | 1.89979100 |
| H | -3.79945800 | 0.54089900 | 3.29641600 |

***(E)* Allylic System/(E) s-*trans***

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.229284 (Hartree/Particle)
Thermal correction to Energy= 0.242539
Thermal correction to Enthalpy= 0.243483
Thermal correction to Gibbs Free Energy= 0.188213
Sum of electronic and zero-point Energies= -669.626959
Sum of electronic and thermal Energies= -669.613704
Sum of electronic and thermal Enthalpies= -669.612760
Sum of electronic and thermal Free Energies= -669.668030

| | | | |
|---|---|---|---|
| O | 0.55494800 | 5.67559000 | -0.32647000 |
| C | 0.38547400 | 6.59219100 | -1.40962300 |
| C | -0.97040300 | 6.22011200 | -2.06598900 |
| H | 0.35924500 | 7.61702200 | -1.00731000 |
| H | 1.23296700 | 6.49615900 | -2.10134500 |
| H | -0.81298300 | 5.59778000 | -2.96616700 |
| N | -1.55073800 | 5.39890300 | -1.01129400 |
| C | -0.61321700 | 5.04370000 | -0.05434500 |
| O | -0.76458000 | 4.29165000 | 0.87369300 |
| C | -2.78124200 | 4.73571900 | -1.09101400 |
| H | -2.97033500 | 4.11629400 | -0.20992100 |
| C | -3.65520700 | 4.81113600 | -2.10627400 |
| H | -3.43547700 | 5.44818700 | -2.96824800 |
| C | -1.78266700 | 7.44192300 | -2.45097300 |
| C | -2.47241800 | 8.18117500 | -1.47883600 |
| C | -1.81149000 | 7.87158700 | -3.78375100 |
| C | -3.18020600 | 9.33070700 | -1.83610900 |
| H | -2.46407100 | 7.84254200 | -0.43975100 |
| C | -2.51458300 | 9.02689000 | -4.14246400 |
| H | -1.28446100 | 7.29516400 | -4.54960800 |
| C | -3.20158400 | 9.75825400 | -3.16924700 |
| H | -3.72095900 | 9.89443300 | -1.07171100 |
| H | -2.52957700 | 9.35179700 | -5.18583900 |
| H | -3.75670900 | 10.65734200 | -3.44819900 |
| C | -4.96093000 | 4.07181400 | -2.12787100 |
| H | -5.02929600 | 3.40311100 | -3.00418200 |
| H | -5.10025600 | 3.45912700 | -1.22325900 |
| H | -5.81507400 | 4.76840100 | -2.20083200 |

***(Z)* Allylic System**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.229135 (Hartree/Particle)
Thermal correction to Energy= 0.242288
Thermal correction to Enthalpy= 0.243233
Thermal correction to Gibbs Free Energy= 0.188188
Sum of electronic and zero-point Energies= -669.622133
Sum of electronic and thermal Energies= -669.608979
Sum of electronic and thermal Enthalpies= -669.608035
Sum of electronic and thermal Free Energies= -669.663080

| | | | |
|---|---|---|---|
| O | -0.09664000 | 7.01830800 | 0.71502800 |
| C | -0.20910900 | 6.57154500 | -0.63781700 |
| C | -1.27009000 | 5.45021500 | -0.59871500 |
| H | 0.77166300 | 6.22569400 | -0.98983200 |
| H | -0.54967500 | 7.40944200 | -1.26838900 |
| N | -1.98206100 | 5.83100500 | 0.61998300 |
| C | -1.19734700 | 6.64228300 | 1.42301300 |
| O | -1.39492000 | 6.97763900 | 2.56145000 |
| C | -3.08547800 | 5.08620000 | 1.08975400 |
| H | -3.02399500 | 4.01215800 | 0.88077200 |
| C | -4.14089200 | 5.60506800 | 1.73312800 |
| H | -4.89074300 | 4.88954600 | 2.08647000 |
| H | -0.78291100 | 4.46715300 | -0.45215900 |
| C | -2.13508900 | 5.39079500 | -1.83898100 |
| C | -3.16275700 | 6.32508700 | -2.04204000 |
| C | -1.88824900 | 4.42393800 | -2.82259800 |
| C | -3.92669300 | 6.29276300 | -3.21072500 |
| H | -3.36871100 | 7.07199200 | -1.27168900 |
| C | -2.64840700 | 4.39435100 | -3.99661300 |
| H | -1.09634300 | 3.68534700 | -2.66817400 |
| C | -3.66984900 | 5.32856900 | -4.19277200 |
| H | -4.72856600 | 7.02126200 | -3.35497500 |
| H | -2.44545700 | 3.63538700 | -4.75637200 |
| H | -4.26892300 | 5.30307600 | -5.10649000 |
| C | -4.37864600 | 7.05571000 | 2.02015800 |
| H | -5.45341300 | 7.29307700 | 1.97845100 |
| H | -4.00748400 | 7.32698200 | 3.02264300 |
| H | -3.84398000 | 7.69992800 | 1.30508300 |

**ii'-3**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.937321 (Hartree/Particle)
Thermal correction to Energy= 0.986032
Thermal correction to Enthalpy= 0.986976
Thermal correction to Gibbs Free Energy= 0.853079
Sum of electronic and zero-point Energies= -3951.045958
Sum of electronic and thermal Energies= -3950.997247
Sum of electronic and thermal Enthalpies= -3950.996302
Sum of electronic and thermal Free Energies= -3951.130199

| | | | |
|---|---|---|---|
| C | 1.58475300 | 0.26527500 | -3.96487800 |
| H | 1.08493600 | -0.62149100 | -4.36800400 |
| C | 0.99230500 | 1.06141800 | -3.04556200 |
| H | 1.55786100 | 1.93941600 | -2.71810100 |
| C | -0.26542200 | 0.80524900 | -2.34220300 |
| H | -0.90886300 | 0.10375000 | -2.89513600 |
| Cu | 0.08961700 | -0.28762900 | -0.58279200 |
| P | -0.77114000 | -0.56040900 | 1.51992100 |
| C | -0.64339400 | 0.90371400 | 2.69811000 |
| C | -2.60742900 | -0.96227700 | 1.42161900 |
| C | -0.02187000 | -1.99176100 | 2.47283000 |
| C | -1.73955100 | 1.96685800 | 2.49705600 |
| C | 0.75754600 | 1.53560700 | 2.57330400 |
| H | -0.75955700 | 0.50413400 | 3.71939800 |
| C | -2.86650500 | -2.46737000 | 1.22582800 |
| C | -3.21170300 | -0.17052900 | 0.24269000 |
| H | -3.08259400 | -0.64299600 | 2.36627400 |
| C | -0.48623300 | -2.15636000 | 3.92902600 |
| C | 1.51387300 | -2.04684100 | 2.37200600 |
| H | -0.39021300 | -2.85609400 | 1.89780300 |
| C | -1.54335900 | 3.17263300 | 3.42593200 |
| H | -1.72486800 | 2.31694500 | 1.45387900 |
| H | -2.73579800 | 1.53175000 | 2.66473600 |
| C | 0.94161500 | 2.75813200 | 3.48030700 |
| H | 0.90704900 | 1.83103200 | 1.52131000 |
| H | 1.53769200 | 0.79180600 | 2.79176100 |
| C | -4.35003800 | -2.77460400 | 0.98250000 |
| H | -2.28287100 | -2.82029000 | 0.36135400 |
| H | -2.51989500 | -3.04471300 | 2.09521000 |
| C | -4.69242800 | -0.47695700 | 0.00697400 |

| | | | |
|---|---|---|---|
| H | -2.65237400 | -0.43184800 | -0.67086000 |
| H | -3.07414200 | 0.91099600 | 0.37441300 |
| C | 0.05476400 | -3.46154800 | 4.53150700 |
| H | -0.11438100 | -1.31058600 | 4.53376300 |
| H | -1.58626300 | -2.13013800 | 3.99665700 |
| C | 2.06088600 | -3.34018700 | 2.99221300 |
| H | 1.96131700 | -1.18625300 | 2.89804400 |
| H | 1.81384500 | -1.96679600 | 1.31657900 |
| C | -0.15694000 | 3.80075100 | 3.25158700 |
| H | -2.33364800 | 3.91789000 | 3.23477800 |
| H | -1.66539400 | 2.84679300 | 4.47532900 |
| H | 1.93838600 | 3.19945800 | 3.30938800 |
| H | 0.91976400 | 2.43244000 | 4.53634800 |
| C | -4.91399100 | -1.97811200 | -0.19786000 |
| H | -4.47061100 | -3.85806300 | 0.81360800 |
| H | -4.92623900 | -2.53067300 | 1.89459800 |
| H | -5.03209600 | 0.09387100 | -0.87168900 |
| H | -5.28791800 | -0.13099600 | 0.87262900 |
| C | 1.58433800 | -3.52344200 | 4.43825200 |
| H | -0.27252200 | -3.55810100 | 5.58042000 |
| H | -0.38016300 | -4.31841700 | 3.98482900 |
| H | 3.16273000 | -3.34247200 | 2.94402500 |
| H | 1.71919000 | -4.20139300 | 2.39087700 |
| H | -0.02891500 | 4.65342000 | 3.93882000 |
| H | -0.06636800 | 4.20774300 | 2.22760600 |
| H | -5.98532700 | -2.20047300 | -0.33775300 |
| H | -4.40013500 | -2.29359300 | -1.12449000 |
| H | 1.95686900 | -4.47735600 | 4.84783500 |
| H | 2.01596100 | -2.72201200 | 5.06643000 |
| C | 2.58844800 | -1.42787000 | -1.79054700 |
| N | 1.38944900 | -1.71481800 | -1.40597100 |
| C | -0.16597100 | -3.66704000 | -1.44698100 |
| C | 0.35560200 | -4.29202700 | -0.30538900 |
| C | -1.44726400 | -4.02960800 | -1.88863100 |
| C | -0.38726500 | -5.25606300 | 0.38160900 |
| H | 1.34989500 | -4.01105200 | 0.04749000 |
| C | -2.18842600 | -5.00327700 | -1.21110200 |
| H | -1.87290800 | -3.53809200 | -2.76799300 |
| C | -1.66155000 | -5.61715700 | -0.07061600 |
| H | 0.02915600 | -5.72650800 | 1.27619200 |
| H | -3.18815800 | -5.26756800 | -1.56446100 |
| H | -2.24393100 | -6.36863300 | 0.46817900 |
| C | 0.65780700 | -2.67071000 | -2.23178100 |
| H | -0.01127000 | -2.09578000 | -2.89300400 |
| H | 1.35106800 | -3.22180200 | -2.89722500 |
| H | 3.03468100 | -1.96820800 | -2.64133000 |
| C | 3.44736200 | -0.41543300 | -1.16970500 |
| C | 4.70845900 | -0.14933600 | -1.73925200 |
| C | 3.05043100 | 0.33243800 | -0.04447800 |
| C | 5.53578600 | 0.84263000 | -1.21310000 |
| H | 5.03059800 | -0.71840600 | -2.61576300 |
| C | 3.87704600 | 1.32368200 | 0.48303100 |
| H | 2.08871400 | 0.12657400 | 0.42528900 |
| C | 5.12076000 | 1.58738500 | -0.10112200 |
| H | 6.50680700 | 1.04137100 | -1.67331700 |
| H | 3.54710200 | 1.89495400 | 1.35406700 |
| H | 5.76547800 | 2.36927100 | 0.30789300 |
| H | 2.58301000 | 0.48969600 | -4.34881400 |
| N | -1.09286600 | 1.98901100 | -2.06731900 |
| C | -0.70450100 | 2.99037600 | -1.08565300 |
| C | -2.45096500 | 1.91077100 | -2.17295700 |
| C | -2.01697700 | 3.79560700 | -0.96092000 |
| O | -3.03199200 | 2.92351700 | -1.44847500 |
| O | -3.11573700 | 1.08205100 | -2.75653100 |
| H | -2.24622000 | 4.08269700 | 0.07511300 |
| H | -1.98720200 | 4.70538500 | -1.58251100 |
| H | -0.46857600 | 2.46170700 | -0.14352900 |
| C | 0.48902100 | 3.84657100 | -1.46030600 |
| C | 1.56828000 | 3.98338700 | -0.57972700 |
| C | 0.53571000 | 4.50668700 | -2.69840600 |
| C | 2.67880000 | 4.76190300 | -0.92464800 |
| H | 1.55257800 | 3.45772900 | 0.37617900 |
| C | 1.64101500 | 5.28389600 | -3.04675000 |
| H | -0.28948400 | 4.37939100 | -3.40391600 |
| C | 2.71795500 | 5.41396900 | -2.15944700 |
| H | 3.51826400 | 4.84623400 | -0.23014000 |
| H | 1.66957200 | 5.78383500 | -4.01831900 |
| H | 3.58644200 | 6.01737600 | -2.43548700 |

**TS-ii'-X**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.937679 (Hartree/Particle)
Thermal correction to Energy= 0.985253
Thermal correction to Enthalpy= 0.986197
Thermal correction to Gibbs Free Energy= 0.855609
Sum of electronic and zero-point Energies= -3951.039139
Sum of electronic and thermal Energies= -3950.991566
Sum of electronic and thermal Enthalpies= -3950.990621
Sum of electronic and thermal Free Energies= -3951.121209

| | | | |
|---|---|---|---|
| C | -2.88683700 | 3.50656300 | -0.00221000 |
| H | -3.37576700 | 2.70120400 | -0.55841200 |
| C | -3.67720800 | 4.44736800 | 0.66169400 |
| H | -3.18322600 | 5.37352500 | 0.96303700 |
| C | -4.98041500 | 4.23107800 | 1.13737200 |
| H | -5.58538700 | 3.44609800 | 0.66956100 |
| Cu | -4.61737800 | 2.95400900 | 3.06342500 |
| P | -5.54255100 | 2.86723100 | 5.13050800 |
| C | -5.39385400 | 4.33344600 | 6.29972400 |
| C | -7.37527600 | 2.45994200 | 5.05446300 |
| C | -4.77085400 | 1.44003200 | 6.07212300 |
| C | -6.48446400 | 5.40358500 | 6.11120100 |
| C | -3.98934300 | 4.95563800 | 6.16972100 |
| H | -5.50532600 | 3.93112500 | 7.32041700 |
| C | -7.62876100 | 0.95358700 | 4.86321100 |
| C | -7.98655200 | 3.24449500 | 3.87599300 |
| H | -7.84291700 | 2.78271900 | 6.00153900 |
| C | -5.21867700 | 1.27879000 | 7.53405700 |
| C | -3.23612300 | 1.38081700 | 5.95232500 |
| H | -5.14704800 | 0.57586800 | 5.50223600 |
| C | -6.27543200 | 6.60127300 | 7.04800500 |
| H | -6.47229800 | 5.76034800 | 5.07061400 |
| H | -7.48281800 | 4.97371600 | 6.28040400 |
| C | -3.79263900 | 6.16616300 | 7.08993000 |
| H | -3.84190100 | 5.26380600 | 5.12132400 |
| H | -3.21322600 | 4.20396900 | 6.37310800 |
| C | -9.11214900 | 0.63978300 | 4.62911000 |
| H | -7.04877600 | 0.60283000 | 3.99536900 |
| H | -7.27360800 | 0.37907500 | 5.73081300 |
| C | -9.46685000 | 2.93161200 | 3.64523700 |
| H | -7.42689700 | 2.97742800 | 2.96396600 |
| H | -7.85349000 | 4.32682300 | 4.00445000 |
| C | -4.67647700 | -0.02934300 | 8.12915500 |
| H | -4.83465700 | 2.12255000 | 8.13402900 |
| H | -6.31766900 | 1.30980900 | 7.61623300 |
| C | -2.68972300 | 0.08354100 | 6.56477100 |
| H | -2.77925800 | 2.23813600 | 6.47552300 |
| H | -2.94697800 | 1.45992200 | 4.89340800 |
| C | -4.88404300 | 7.21953900 | 6.87622000 |
| H | -7.06010300 | 7.35446400 | 6.86489300 |
| H | -6.39805800 | 6.26792300 | 8.09486100 |
| H | -2.79319900 | 6.60149800 | 6.92029600 |
| H | -3.81355400 | 5.82845200 | 8.14215600 |
| C | -9.68426900 | 1.42893800 | 3.44786500 |
| H | -9.22850100 | -0.44460700 | 4.46457200 |
| H | -9.68499400 | 0.88485300 | 5.54300300 |
| H | -9.81313200 | 3.49735400 | 2.76584200 |
| H | -10.05984900 | 3.27980100 | 4.51159400 |
| C | -3.14863800 | -0.09931200 | 8.01645100 |
| H | -4.99148600 | -0.12418500 | 9.18196800 |
| H | -5.12294000 | -0.88355800 | 7.58769900 |

| | | | |
|---|---|---|---|
| H | -1.58871200 | 0.07542500 | 6.50227900 |
| H | -3.04352500 | -0.77470700 | 5.96609000 |
| H | -4.74772800 | 8.06333600 | 7.57269800 |
| H | -4.79266300 | 7.63780800 | 5.85679100 |
| H | -10.75555700 | 1.20297400 | 3.31401600 |
| H | -9.17347600 | 1.11080400 | 2.52062100 |
| H | -2.77662000 | -1.05589700 | 8.42025300 |
| H | -2.70482700 | 0.69884400 | 8.64032300 |
| C | -2.22945800 | 2.17747900 | 1.61087700 |
| N | -3.35379200 | 1.70453200 | 2.15215900 |
| C | -4.91920800 | -0.23807900 | 2.11569900 |
| C | -4.44530300 | -0.86136300 | 3.28013100 |
| C | -6.20550600 | -0.56016000 | 1.65859100 |
| C | -5.23219100 | -1.79047800 | 3.96495700 |
| H | -3.44910600 | -0.60345400 | 3.64477800 |
| C | -6.99427900 | -1.49716900 | 2.33625100 |
| H | -6.59557000 | -0.06933900 | 0.76227200 |
| C | -6.50964300 | -2.11569200 | 3.49238600 |
| H | -4.84874800 | -2.26277600 | 4.87348100 |
| H | -7.99662200 | -1.73055600 | 1.96834300 |
| H | -7.12721800 | -2.84032300 | 4.02897500 |
| C | -4.02962500 | 0.70503000 | 1.33529600 |
| H | -4.63812700 | 1.19690100 | 0.55069700 |
| H | -3.28426200 | 0.09335000 | 0.78566500 |
| H | -1.71349300 | 1.54893000 | 0.86917300 |
| C | -1.32759900 | 3.10273800 | 2.33592300 |
| C | -0.04324100 | 3.36533000 | 1.81731100 |
| C | -1.70682700 | 3.77339000 | 3.51209300 |
| C | 0.81406600 | 4.27456100 | 2.43611100 |
| H | 0.27728200 | 2.85425600 | 0.90464900 |
| C | -0.85243800 | 4.68779800 | 4.13352100 |
| H | -2.68098400 | 3.56912500 | 3.95793400 |
| C | 0.41153100 | 4.94872800 | 3.59779200 |
| H | 1.80350500 | 4.46203500 | 2.01058200 |
| H | -1.17883200 | 5.19623300 | 5.04464000 |
| H | 1.08087500 | 5.66497900 | 4.08091900 |
| H | -1.91965400 | 3.82777800 | -0.39360400 |
| N | -5.81713700 | 5.33283500 | 1.53601600 |
| C | -5.42443400 | 6.34005500 | 2.51462600 |
| C | -7.17975700 | 5.23083600 | 1.44539100 |
| C | -6.75559700 | 7.11049200 | 2.66877600 |
| O | -7.76153900 | 6.22109000 | 2.18899800 |
| O | -7.82738400 | 4.39823500 | 0.85266000 |
| H | -6.97461400 | 7.38222300 | 3.71033600 |
| H | -6.75800400 | 8.02513200 | 2.05487000 |
| H | -5.15590000 | 5.81156300 | 3.44731900 |
| C | -4.26635700 | 7.23458200 | 2.11916900 |
| C | -3.17262800 | 7.39548600 | 2.97800900 |
| C | -4.26820500 | 7.90476300 | 0.88578300 |
| C | -2.09340400 | 8.20795500 | 2.61401500 |
| H | -3.14889600 | 6.86012700 | 3.92840300 |
| C | -3.19296000 | 8.71523500 | 0.51897300 |
| H | -5.10590600 | 7.76226800 | 0.19787900 |
| C | -2.10086200 | 8.86911600 | 1.38329000 |
| H | -1.24090500 | 8.31026200 | 3.28972600 |
| H | -3.20034500 | 9.22277800 | -0.44893500 |
| H | -1.25592200 | 9.49828400 | 1.09242100 |

**X**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.939616 (Hartree/Particle)

Thermal correction to Energy= 0.987510

Thermal correction to Enthalpy= 0.988454

Thermal correction to Gibbs Free Energy= 0.854780

Sum of electronic and zero-point Energies= -3951.064559

Sum of electronic and thermal Energies= -3951.016665

Sum of electronic and thermal Enthalpies= -3951.015721

Sum of electronic and thermal Free Energies= -3951.149395

| | | | |
|---|---|---|---|
| C | 1.88090600 | 0.01095400 | -3.43290200 |
| H | 1.37055000 | -0.61894900 | -4.17814900 |
| C | 0.93886700 | 1.03876100 | -2.89507200 |
| H | 1.37977800 | 1.83833000 | -2.30099000 |
| C | -0.39541200 | 0.98761200 | -3.02175600 |
| H | -0.90465400 | 0.21054400 | -3.59736800 |
| Cu | 0.42487200 | -1.01839700 | -0.25577100 |
| P | -0.61697800 | -0.72014300 | 1.65765100 |
| C | -0.16995500 | 0.82414600 | 2.62950600 |
| C | -2.46804100 | -0.87949800 | 1.45997400 |
| C | -0.11549900 | -2.11710800 | 2.78913100 |
| C | -1.23641500 | 1.92964200 | 2.69852600 |
| C | 1.15509400 | 1.38567100 | 2.07419200 |
| H | 0.00811400 | 0.48220500 | 3.66380000 |
| C | -2.79138800 | -2.34013200 | 1.07752000 |
| C | -2.94729100 | 0.06890900 | 0.34176600 |
| H | -2.97200400 | -0.62241000 | 2.40785300 |
| C | -0.85272200 | -2.19649800 | 4.13534000 |
| C | 1.41152700 | -2.14469800 | 2.98721700 |
| H | -0.37259700 | -3.01068400 | 2.19573800 |
| C | -0.74202500 | 3.11210800 | 3.54359700 |
| H | -1.45546100 | 2.29413900 | 1.68113500 |
| H | -2.18233400 | 1.53812800 | 3.10438100 |
| C | 1.64685100 | 2.59702800 | 2.87408700 |
| H | 0.99965000 | 1.66524500 | 1.01706000 |
| H | 1.93138800 | 0.60694900 | 2.04730000 |
| C | -4.26189400 | -2.54142200 | 0.69444700 |
| H | -2.15411200 | -2.62535800 | 0.22268200 |
| H | -2.53480300 | -3.02816800 | 1.89575400 |
| C | -4.42395900 | -0.13251300 | -0.01400200 |
| H | -2.33001900 | -0.13217800 | -0.55247000 |
| H | -2.77172000 | 1.11778300 | 0.61384000 |
| C | -0.41652000 | -3.44213500 | 4.92262400 |
| H | -0.62999600 | -1.29553200 | 4.73484800 |
| H | -1.94407000 | -2.21097000 | 3.98492300 |
| C | 1.83906000 | -3.39231600 | 3.77022600 |
| H | 1.73524300 | -1.24502900 | 3.54085400 |
| H | 1.91222500 | -2.10755100 | 2.00703200 |
| C | 0.56992300 | 3.68315600 | 2.99196400 |
| H | -1.51761100 | 3.89537600 | 3.58062700 |
| H | -0.58685900 | 2.77311700 | 4.58434000 |
| H | 2.56001000 | 3.00122000 | 2.40573300 |
| H | 1.93657000 | 2.26299500 | 3.88730500 |
| C | -4.69684400 | -1.58311600 | -0.41702500 |
| H | -4.41049800 | -3.58980400 | 0.38671900 |
| H | -4.89679600 | -2.37835000 | 1.58524900 |
| H | -4.69515500 | 0.55636700 | -0.82730200 |
| H | -5.04899800 | 0.13266500 | 0.85915700 |
| C | 1.10476400 | -3.48754500 | 5.11339300 |
| H | -0.92909600 | -3.46951000 | 5.89881300 |
| H | -0.74083300 | -4.34383100 | 4.37135400 |
| H | 2.93090700 | -3.38436800 | 3.92543000 |
| H | 1.61334700 | -4.28954400 | 3.16511600 |
| H | 0.92697900 | 4.51047800 | 3.62754200 |
| H | 0.37792000 | 4.11868800 | 1.99475800 |
| H | -5.76369200 | -1.72615800 | -0.65706000 |
| H | -4.13016200 | -1.80807100 | -1.33878800 |
| H | 1.39662300 | -4.40701000 | 5.64783200 |
| H | 1.41369900 | -2.64041900 | 5.75382300 |
| C | 2.44874100 | -0.94731300 | -2.32570200 |
| N | 1.43359300 | -1.73639300 | -1.68357800 |
| C | -0.03276600 | -3.69518600 | -1.69419000 |
| C | 0.43674600 | -4.22782300 | -0.48000500 |
| C | -1.32374500 | -4.04429400 | -2.11506700 |
| C | -0.35432000 | -5.09159500 | 0.28063300 |
| H | 1.42999500 | -3.93416800 | -0.13458400 |
| C | -2.12103200 | -4.91219200 | -1.35749800 |
| H | -1.71424300 | -3.62304300 | -3.04615900 |
| C | -1.63919400 | -5.43932800 | -0.15636000 |
| H | 0.03090000 | -5.49428900 | 1.22173300 |
| H | -3.12796500 | -5.16335800 | -1.70127200 |
| H | -2.26317000 | -6.10865400 | 0.44159300 |

| | | | |
|---|---|---|---|
| C | 0.84529100 | -2.75958000 | -2.50737200 |
| H | 0.22826600 | -2.37757600 | -3.35600300 |
| H | 1.64092200 | -3.37253200 | -2.99946800 |
| H | 3.15341300 | -1.61945400 | -2.87448900 |
| C | 3.29526600 | -0.22269300 | -1.26644600 |
| C | 3.79952700 | 1.07945400 | -1.41764600 |
| C | 3.59430500 | -0.89756800 | -0.06787300 |
| C | 4.53391900 | 1.69850800 | -0.39759800 |
| H | 3.61906000 | 1.64043600 | -2.33540900 |
| C | 4.33567300 | -0.29134100 | 0.94812900 |
| H | 3.20779200 | -1.90986900 | 0.05298500 |
| C | 4.80037700 | 1.02023700 | 0.79446900 |
| H | 4.89370300 | 2.72128000 | -0.54015400 |
| H | 4.54265300 | -0.84253200 | 1.86984600 |
| H | 5.36742100 | 1.50564200 | 1.59313800 |
| H | 2.71737400 | 0.49879800 | -3.96351900 |
| N | -1.28806500 | 1.90199300 | -2.44020000 |
| C | -0.91761700 | 2.85494700 | -1.39853300 |
| C | -2.65255800 | 1.69967800 | -2.48772400 |
| C | -2.30076100 | 3.47837400 | -1.08911600 |
| O | -3.26100100 | 2.58436300 | -1.65434600 |
| O | -3.25386700 | 0.87083800 | -3.12404000 |
| H | -2.49029400 | 3.57755300 | -0.01159900 |
| H | -2.40807700 | 4.46502300 | -1.56527000 |
| H | -0.53472600 | 2.28364100 | -0.53379900 |
| C | 0.11974100 | 3.88661600 | -1.79909100 |
| C | 1.19573400 | 4.17276100 | -0.94914100 |
| C | 0.01427500 | 4.56796900 | -3.02013000 |
| C | 2.15092100 | 5.12943200 | -1.30804600 |
| H | 1.30477200 | 3.62580100 | -0.01118500 |
| C | 0.96882600 | 5.52044500 | -3.38282600 |
| H | -0.81098900 | 4.33382200 | -3.69785900 |
| C | 2.03965400 | 5.80545700 | -2.52634200 |
| H | 2.98791200 | 5.33663400 | -0.63670600 |
| H | 0.88155000 | 6.03886400 | -4.34096300 |
| H | 2.78809700 | 6.54845600 | -2.81281500 |

**TS-iii'-iv-3 *cis (S,S,S)* conf2**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.937168 (Hartree/Particle)
Thermal correction to Energy= 0.984737
Thermal correction to Enthalpy= 0.985681
Thermal correction to Gibbs Free Energy= 0.853783
Sum of electronic and zero-point Energies= -3951.035426
Sum of electronic and thermal Energies= -3950.987856
Sum of electronic and thermal Enthalpies= -3950.986912
Sum of electronic and thermal Free Energies= -3951.118811

| | | | |
|---|---|---|---|
| O | -2.12828200 | 6.06770400 | -2.49252800 |
| C | -1.65618400 | 6.73328500 | -1.31590800 |
| C | -2.13505000 | 5.84519100 | -0.15142400 |
| H | -0.55672500 | 6.79229700 | -1.35609300 |
| H | -2.07178900 | 7.74900500 | -1.28395600 |
| H | -3.12468500 | 6.18130700 | 0.20777300 |
| N | -2.31245600 | 4.56194500 | -0.85574700 |
| C | -2.42170200 | 4.77281500 | -2.19192300 |
| O | -2.75047200 | 3.99006400 | -3.06705300 |
| C | -2.79556700 | 3.40441100 | -0.15092300 |
| H | -2.27276200 | 3.29585600 | 0.80206200 |
| C | -4.19613100 | 3.12248000 | -0.15418100 |
| H | -4.49826200 | 2.40377100 | 0.61830500 |
| C | -5.12521700 | 3.43981700 | -1.10469200 |
| H | -6.14810400 | 3.06989100 | -1.01606100 |
| H | -4.95097500 | 4.20153300 | -1.86529200 |
| Cu | -4.00379100 | 2.07140900 | -3.16676000 |
| P | -5.05202900 | 2.20440300 | -5.12353100 |
| C | -4.91240200 | 3.88350500 | -5.94438400 |
| C | -6.91535600 | 1.91686300 | -5.03233300 |
| C | -4.40295600 | 0.95399200 | -6.35502100 |
| C | -5.49496400 | 4.95957600 | -5.00392400 |
| C | -3.44791600 | 4.21094900 | -6.30321600 |
| H | -5.51431900 | 3.85630800 | -6.87141600 |
| C | -7.35229900 | 0.48501300 | -5.39327000 |
| C | -7.39927400 | 2.26368100 | -3.60797100 |
| H | -7.38322400 | 2.61535100 | -5.75009400 |
| C | -4.77909800 | 1.19124800 | -7.82730000 |
| C | -2.88816300 | 0.71493600 | -6.19009900 |
| H | -4.88684100 | 0.02007200 | -6.02259000 |
| C | -5.31508200 | 6.38012700 | -5.55364100 |
| H | -4.97775900 | 4.87696200 | -4.03370200 |
| H | -6.56411700 | 4.77097500 | -4.81961300 |
| C | -3.28814500 | 5.63915700 | -6.84262900 |
| H | -2.83107400 | 4.09420400 | -5.39852200 |
| H | -3.07027400 | 3.49885300 | -7.05138300 |
| C | -8.86500400 | 0.28654600 | -5.21919600 |
| H | -6.82130300 | -0.22919200 | -4.74344500 |
| H | -7.07577400 | 0.23918600 | -6.42910900 |
| C | -8.91088300 | 2.07526400 | -3.44390800 |
| H | -6.86473800 | 1.60807800 | -2.89822600 |
| H | -7.11040200 | 3.28988100 | -3.33864400 |
| C | -4.29755000 | 0.03073100 | -8.71069600 |
| H | -4.31393800 | 2.12633800 | -8.18259200 |
| H | -5.86758400 | 1.32698800 | -7.93593300 |
| C | -2.41441500 | -0.43827000 | -7.08345400 |
| H | -2.32459400 | 1.62730700 | -6.44473900 |
| H | -2.67056600 | 0.50096700 | -5.13262400 |
| C | -3.84515100 | 6.67777200 | -5.86422200 |
| H | -5.71528600 | 7.10875000 | -4.82814000 |
| H | -5.91406900 | 6.49390400 | -6.47661500 |
| H | -2.22270600 | 5.83529900 | -7.05132300 |
| H | -3.81929900 | 5.72848700 | -7.80910100 |
| C | -9.33112900 | 0.64734100 | -3.80518000 |
| H | -9.12705100 | -0.75853700 | -5.45691300 |
| H | -9.40079800 | 0.91947800 | -5.95097000 |
| H | -9.20590200 | 2.31704300 | -2.40874500 |
| H | -9.44274700 | 2.79123300 | -4.09798900 |
| C | -2.79008600 | -0.20542600 | -8.55231100 |
| H | -4.54842600 | 0.22987000 | -9.76630700 |
| H | -4.84152200 | -0.88867200 | -8.42528000 |
| H | -1.32474000 | -0.57276600 | -6.97876500 |
| H | -2.88229600 | -1.37729400 | -6.73526000 |
| H | -3.73623400 | 7.69514000 | -6.27721800 |
| H | -3.26218900 | 6.64504300 | -4.92669900 |
| H | -10.42414800 | 0.52779300 | -3.71649000 |
| H | -8.87340000 | -0.05539900 | -3.08571600 |
| H | -2.46805300 | -1.05890800 | -9.17239700 |
| H | -2.24497900 | 0.68019800 | -8.92877600 |
| C | -1.18733400 | 5.78277600 | 1.02595300 |
| C | 0.13001500 | 5.32749000 | 0.85974500 |
| C | -1.61506200 | 6.17229400 | 2.30169700 |
| C | 1.00122600 | 5.26428500 | 1.94867900 |
| H | 0.46780100 | 4.99896500 | -0.12447000 |
| C | -0.74207800 | 6.11621100 | 3.39415800 |
| H | -2.64294100 | 6.51780400 | 2.44302100 |
| C | 0.56792900 | 5.66097400 | 3.22000600 |
| H | 2.02215200 | 4.90078700 | 1.80537200 |
| H | -1.08939700 | 6.42386500 | 4.38371200 |
| H | 1.25005600 | 5.61186500 | 4.07259400 |
| C | -2.08240100 | 1.51162900 | -1.07649600 |
| N | -3.04354400 | 0.97816100 | -1.83839800 |
| C | -4.63974000 | -0.88887900 | -2.14954800 |
| C | -3.97190400 | -1.41229900 | -3.26867500 |
| C | -5.97380600 | -1.26284300 | -1.93347500 |
| C | -4.61731800 | -2.29129400 | -4.14167900 |
| H | -2.93854300 | -1.10950700 | -3.44767400 |
| C | -6.62258600 | -2.14985700 | -2.80059100 |
| H | -6.51449700 | -0.84965400 | -1.07679900 |
| C | -5.94624200 | -2.66779900 | -3.90901200 |
| H | -4.08084000 | -2.68692700 | -5.00819200 |
| H | -7.66452100 | -2.42490400 | -2.61679900 |
| H | -6.45337100 | -3.35253400 | -4.59354600 |

| | | | |
|---|---|---|---|
| C | -3.91859400 | 0.02248700 | -1.17542800 |
| H | -4.67380900 | 0.52463100 | -0.54205600 |
| H | -3.33124100 | -0.61845100 | -0.48367200 |
| H | -1.94050300 | 1.06792800 | -0.07794700 |
| C | -0.79701800 | 1.98377500 | -1.65871100 |
| C | 0.26417600 | 2.32334400 | -0.80062500 |
| C | -0.56911600 | 2.04029900 | -3.04518600 |
| C | 1.50462800 | 2.72043400 | -1.30522600 |
| H | 0.10844600 | 2.28499100 | 0.28108700 |
| C | 0.66732100 | 2.44106200 | -3.55324700 |
| H | -1.37831100 | 1.77206200 | -3.72321400 |
| C | 1.71212300 | 2.78784800 | -2.68775100 |
| H | 2.31262200 | 2.97968800 | -0.61531600 |
| H | 0.81741500 | 2.48126300 | -4.63573400 |
| H | 2.68053000 | 3.10075200 | -3.08677600 |

**TS-iii'-iv-3 *cis (S,S,S)* conf3**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.936949 (Hartree/Particle)

Thermal correction to Energy= 0.984425

Thermal correction to Enthalpy= 0.985369

Thermal correction to Gibbs Free Energy= 0.853943

Sum of electronic and zero-point Energies= -3951.031304

Sum of electronic and thermal Energies= -3950.983828

Sum of electronic and thermal Enthalpies= -3950.982884

Sum of electronic and thermal Free Energies= -3951.114310

| | | | |
|---|---|---|---|
| O | -9.44369200 | 2.58291500 | 1.90438300 |
| C | -9.61424800 | 2.59550600 | 3.32569400 |
| C | -8.56375300 | 1.59820400 | 3.85305600 |
| H | -9.42923700 | 3.61567300 | 3.69818000 |
| H | -10.64471000 | 2.30440500 | 3.56864000 |
| H | -9.00376600 | 0.58859300 | 3.94657300 |
| N | -7.62014500 | 1.59000600 | 2.72229000 |
| C | -8.22520400 | 2.06026400 | 1.59921600 |
| O | -7.82316300 | 2.03654700 | 0.45004400 |
| C | -6.45131900 | 0.74612700 | 2.74500600 |
| H | -5.95102500 | 0.82917600 | 3.71386000 |
| C | -6.56562500 | -0.58231300 | 2.20841000 |
| H | -5.72458300 | -1.23723300 | 2.46865500 |
| C | -7.42495500 | -1.02078000 | 1.24357500 |
| H | -7.34189700 | -2.03440400 | 0.84442600 |
| H | -8.33340800 | -0.47291400 | 0.98620000 |
| Cu | -6.50123600 | 0.47609000 | -0.64668400 |
| P | -7.56097100 | 0.20167200 | -2.59337300 |
| C | -7.17780000 | 1.71975000 | -3.62895300 |
| C | -9.44743800 | 0.11511900 | -2.64951200 |
| C | -6.96644300 | -1.27259600 | -3.58256300 |
| C | -7.79997000 | 2.97378100 | -2.97853500 |
| C | -5.65175300 | 1.87873400 | -3.76632100 |
| H | -7.62429300 | 1.57988200 | -4.62968200 |
| C | -10.02883200 | -1.30262700 | -2.81123200 |
| C | -10.03426700 | 0.77468000 | -1.38431800 |
| H | -9.75404900 | 0.70620200 | -3.53215300 |
| C | -7.14268400 | -1.17135700 | -5.10739500 |
| C | -5.52945800 | -1.67674600 | -3.20090200 |
| H | -7.61401500 | -2.09018700 | -3.22276700 |
| C | -7.37847500 | 4.26910900 | -3.68511800 |
| H | -7.49626600 | 3.01482000 | -1.91841300 |
| H | -8.89833000 | 2.90031800 | -2.98206500 |
| C | -5.24899500 | 3.18013600 | -4.46750300 |
| H | -5.21124400 | 1.85392000 | -2.75581900 |
| H | -5.21706900 | 1.02188800 | -4.30107200 |
| C | -11.56530800 | -1.28272900 | -2.82321200 |
| H | -9.68016000 | -1.93743900 | -1.97537600 |
| H | -9.67050300 | -1.77364000 | -3.73884800 |
| C | -11.56562100 | 0.80181200 | -1.40342300 |
| H | -9.69167700 | 0.20091400 | -0.50715600 |
| H | -9.63089500 | 1.78355300 | -1.23579400 |
| C | -6.71416700 | -2.47169300 | -5.80330100 |
| H | -6.52492700 | -0.34375300 | -5.49517900 |
| H | -8.18712500 | -0.92668200 | -5.36376700 |
| C | -5.11647500 | -2.97344500 | -3.90618100 |
| H | -4.81557700 | -0.87949400 | -3.46194800 |
| H | -5.45817700 | -1.78849800 | -2.10779000 |
| C | -5.85470400 | 4.40063500 | -3.76925400 |
| H | -7.81402300 | 5.13365100 | -3.15618800 |
| H | -7.79853000 | 4.28152000 | -4.70812000 |
| H | -4.14868700 | 3.25380800 | -4.49862000 |
| H | -5.59282600 | 3.15349400 | -5.51829200 |
| C | -12.14385800 | -0.60614000 | -1.57606200 |
| H | -11.94819900 | -2.31292300 | -2.91870400 |
| H | -11.90675800 | -0.73701700 | -3.72227300 |
| H | -11.93662700 | 1.26518800 | -0.47371300 |
| H | -11.91043000 | 1.44431200 | -2.23505200 |
| C | -5.27901200 | -2.86061700 | -5.42666600 |
| H | -6.81262100 | -2.36319600 | -6.89671500 |
| H | -7.40111700 | -3.28510200 | -5.50454700 |
| H | -4.07491000 | -3.21925200 | -3.64517400 |
| H | -5.74413300 | -3.80563500 | -3.53576100 |
| H | -5.57409600 | 5.32929300 | -4.29399500 |
| H | -5.43831300 | 4.47582500 | -2.74823100 |
| H | -13.24507200 | -0.57377400 | -1.63229500 |
| H | -11.89066400 | -1.21134800 | -0.68579200 |
| H | -4.99692100 | -3.80741300 | -5.91738100 |
| H | -4.58296900 | -2.08937600 | -5.80599800 |
| C | -7.93978800 | 1.97891000 | 5.17803200 |
| C | -7.27702100 | 3.20721900 | 5.33160700 |
| C | -8.00634000 | 1.10340300 | 6.26947100 |
| C | -6.69430500 | 3.55112500 | 6.55274400 |
| H | -7.20020500 | 3.88959700 | 4.48318400 |
| C | -7.42817500 | 1.44770100 | 7.49663200 |
| H | -8.51120500 | 0.13993900 | 6.15661500 |
| C | -6.76979200 | 2.67211800 | 7.64047400 |
| H | -6.17649100 | 4.50824800 | 6.65585300 |
| H | -7.48863000 | 0.75449200 | 8.33942100 |
| H | -6.31372600 | 2.94152400 | 8.59650900 |
| N | -4.83086300 | 0.81361600 | 0.34424700 |
| C | -3.90225600 | -0.29880300 | 0.28383900 |
| H | -3.17216100 | -0.24529900 | 1.11999400 |
| H | -4.41194400 | -1.27506700 | 0.40792100 |
| C | -3.11471400 | -0.34052700 | -1.01644200 |
| C | -2.87857300 | 0.82864500 | -1.75245600 |
| C | -2.59957800 | -1.55168200 | -1.50178600 |
| C | -2.16562500 | 0.78702500 | -2.95447700 |
| H | -3.28612800 | 1.76769200 | -1.37478300 |
| C | -1.87903900 | -1.59839400 | -2.69866400 |
| H | -2.78592800 | -2.47558900 | -0.94533200 |
| C | -1.66658700 | -0.42807500 | -3.43657500 |
| H | -2.00510300 | 1.70841600 | -3.52145700 |
| H | -1.49428400 | -2.55398600 | -3.06528600 |
| H | -1.11555500 | -0.46396100 | -4.38004600 |
| C | -5.15090100 | 2.95910200 | 1.51421800 |
| C | -5.06904000 | 3.68302200 | 2.71499100 |
| C | -5.41788400 | 3.66751300 | 0.33045100 |
| C | -5.26891000 | 5.06614300 | 2.73949400 |
| H | -4.85416500 | 3.15081100 | 3.64541700 |
| C | -5.62189600 | 5.04768000 | 0.34947000 |
| H | -5.47323200 | 3.10901600 | -0.60371100 |
| C | -5.55355300 | 5.75629600 | 1.55565200 |
| H | -5.20138400 | 5.60731700 | 3.68759100 |
| H | -5.83705000 | 5.57534000 | -0.58397600 |
| H | -5.71349800 | 6.83757800 | 1.57157100 |
| C | -4.88550300 | 1.48839700 | 1.50790300 |
| H | -4.11467700 | 1.22233700 | 2.25116200 |

**TS-iii'-iv-3 *cis (S,S,S)* conf4**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.937012 (Hartree/Particle)

Thermal correction to Energy= 0.984481

Thermal correction to Enthalpy= 0.985425

Thermal correction to Gibbs Free Energy= 0.852890
Sum of electronic and zero-point Energies= -3951.029482
Sum of electronic and thermal Energies= -3950.982013
Sum of electronic and thermal Enthalpies= -3950.981069
Sum of electronic and thermal Free Energies= -3951.113603

| | | | |
|---|---|---|---|
| O | -9.28922500 | 2.52298700 | 1.91218300 |
| C | -9.33926300 | 2.48527200 | 3.34213900 |
| C | -8.21674500 | 1.50911400 | 3.74391500 |
| H | -9.15433900 | 3.49877400 | 3.73277500 |
| H | -10.33571200 | 2.15175400 | 3.66065200 |
| H | -8.61315000 | 0.48113500 | 3.83195700 |
| N | -7.36807000 | 1.57744100 | 2.54151100 |
| C | -8.08083800 | 2.06191200 | 1.48914200 |
| O | -7.77788800 | 2.09563500 | 0.30968700 |
| C | -6.17033100 | 0.78198100 | 2.44481600 |
| H | -5.59405500 | 0.85508600 | 3.37077000 |
| C | -6.26053500 | -0.51991200 | 1.85176000 |
| H | -5.37328100 | -1.14282500 | 2.02166100 |
| C | -7.16396500 | -0.95860500 | 0.92550400 |
| H | -7.05757100 | -1.94627700 | 0.47171500 |
| H | -8.11805600 | -0.45426200 | 0.76368100 |
| Cu | -6.47048500 | 0.66767700 | -0.94186000 |
| P | -7.68260600 | 0.26922600 | -2.75491500 |
| C | -7.66477400 | 1.74392800 | -3.92816400 |
| C | -9.51691800 | -0.11385400 | -2.51855100 |
| C | -7.05139000 | -1.18313300 | -3.76994600 |
| C | -8.71311300 | 2.82293700 | -3.59229400 |
| C | -6.25965700 | 2.38197400 | -3.91750700 |
| H | -7.88368000 | 1.35563600 | -4.94001100 |
| C | -9.85379200 | -1.60119400 | -2.28974900 |
| C | -10.08969400 | 0.71147100 | -1.34746700 |
| H | -10.01169800 | 0.19623700 | -3.45791500 |
| C | -5.92067000 | -0.86703600 | -4.76634000 |
| C | -6.57814500 | -2.29982200 | -2.81446400 |
| H | -7.91386900 | -1.55022900 | -4.35519500 |
| C | -8.61335200 | 4.02312600 | -4.54555400 |
| H | -8.54996800 | 3.16919000 | -2.55614200 |
| H | -9.73238000 | 2.41146100 | -3.63706800 |
| C | -6.15429000 | 3.57838500 | -4.86870100 |
| H | -6.04831600 | 2.71460000 | -2.88627900 |
| H | -5.48241000 | 1.64494000 | -4.15069200 |
| C | -11.36854300 | -1.81121200 | -2.14130400 |
| H | -9.35249600 | -1.94914500 | -1.36917600 |
| H | -9.48219600 | -2.22836100 | -3.11339800 |
| C | -11.60151500 | 0.51590900 | -1.19288000 |
| H | -9.58396400 | 0.39183400 | -0.42355700 |
| H | -9.84991500 | 1.77662800 | -1.44248200 |
| C | -5.51754700 | -2.12430800 | -5.55255800 |
| H | -5.04227500 | -0.48882200 | -4.21773400 |
| H | -6.22490900 | -0.08126600 | -5.47421200 |
| C | -6.18530000 | -3.56751300 | -3.58245300 |
| H | -5.70883700 | -1.91556900 | -2.25130100 |
| H | -7.34430700 | -2.53598100 | -2.06291500 |
| C | -7.21054300 | 4.63893500 | -4.54417700 |
| H | -9.36794400 | 4.77829900 | -4.26784300 |
| H | -8.86331500 | 3.69142600 | -5.57045600 |
| H | -5.13998200 | 4.00847800 | -4.81110700 |
| H | -6.28998200 | 3.23097100 | -5.90984800 |
| C | -11.95472800 | -0.96326000 | -1.00757000 |
| H | -11.57914000 | -2.88096600 | -1.97301100 |
| H | -11.86304900 | -1.53995800 | -3.09241700 |
| H | -11.96404600 | 1.11141200 | -0.33813400 |
| H | -12.11558300 | 0.90683000 | -2.09077600 |
| C | -5.10338900 | -3.27378600 | -4.62701700 |
| H | -4.69421700 | -1.87641300 | -6.24370800 |
| H | -6.36991300 | -2.44669300 | -6.17938100 |
| H | -5.83864000 | -4.34121200 | -2.87648900 |
| H | -7.08226900 | -3.97829500 | -4.08258600 |
| H | -7.15542800 | 5.47771800 | -5.25837000 |
| H | -7.00161600 | 5.06023300 | -3.54319000 |
| H | -13.04766200 | -1.10067800 | -0.94834200 |
| H | -11.53946400 | -1.31352700 | -0.04442100 |
| H | -4.87728500 | -4.17893700 | -5.21589400 |
| H | -4.17370800 | -2.99076600 | -4.10621500 |
| C | -7.50242700 | 1.86466500 | 5.02939600 |
| C | -6.85512600 | 3.10261500 | 5.16945500 |
| C | -7.47152600 | 0.95834300 | 6.09697200 |
| C | -6.19123700 | 3.42579000 | 6.35424400 |
| H | -6.85367800 | 3.80856900 | 4.33711700 |
| C | -6.81219800 | 1.28197200 | 7.28832800 |
| H | -7.96367500 | -0.01273000 | 5.99335200 |
| C | -6.16955700 | 2.51625100 | 7.41902200 |
| H | -5.68600500 | 4.39075100 | 6.44646300 |
| H | -6.79688600 | 0.56498300 | 8.11307200 |
| H | -5.65009200 | 2.76944500 | 8.34673300 |
| N | -4.74142500 | 1.04813800 | -0.08499300 |
| C | -3.79491900 | -0.03016800 | -0.29236300 |
| H | -2.93494100 | 0.06295900 | 0.40528500 |
| H | -4.23760300 | -1.02315500 | -0.07571700 |
| C | -3.23665500 | -0.06121400 | -1.70629000 |
| C | -3.21882900 | 1.09272400 | -2.50270300 |
| C | -2.69123300 | -1.24332700 | -2.23005700 |
| C | -2.67294200 | 1.06676100 | -3.78968700 |
| H | -3.66265400 | 2.00375100 | -2.09968200 |
| C | -2.13460600 | -1.27147400 | -3.51259100 |
| H | -2.70989100 | -2.15661000 | -1.62707200 |
| C | -2.12745600 | -0.11562800 | -4.30136700 |
| H | -2.67974500 | 1.97491200 | -4.39886800 |
| H | -1.71573800 | -2.20264700 | -3.90322100 |
| H | -1.70415000 | -0.13892000 | -5.30887000 |
| C | -5.03952300 | 3.10733000 | 1.23563200 |
| C | -4.83291800 | 3.76815400 | 2.45834500 |
| C | -5.48699200 | 3.86590400 | 0.14040400 |
| C | -5.08143100 | 5.13684600 | 2.59102800 |
| H | -4.48034900 | 3.19636200 | 3.32108500 |
| C | -5.73828100 | 5.23245700 | 0.26808700 |
| H | -5.64362100 | 3.35972200 | -0.81155600 |
| C | -5.54177600 | 5.87698900 | 1.49589500 |
| H | -4.91401000 | 5.62765100 | 3.55401000 |
| H | -6.09030000 | 5.79969200 | -0.59829200 |
| H | -5.73859400 | 6.94759600 | 1.59632600 |
| C | -4.71171500 | 1.65705400 | 1.11137400 |
| H | -3.87906500 | 1.37546800 | 1.77790500 |

**TS-iii'-iv-3 *cis (S,S,S)* conf5**
B3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.936991 (Hartree/Particle)
Thermal correction to Energy= 0.984466
Thermal correction to Enthalpy= 0.985410
Thermal correction to Gibbs Free Energy= 0.852590
Sum of electronic and zero-point Energies= -3951.029489
Sum of electronic and thermal Energies= -3950.982015
Sum of electronic and thermal Enthalpies= -3950.981070
Sum of electronic and thermal Free Energies= -3951.113890

| | | | |
|---|---|---|---|
| O | -9.28832100 | 2.47820400 | 1.90632900 |
| C | -9.36765000 | 2.46962200 | 3.33543600 |
| C | -8.28313300 | 1.46860500 | 3.77840700 |
| H | -9.16028900 | 3.48460000 | 3.71063900 |
| H | -10.37974900 | 2.17194100 | 3.63981600 |
| H | -8.71212300 | 0.45498100 | 3.87913000 |
| N | -7.40995800 | 1.48679900 | 2.59183000 |
| C | -8.08662600 | 1.97250500 | 1.51647600 |
| O | -7.75951600 | 1.97449300 | 0.34301600 |
| C | -6.23556900 | 0.65357900 | 2.53453200 |
| H | -5.67517900 | 0.72793600 | 3.47010000 |
| C | -6.35434700 | -0.65666200 | 1.96553400 |
| H | -5.49020000 | -1.30274800 | 2.16533700 |
| C | -7.25274700 | -1.08602200 | 1.02998600 |
| H | -7.16859400 | -2.08559000 | 0.59800800 |
| H | -8.18771100 | -0.55628500 | 0.84016100 |

| | | | |
|---|---|---|---|
| Cu | -6.47473000 | 0.47981200 | -0.85424700 |
| P | -7.66699000 | 0.09517800 | -2.68361100 |
| C | -7.58304300 | 1.55911900 | -3.86746400 |
| C | -9.51584600 | -0.22939900 | -2.47366400 |
| C | -7.06520500 | -1.38597500 | -3.67489800 |
| C | -8.59843900 | 2.67509400 | -3.55138200 |
| C | -6.15715700 | 2.14892500 | -3.84159600 |
| H | -7.80181600 | 1.17185000 | -4.87972500 |
| C | -9.89826000 | -1.70358300 | -2.23100800 |
| C | -10.08345900 | 0.62683400 | -1.32239900 |
| H | -9.98602000 | 0.08257100 | -3.42504500 |
| C | -5.91599400 | -1.11426700 | -4.66319600 |
| C | -6.63431900 | -2.50416600 | -2.70126300 |
| H | -7.93135200 | -1.73556700 | -4.26534300 |
| C | -8.44456600 | 3.86713000 | -4.50759500 |
| H | -8.43870100 | 3.01977200 | -2.51414200 |
| H | -9.63029000 | 2.29815700 | -3.60977900 |
| C | -5.99850400 | 3.33703900 | -4.79578200 |
| H | -5.94779600 | 2.47836200 | -2.80905800 |
| H | -5.40266600 | 1.38476500 | -4.06166500 |
| C | -11.42028500 | -1.86953200 | -2.10303400 |
| H | -9.42059200 | -2.05262100 | -1.29833900 |
| H | -9.53215700 | -2.35215300 | -3.04041000 |
| C | -11.60226500 | 0.47518500 | -1.18838700 |
| H | -9.60060200 | 0.30559200 | -0.38694400 |
| H | -9.81315700 | 1.68358400 | -1.42739200 |
| C | -5.54199100 | -2.39186200 | -5.43072300 |
| H | -5.03204300 | -0.75576800 | -4.11029500 |
| H | -6.19020300 | -0.32823000 | -5.38299700 |
| C | -6.26811600 | -3.79134100 | -3.44999100 |
| H | -5.76144000 | -2.13748600 | -2.13192000 |
| H | -7.41566100 | -2.71029200 | -1.95634800 |
| C | -7.02167800 | 4.43455200 | -4.48898800 |
| H | -9.17666800 | 4.64871200 | -4.24307000 |
| H | -8.69157700 | 3.54003000 | -5.53470000 |
| H | -4.97081500 | 3.73221200 | -4.72640300 |
| H | -6.13252500 | 2.99032600 | -5.83738600 |
| C | -11.99942200 | -0.99092100 | -0.98927500 |
| H | -11.66308000 | -2.93076400 | -1.92445000 |
| H | -11.89281400 | -1.59717100 | -3.06493500 |
| H | -11.96054200 | 1.09204200 | -0.34709300 |
| H | -12.09182400 | 0.86812200 | -2.09900800 |
| C | -5.16831600 | -3.54035000 | -4.48709700 |
| H | -4.70620200 | -2.17596200 | -6.11765900 |
| H | -6.39777000 | -2.69798300 | -6.06104400 |
| H | -5.94976100 | -4.56534100 | -2.73113900 |
| H | -7.17087000 | -4.18387000 | -3.95437100 |
| H | -6.92803700 | 5.26832800 | -5.20502100 |
| H | -6.81192200 | 4.85200900 | -3.48655400 |
| H | -13.09652200 | -1.09723100 | -0.94491700 |
| H | -11.60837200 | -1.33975900 | -0.01552900 |
| H | -4.96139500 | -4.45877900 | -5.06231300 |
| H | -4.23630200 | -3.27606100 | -3.96058300 |
| C | -7.58232500 | 1.82881200 | 5.07005100 |
| C | -6.90201200 | 3.05022300 | 5.19822300 |
| C | -7.59626700 | 0.94293800 | 6.15499100 |
| C | -6.24996900 | 3.37743300 | 6.38846200 |
| H | -6.86537000 | 3.73928400 | 4.35263900 |
| C | -6.94880800 | 1.27078900 | 7.35169500 |
| H | -8.11427200 | -0.01556800 | 6.06089900 |
| C | -6.27324400 | 2.48857500 | 7.47054800 |
| H | -5.71871900 | 4.32917300 | 6.47141100 |
| H | -6.96858400 | 0.56984900 | 8.19002600 |
| H | -5.76302000 | 2.74488700 | 8.40252100 |
| N | -4.75129700 | 0.82457600 | 0.02873900 |
| C | -3.83552000 | -0.28663000 | -0.13902700 |
| H | -2.98541800 | -0.20541700 | 0.57208900 |
| H | -4.31276800 | -1.26069100 | 0.08982100 |
| C | -3.25380000 | -0.36449900 | -1.54160900 |
| C | -3.18683400 | 0.77129700 | -2.36118500 |
| C | -2.73523200 | -1.57327100 | -2.03065000 |
| C | -2.61848900 | 0.70185900 | -3.63680100 |
| H | -3.61007300 | 1.70344400 | -1.98521700 |
| C | -2.15625600 | -1.64506200 | -3.30152600 |
| H | -2.79235000 | -2.47259400 | -1.40937600 |
| C | -2.09951700 | -0.50677800 | -4.11354500 |
| H | -2.58666100 | 1.59673200 | -4.26456400 |
| H | -1.75825300 | -2.59625400 | -3.66477700 |
| H | -1.65848200 | -0.56389700 | -5.11205600 |
| C | -5.00968700 | 2.91818600 | 1.30291300 |
| C | -4.80742600 | 3.59655400 | 2.51670100 |
| C | -5.41098000 | 3.66830600 | 0.18420200 |
| C | -5.01603300 | 4.97458300 | 2.61781800 |
| H | -4.49043300 | 3.03153900 | 3.39750400 |
| C | -5.62245700 | 5.04412400 | 0.28029600 |
| H | -5.56394700 | 3.14835600 | -0.76083400 |
| C | -5.43100200 | 5.70659900 | 1.49932700 |
| H | -4.85306300 | 5.47902900 | 3.57449000 |
| H | -5.93920000 | 5.60447000 | -0.60400400 |
| H | -5.59660500 | 6.78449400 | 1.57505200 |
| C | -4.72517000 | 1.45623900 | 1.21333200 |
| H | -3.91470300 | 1.16234400 | 1.90154000 |

**TS-iii'-iv-3 *cis (S,S,S)* conf6**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.937699 (Hartree/Particle)
Thermal correction to Energy= 0.985204
Thermal correction to Enthalpy= 0.986148
Thermal correction to Gibbs Free Energy= 0.855011
Sum of electronic and zero-point Energies= -3951.026885
Sum of electronic and thermal Energies= -3950.979380
Sum of electronic and thermal Enthalpies= -3950.978436
Sum of electronic and thermal Free Energies= -3951.109573

| | | | |
|---|---|---|---|
| O | -8.21255500 | 3.88937300 | 0.90566600 |
| C | -8.09133400 | 4.54999800 | 2.17053500 |
| C | -7.83602400 | 3.41197400 | 3.17706900 |
| H | -7.24471700 | 5.25340900 | 2.12570900 |
| H | -9.01377600 | 5.10899700 | 2.37643900 |
| H | -8.79257200 | 3.04349200 | 3.59034700 |
| N | -7.30060400 | 2.37738700 | 2.27229500 |
| C | -7.65800900 | 2.64723300 | 0.99354800 |
| O | -7.55942700 | 1.93541800 | 0.00940100 |
| C | -6.94925300 | 1.07860400 | 2.76495600 |
| H | -6.33623300 | 1.15297000 | 3.66518900 |
| C | -7.89179600 | 0.01481700 | 2.69943800 |
| H | -7.66034700 | -0.81802600 | 3.37703400 |
| C | -8.92092300 | -0.17494100 | 1.81765300 |
| H | -9.54366700 | -1.06996800 | 1.88562100 |
| H | -9.24680600 | 0.58995400 | 1.11438300 |
| Cu | -7.24299100 | -0.28050600 | -0.64219900 |
| P | -8.18348900 | -0.15383300 | -2.66599100 |
| C | -8.37728000 | 1.60155800 | -3.32404100 |
| C | -9.93819100 | -0.85148800 | -2.72110000 |
| C | -7.26945600 | -1.09931700 | -4.01503500 |
| C | -9.57097800 | 2.34561500 | -2.68742200 |
| C | -7.08333200 | 2.41402200 | -3.09124000 |
| H | -8.56674100 | 1.50862100 | -4.41067600 |
| C | -10.05046600 | -2.33880200 | -3.10627800 |
| C | -10.60414700 | -0.62958600 | -1.34713400 |
| H | -10.47927300 | -0.26684200 | -3.48720000 |
| C | -6.16976700 | -0.32413200 | -4.76329200 |
| C | -6.66751500 | -2.37816500 | -3.40041500 |
| H | -8.03164600 | -1.37941100 | -4.76342900 |
| C | -9.68202800 | 3.78917900 | -3.19877000 |
| H | -9.42838300 | 2.36300200 | -1.59480700 |
| H | -10.51610400 | 1.82054600 | -2.89229700 |
| C | -7.20139200 | 3.85505100 | -3.60241400 |
| H | -6.89004800 | 2.43371500 | -2.01118500 |
| H | -6.21705500 | 1.92992800 | -3.55857300 |
| C | -11.51205500 | -2.80999700 | -3.09816200 |

| | | | |
|---|---|---|---|
| H | -9.47835100 | -2.94375300 | -2.38545200 |
| H | -9.61269500 | -2.52722300 | -4.09768800 |
| C | -12.06217200 | -1.10045100 | -1.32624600 |
| H | -10.02059500 | -1.18866700 | -0.59588600 |
| H | -10.54220600 | 0.42465500 | -1.04310100 |
| C | -5.49952400 | -1.20432300 | -5.82945100 |
| H | -5.40207600 | 0.01047500 | -4.04305600 |
| H | -6.57893200 | 0.57789500 | -5.24206200 |
| C | -5.99417800 | -3.26181000 | -4.45495500 |
| H | -5.92827300 | -2.07634900 | -2.63792400 |
| H | -7.42383600 | -2.95568700 | -2.85443100 |
| C | -8.38975200 | 4.57528600 | -2.95865800 |
| H | -10.53568600 | 4.28679100 | -2.70773700 |
| H | -9.90626800 | 3.77652800 | -4.28208500 |
| H | -6.26185900 | 4.39409800 | -3.39164100 |
| H | -7.32442200 | 3.85348600 | -4.70215300 |
| C | -12.17739500 | -2.57135500 | -1.73847300 |
| H | -11.55668900 | -3.87890300 | -3.36768500 |
| H | -12.07432700 | -2.26534600 | -3.87924000 |
| H | -12.48949500 | -0.94432200 | -0.32141800 |
| H | -12.65624700 | -0.47811300 | -2.02112500 |
| C | -4.92066400 | -2.48897400 | -5.22720400 |
| H | -4.71157800 | -0.62786200 | -6.34307800 |
| H | -6.24760900 | -1.46848100 | -6.59983600 |
| H | -5.56105900 | -4.15042300 | -3.96770700 |
| H | -6.75989500 | -3.63237800 | -5.16198200 |
| H | -8.48318800 | 5.60229900 | -3.35122400 |
| H | -8.21675600 | 4.65810000 | -1.87084600 |
| H | -13.23362700 | -2.88815500 | -1.76342300 |
| H | -11.67740400 | -3.19848000 | -0.97706500 |
| H | -4.47681800 | -3.11909000 | -6.01644000 |
| H | -4.09999700 | -2.22484600 | -4.53481400 |
| C | -6.91910900 | 3.76683000 | 4.32695000 |
| C | -5.63275700 | 4.27744600 | 4.09146300 |
| C | -7.33778000 | 3.57141200 | 5.64956300 |
| C | -4.78520900 | 4.58746000 | 5.15671700 |
| H | -5.28654100 | 4.41614800 | 3.06619600 |
| C | -6.49282400 | 3.88558900 | 6.71997200 |
| H | -8.33368500 | 3.16363800 | 5.84357200 |
| C | -5.21384900 | 4.39354300 | 6.47575400 |
| H | -3.78466800 | 4.97997700 | 4.95723300 |
| H | -6.83418100 | 3.72792400 | 7.74619000 |
| H | -4.55060100 | 4.63633300 | 7.30987500 |
| C | -5.26402500 | 0.13131500 | 1.39078800 |
| N | -5.82467100 | -0.79799500 | 0.62529800 |
| C | -5.85110500 | -2.12939200 | 1.23511300 |
| H | -4.82471700 | -2.42294200 | 1.52529700 |
| H | -6.43905200 | -2.10886900 | 2.17216800 |
| C | -6.41732300 | -3.20681000 | 0.33844000 |
| C | -7.80287100 | -3.42671900 | 0.27604400 |
| C | -5.57549100 | -4.02316500 | -0.43009500 |
| C | -8.33095700 | -4.44965900 | -0.51673000 |
| H | -8.46413300 | -2.78439100 | 0.86003400 |
| C | -6.09885800 | -5.04628300 | -1.22797400 |
| H | -4.49445200 | -3.85990900 | -0.39548100 |
| C | -7.47943400 | -5.26463300 | -1.27146100 |
| H | -9.41103800 | -4.61550000 | -0.54046100 |
| H | -5.42619800 | -5.67730300 | -1.81459500 |
| H | -7.89063800 | -6.06546100 | -1.89138000 |
| C | -4.66422100 | 1.37122400 | 0.84431800 |
| C | -4.05888600 | 2.29317900 | 1.71757600 |
| C | -4.60877100 | 1.63832800 | -0.53610000 |
| C | -3.44203600 | 3.44902500 | 1.23434500 |
| H | -4.08773000 | 2.10414800 | 2.79358600 |
| C | -4.00190100 | 2.79619900 | -1.02233600 |
| H | -5.05594400 | 0.92744600 | -1.23235000 |
| C | -3.41772300 | 3.71332800 | -0.14030000 |
| H | -2.97925000 | 4.14958000 | 1.93512900 |
| H | -3.98545700 | 2.98328000 | -2.09948300 |
| H | -2.94189000 | 4.62097000 | -0.52044300 |
| H | -4.78419200 | -0.19855500 | 2.32349300 |

**TS-iii'-iv-3 *trans (S,S,S)* conf2**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.936459 (Hartree/Particle)
Thermal correction to Energy= 0.984373
Thermal correction to Enthalpy= 0.985317
Thermal correction to Gibbs Free Energy= 0.850530
Sum of electronic and zero-point Energies= -3951.034061
Sum of electronic and thermal Energies= -3950.986148
Sum of electronic and thermal Enthalpies= -3950.985203
Sum of electronic and thermal Free Energies= -3951.119991

| | | | |
|---|---|---|---|
| O | -0.02406400 | 6.77527700 | -0.19506300 |
| C | -0.03364400 | 6.04358500 | 1.02932700 |
| C | -1.35345100 | 5.25250900 | 0.99941200 |
| H | 0.84426200 | 5.37784500 | 1.06012900 |
| H | 0.02215000 | 6.74362800 | 1.87390200 |
| H | -2.15816600 | 5.84792200 | 1.47155500 |
| N | -1.59018800 | 5.20716200 | -0.44833700 |
| C | -0.89833600 | 6.20507700 | -1.08486000 |
| O | -1.00252900 | 6.59948300 | -2.22170000 |
| C | -2.70799700 | 4.48233300 | -0.98271900 |
| H | -3.19872600 | 3.92777200 | -0.17878600 |
| C | -3.59392000 | 5.07159600 | -1.93439000 |
| H | -3.18787600 | 5.86646800 | -2.56532600 |
| C | -4.84211000 | 4.55918100 | -2.22946500 |
| H | -5.35337300 | 3.90302500 | -1.51322500 |
| H | -5.49048300 | 5.10203800 | -2.92127500 |
| Cu | -4.32816700 | 2.79233600 | -3.58846400 |
| P | -5.42876900 | 2.52043300 | -5.50174800 |
| C | -5.36525800 | 3.97958500 | -6.67290900 |
| C | -7.27291700 | 2.21493600 | -5.26573700 |
| C | -4.76860500 | 1.04957400 | -6.45110800 |
| C | -6.12165700 | 5.19355600 | -6.09783600 |
| C | -3.90554300 | 4.36447500 | -6.98323300 |
| H | -5.86382500 | 3.67080400 | -7.60915700 |
| C | -7.67977100 | 0.73012400 | -5.28134300 |
| C | -7.71142900 | 2.86520900 | -3.93462300 |
| H | -7.79087300 | 2.72164300 | -6.10000100 |
| C | -5.17072200 | 0.95702900 | -7.93154100 |
| C | -3.24683600 | 0.87027900 | -6.27521600 |
| H | -5.23021600 | 0.20412700 | -5.91316900 |
| C | -6.02393200 | 6.41686800 | -7.01958800 |
| H | -5.68911700 | 5.44331400 | -5.11319600 |
| H | -7.18119100 | 4.94874900 | -5.92740800 |
| C | -3.81307800 | 5.58850000 | -7.90290900 |
| H | -3.39309000 | 4.58919500 | -6.03162200 |
| H | -3.36794900 | 3.51896700 | -7.43690700 |
| C | -9.18048100 | 0.55060700 | -5.00948700 |
| H | -7.10887300 | 0.18811200 | -4.50994200 |
| H | -7.43082400 | 0.26658200 | -6.24773600 |
| C | -9.21094800 | 2.68948500 | -3.67253200 |
| H | -7.13477200 | 2.39435400 | -3.11772100 |
| H | -7.44351400 | 3.93193400 | -3.91526700 |
| C | -4.70326700 | -0.37362000 | -8.54080000 |
| H | -4.70724800 | 1.78920000 | -8.48993500 |
| H | -6.26095500 | 1.06977300 | -8.05190200 |
| C | -2.78833400 | -0.46199500 | -6.88058800 |
| H | -2.70456100 | 1.69474000 | -6.76773900 |
| H | -2.98746100 | 0.92842900 | -5.20701600 |
| C | -4.56713100 | 6.78593300 | -7.31678800 |
| H | -6.55442200 | 7.26833400 | -6.56144800 |
| H | -6.54481500 | 6.19562100 | -7.96950600 |
| H | -2.75368000 | 5.84269700 | -8.07386300 |
| H | -4.24041500 | 5.33410600 | -8.89043100 |
| C | -9.60658300 | 1.20973200 | -3.69369500 |
| H | -9.42455300 | -0.52521700 | -4.99858600 |
| H | -9.75595700 | 0.99514300 | -5.84269100 |
| H | -9.47618600 | 3.14889300 | -2.70547200 |
| H | -9.78268700 | 3.23406800 | -4.44687700 |

| | | | |
|---|---|---|---|
| C | -3.19400300 | -0.57794800 | -8.35571000 |
| H | -4.96970300 | -0.41362400 | -9.61043500 |
| H | -5.24598700 | -1.20234700 | -8.04972900 |
| H | -1.69639900 | -0.56964000 | -6.77039000 |
| H | -3.24574700 | -1.29154100 | -6.30976300 |
| H | -4.51897300 | 7.64789000 | -8.00294900 |
| H | -4.07353500 | 7.09981000 | -6.37870300 |
| H | -10.69259000 | 1.09508300 | -3.53889400 |
| H | -9.10770800 | 0.69221000 | -2.85489600 |
| H | -2.88727200 | -1.55518800 | -8.76482800 |
| H | -2.65263600 | 0.19029700 | -8.93859700 |
| C | -1.33139200 | 3.88980000 | 1.66468400 |
| C | -0.31869200 | 2.95420500 | 1.39896100 |
| C | -2.37972500 | 3.51795300 | 2.51838400 |
| C | -0.35506600 | 1.68008000 | 1.96946000 |
| H | 0.50467400 | 3.21610600 | 0.73211800 |
| C | -2.42184000 | 2.24239500 | 3.09128900 |
| H | -3.17907000 | 4.23398100 | 2.72870900 |
| C | -1.40991200 | 1.31859900 | 2.81559000 |
| H | 0.44033400 | 0.96425400 | 1.74789200 |
| H | -3.24956100 | 1.96999200 | 3.75080500 |
| H | -1.44124900 | 0.31988500 | 3.25820000 |
| C | -2.00183500 | 2.76139500 | -1.88321800 |
| N | -3.06349800 | 2.03376300 | -2.30056700 |
| C | -4.67952700 | 0.23731300 | -1.81968000 |
| C | -4.26454300 | -0.59763900 | -2.87161300 |
| C | -5.97168400 | 0.06786900 | -1.30358300 |
| C | -5.11221000 | -1.58284800 | -3.38194400 |
| H | -3.26638300 | -0.45530200 | -3.29011400 |
| C | -6.82380000 | -0.92276000 | -1.80783100 |
| H | -6.31689900 | 0.72157500 | -0.49710600 |
| C | -6.39612000 | -1.75318800 | -2.84749200 |
| H | -4.77115100 | -2.22112700 | -4.20169700 |
| H | -7.82771800 | -1.03953400 | -1.39139600 |
| H | -7.06266000 | -2.52117800 | -3.24813900 |
| C | -3.73210200 | 1.27797100 | -1.25565500 |
| H | -4.30210400 | 1.93537100 | -0.56329800 |
| H | -2.98731500 | 0.76267700 | -0.61193500 |
| H | -1.51429500 | 2.42301400 | -0.95639600 |
| C | -1.02540800 | 3.29291700 | -2.86950300 |
| C | 0.29031900 | 3.58224700 | -2.46270100 |
| C | -1.36440000 | 3.54780800 | -4.20993900 |
| C | 1.21533100 | 4.14142500 | -3.34667700 |
| H | 0.58810400 | 3.37105700 | -1.43462400 |
| C | -0.44415300 | 4.10262700 | -5.09869700 |
| H | -2.36606000 | 3.29887600 | -4.56602800 |
| C | 0.85164900 | 4.41244200 | -4.66934700 |
| H | 2.22709800 | 4.36787400 | -2.99972000 |
| H | -0.74240200 | 4.29536500 | -6.13314600 |
| H | 1.57275800 | 4.85475700 | -5.36145700 |

**TS-iii'-iv-3 *trans (S,S,S)* conf3**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.936459 (Hartree/Particle)
Thermal correction to Energy= 0.984373
Thermal correction to Enthalpy= 0.985317
Thermal correction to Gibbs Free Energy= 0.850530
Sum of electronic and zero-point Energies= -3951.034061
Sum of electronic and thermal Energies= -3950.986148
Sum of electronic and thermal Enthalpies= -3950.985203
Sum of electronic and thermal Free Energies= -3951.119991

| | | | |
|---|---|---|---|
| O | -0.00147600 | 6.73280500 | -0.15896400 |
| C | -0.00018700 | 5.97968700 | 1.05236400 |
| C | -1.31715400 | 5.18387000 | 1.01762800 |
| H | 0.88070300 | 5.31736900 | 1.06584300 |
| H | 0.05840300 | 6.66504500 | 1.90872500 |
| H | -2.12025700 | 5.76626900 | 1.50834500 |
| N | -1.56635200 | 5.16618100 | -0.42863900 |
| C | -0.88126600 | 6.17675800 | -1.05222900 |
| O | -0.99458600 | 6.59109400 | -2.18109100 |
| C | -2.68714300 | 4.44895900 | -0.96702300 |
| H | -3.17273000 | 3.88223400 | -0.16848600 |
| C | -3.57941100 | 5.05175200 | -1.90417200 |
| H | -3.17776900 | 5.85564100 | -2.52640000 |
| C | -4.82955500 | 4.54340300 | -2.19785300 |
| H | -5.33603900 | 3.87734400 | -1.48737900 |
| H | -5.48249000 | 5.09560900 | -2.87786500 |
| Cu | -4.32672100 | 2.79355300 | -3.58406500 |
| P | -5.44442800 | 2.54641600 | -5.49058000 |
| C | -5.38831300 | 4.01892100 | -6.64529100 |
| C | -7.28703200 | 2.24121200 | -5.24207000 |
| C | -4.79586000 | 1.08575300 | -6.46327100 |
| C | -6.13752100 | 5.22767700 | -6.05018000 |
| C | -3.93061700 | 4.40478900 | -6.96382100 |
| H | -5.89545700 | 3.72169500 | -7.58067500 |
| C | -7.69607500 | 0.75717600 | -5.27049100 |
| C | -7.71310300 | 2.87723500 | -3.90010400 |
| H | -7.81130200 | 2.75785500 | -6.06623900 |
| C | -5.21317700 | 1.01101000 | -7.94050500 |
| C | -3.27268300 | 0.90205000 | -6.30513700 |
| H | -5.25332300 | 0.23476600 | -5.93055900 |
| C | -6.04559800 | 6.46096400 | -6.95916900 |
| H | -5.69604500 | 5.46583400 | -5.06662500 |
| H | -7.19598300 | 4.98277800 | -5.87334900 |
| C | -3.84389300 | 5.63876000 | -7.87067200 |
| H | -3.40966200 | 4.61804900 | -6.01420200 |
| H | -3.39831900 | 3.56354700 | -7.43146100 |
| C | -9.19453800 | 0.57646500 | -4.98735400 |
| H | -7.11905000 | 0.20596800 | -4.51023400 |
| H | -7.45634600 | 0.30400900 | -6.24408700 |
| C | -9.21045300 | 2.70034000 | -3.62665100 |
| H | -7.12989600 | 2.39668300 | -3.09359700 |
| H | -7.44376200 | 3.94337800 | -3.87127600 |
| C | -4.75468900 | -0.31348700 | -8.56959200 |
| H | -4.75367800 | 1.84865000 | -8.49400900 |
| H | -6.30433800 | 1.12726400 | -8.04842600 |
| C | -2.82285300 | -0.42403900 | -6.93036000 |
| H | -2.73419000 | 1.73116800 | -6.79395300 |
| H | -3.00207500 | 0.94763700 | -5.23908200 |
| C | -4.59078500 | 6.83089800 | -7.26493300 |
| H | -6.57058700 | 7.30818900 | -6.48704500 |
| H | -6.57509900 | 6.25113500 | -7.90691200 |
| H | -2.78555300 | 5.89306600 | -8.04791900 |
| H | -4.28012300 | 5.39599400 | -8.85723300 |
| C | -9.60806600 | 1.22136100 | -3.66056600 |
| H | -9.43992700 | -0.49911400 | -4.98634800 |
| H | -9.77678700 | 1.03104000 | -5.81037100 |
| H | -9.46649900 | 3.14939100 | -2.65227900 |
| H | -9.78839400 | 3.25404400 | -4.38984100 |
| C | -3.24402900 | -0.52266400 | -8.40245900 |
| H | -5.03221100 | -0.34088300 | -9.63680400 |
| H | -5.29394300 | -1.14672300 | -8.08235000 |
| H | -1.73003000 | -0.53478500 | -6.83276400 |
| H | -3.27582200 | -1.25922200 | -6.36424500 |
| H | -4.54710100 | 7.70025700 | -7.94199700 |
| H | -4.08855300 | 7.13367800 | -6.32778500 |
| H | -10.69277300 | 1.10618900 | -3.49728400 |
| H | -9.10228200 | 0.69402700 | -2.83205600 |
| H | -2.94342700 | -1.49581600 | -8.82562700 |
| H | -2.70722900 | 0.25108600 | -8.98227600 |
| C | -1.28425800 | 3.80802400 | 1.65509700 |
| C | -0.26700200 | 2.88412100 | 1.36695400 |
| C | -2.32782800 | 3.41219800 | 2.50386300 |
| C | -0.29429000 | 1.59809800 | 1.91064400 |
| H | 0.55290000 | 3.16463700 | 0.70340900 |
| C | -2.36097000 | 2.12462200 | 3.04982700 |
| H | -3.13064300 | 4.11898100 | 2.73155100 |
| C | -1.34456700 | 1.21271400 | 2.75186200 |
| H | 0.50459900 | 0.89177500 | 1.67181700 |
| H | -3.18516300 | 1.83360600 | 3.70580400 |

| | | | |
|---|---|---|---|
| H | -1.36885500 | 0.20474400 | 3.17342500 |
| C | -1.98657500 | 2.74205000 | -1.89818800 |
| N | -3.05107900 | 2.01919100 | -2.31664500 |
| C | -4.66211800 | 0.21548900 | -1.84638700 |
| C | -4.25479300 | -0.60642400 | -2.91147600 |
| C | -5.95073100 | 0.04008100 | -1.32346800 |
| C | -5.10644200 | -1.58484800 | -3.42820700 |
| H | -3.25946900 | -0.45929800 | -3.33506900 |
| C | -6.80677600 | -0.94387000 | -1.83408200 |
| H | -6.29003600 | 0.68381500 | -0.50653100 |
| C | -6.38669400 | -1.76137200 | -2.88701200 |
| H | -4.77133200 | -2.21301600 | -4.25816200 |
| H | -7.80785500 | -1.06544500 | -1.41221700 |
| H | -7.05631400 | -2.52408600 | -3.29257400 |
| C | -3.71046800 | 1.24894200 | -1.27638800 |
| H | -4.27499400 | 1.89665200 | -0.57055800 |
| H | -2.96001700 | 0.72555900 | -0.64591900 |
| H | -1.49064900 | 2.39114600 | -0.98054900 |
| C | -1.01955000 | 3.28908100 | -2.88522800 |
| C | 0.29815100 | 3.57842800 | -2.48481600 |
| C | -1.36949800 | 3.55874400 | -4.21997600 |
| C | 1.21433900 | 4.15198300 | -3.36871600 |
| H | 0.60430400 | 3.35593800 | -1.46164900 |
| C | -0.45805000 | 4.12810200 | -5.10867200 |
| H | -2.37265300 | 3.30964200 | -4.57173800 |
| C | 0.83972000 | 4.43776100 | -4.68523400 |
| H | 2.22780000 | 4.37813500 | -3.02654600 |
| H | -0.76468300 | 4.33207200 | -6.13850500 |
| H | 1.55392000 | 4.89132000 | -5.37723000 |

**TS-iii'-iv-3** ***trans (S,S,S)*** **conf4**

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.936910 (Hartree/Particle)

Thermal correction to Energy= 0.984581

Thermal correction to Enthalpy= 0.985525

Thermal correction to Gibbs Free Energy= 0.852936

Sum of electronic and zero-point Energies= -3951.033454

Sum of electronic and thermal Energies= -3950.985783

Sum of electronic and thermal Enthalpies= -3950.984839

Sum of electronic and thermal Free Energies= -3951.117428

| | | | |
|---|---|---|---|
| O | -0.77329900 | 6.73445400 | -1.02162300 |
| C | -1.07386200 | 6.78865300 | 0.37372400 |
| C | -1.69657300 | 5.41641600 | 0.70983700 |
| H | -0.15538300 | 7.00360200 | 0.93469200 |
| H | -1.79666300 | 7.60187600 | 0.55258500 |
| H | -2.60849700 | 5.55329500 | 1.31306900 |
| N | -2.07752000 | 4.96976300 | -0.63490600 |
| C | -1.53510800 | 5.75753400 | -1.61180300 |
| O | -1.67619600 | 5.68565600 | -2.81107800 |
| C | -3.05249300 | 3.93186800 | -0.85160700 |
| H | -3.34033800 | 3.50023200 | 0.11096900 |
| C | -4.16124000 | 4.26323400 | -1.70841000 |
| H | -3.99418700 | 5.07172600 | -2.42584200 |
| C | -5.31719000 | 3.53557600 | -1.81679000 |
| H | -5.58885400 | 2.78269600 | -1.07086700 |
| H | -6.12623000 | 3.88638900 | -2.46217000 |
| Cu | -4.38604400 | 2.02149300 | -3.36673000 |
| P | -5.33879200 | 2.33814100 | -5.35031500 |
| C | -4.88312200 | 3.98643600 | -6.10490400 |
| C | -7.19194900 | 2.33214500 | -5.16538900 |
| C | -4.96143400 | 1.02174500 | -6.63329700 |
| C | -5.51533000 | 5.15802500 | -5.32800100 |
| C | -3.34664400 | 4.11790700 | -6.10423100 |
| H | -5.25349400 | 4.01571100 | -7.14375700 |
| C | -8.01886300 | 2.48230600 | -6.45137700 |
| C | -7.63288900 | 1.09820500 | -4.35575900 |
| H | -7.37917600 | 3.21535300 | -4.52887600 |
| C | -4.98694500 | 1.46571100 | -8.10700700 |
| C | -3.64309700 | 0.29017200 | -6.31001400 |
| H | -5.77843800 | 0.29203600 | -6.48425800 |
| C | -5.02861400 | 6.51753900 | -5.85027100 |
| H | -5.24332400 | 5.06352500 | -4.26383400 |
| H | -6.61466000 | 5.11379900 | -5.38312700 |
| C | -2.87462300 | 5.47308200 | -6.64022400 |
| H | -2.99090200 | 4.00986000 | -5.06725200 |
| H | -2.88458200 | 3.29900200 | -6.67867300 |
| C | -9.52182600 | 2.52629000 | -6.13592100 |
| H | -7.82049500 | 1.62197000 | -7.11441000 |
| H | -7.71823600 | 3.38680800 | -7.00555600 |
| C | -9.13475400 | 1.13723400 | -4.05304400 |
| H | -7.40370700 | 0.17750900 | -4.92056500 |
| H | -7.05171200 | 1.03201500 | -3.42245000 |
| C | -4.76981000 | 0.26843600 | -9.04473400 |
| H | -4.18407300 | 2.20299800 | -8.27991700 |
| H | -5.93367200 | 1.97023800 | -8.35225300 |
| C | -3.42271600 | -0.90178700 | -7.24852400 |
| H | -2.79785200 | 0.99412800 | -6.41049900 |
| H | -3.64739100 | -0.03347700 | -5.25796400 |
| C | -3.49902500 | 6.62046600 | -5.83962200 |
| H | -5.47617500 | 7.32415000 | -5.24536000 |
| H | -5.39697700 | 6.65860400 | -6.88359500 |
| H | -1.77433000 | 5.52164200 | -6.58886900 |
| H | -3.15115100 | 5.56726000 | -7.70714200 |
| C | -9.96344400 | 1.29508800 | -5.33385400 |
| H | -10.10070700 | 2.60607000 | -7.07140300 |
| H | -9.74034000 | 3.43921200 | -5.55179000 |
| H | -9.42650100 | 0.22393600 | -3.50874400 |
| H | -9.34298900 | 1.98681600 | -3.37670200 |
| C | -3.46745600 | -0.47373500 | -8.72055200 |
| H | -4.76853900 | 0.60985900 | -10.09356000 |
| H | -5.62209000 | -0.42847900 | -8.94186000 |
| H | -2.46190000 | -1.39082900 | -7.01646300 |
| H | -4.21192900 | -1.65415100 | -7.06313900 |
| H | -3.17948200 | 7.59483900 | -6.24604400 |
| H | -3.12604400 | 6.56774900 | -4.80136200 |
| H | -11.03784500 | 1.35960600 | -5.09309900 |
| H | -9.83543400 | 0.39250800 | -5.96015400 |
| H | -3.34947300 | -1.34901500 | -9.38109900 |
| H | -2.61097000 | 0.19436100 | -8.92760400 |
| C | -0.79232000 | 4.42721900 | 1.42912500 |
| C | 0.59420100 | 4.40301500 | 1.20884200 |
| C | -1.35523500 | 3.47025300 | 2.28518500 |
| C | 1.39652800 | 3.44074000 | 1.82687400 |
| H | 1.05140400 | 5.12478600 | 0.52782700 |
| C | -0.55624300 | 2.50010800 | 2.89962500 |
| H | -2.43244300 | 3.48311800 | 2.47440500 |
| C | 0.82286700 | 2.48344200 | 2.67138400 |
| H | 2.47354300 | 3.43323700 | 1.64171200 |
| H | -1.01220800 | 1.75892200 | 3.56085700 |
| H | 1.45035200 | 1.72848600 | 3.15156200 |
| C | -2.22185700 | 2.17218000 | -1.50501300 |
| N | -3.21283300 | 1.35646300 | -1.95444800 |
| C | -4.98000200 | -0.28783800 | -1.51553400 |
| C | -4.71671800 | -1.07006800 | -2.65419400 |
| C | -6.26848900 | -0.32549000 | -0.96515200 |
| C | -5.71222000 | -1.86639800 | -3.22388800 |
| H | -3.71795900 | -1.03212400 | -3.09356400 |
| C | -7.26907900 | -1.12631200 | -1.52991000 |
| H | -6.49515700 | 0.28746300 | -0.08785400 |
| C | -6.99458200 | -1.89796200 | -2.66221300 |
| H | -5.48813900 | -2.46154800 | -4.11345100 |
| H | -8.26995200 | -1.13563200 | -1.09032800 |
| H | -7.77778300 | -2.51451700 | -3.11080300 |
| C | -3.88727700 | 0.58241800 | -0.92715800 |
| H | -4.33619500 | 1.22369800 | -0.13638700 |
| H | -3.16219900 | -0.06809900 | -0.39193500 |
| H | -1.81907100 | 1.93132800 | -0.50724700 |
| C | -1.12315400 | 2.56329000 | -2.43772100 |
| C | 0.08761200 | 3.04609900 | -1.91177600 |
| C | -1.22764800 | 2.44305500 | -3.83277400 |

| | | | |
|---|---|---|---|
| C | 1.12808900 | 3.45778100 | -2.74680100 |
| H | 0.21224200 | 3.09875000 | -0.83109600 |
| C | -0.19024600 | 2.84879500 | -4.67292300 |
| H | -2.13348900 | 2.01564100 | -4.26444100 |
| C | 0.99028800 | 3.37509200 | -4.13610800 |
| H | 2.05324800 | 3.84238800 | -2.30816900 |
| H | -0.30636100 | 2.75525000 | -5.75651300 |
| H | 1.79952800 | 3.70287400 | -4.79389100 |

**(E) s-*cis***

B3LYP-D3/def2-SVP-CPCM(toluene)

Zero-point correction= 0.229153 (Hartree/Particle)
Thermal correction to Energy= 0.242458
Thermal correction to Enthalpy= 0.243402
Thermal correction to Gibbs Free Energy= 0.187828
Sum of electronic and zero-point Energies= -669.623243
Sum of electronic and thermal Energies= -669.609938
Sum of electronic and thermal Enthalpies= -669.608994
Sum of electronic and thermal Free Energies= -669.664568

| | | | |
|---|---|---|---|
| O | -0.05458200 | 7.14047700 | 0.80312300 |
| C | -0.16285400 | 6.70856300 | -0.55020900 |
| C | -1.18450700 | 5.54985300 | -0.52257600 |
| H | 0.82468700 | 6.39666700 | -0.91672200 |
| H | -0.53158400 | 7.54285700 | -1.17044200 |
| N | -1.85731200 | 5.82569600 | 0.74262100 |
| C | -1.13171200 | 6.69243000 | 1.52150700 |
| O | -1.34780200 | 7.06415800 | 2.65058700 |
| C | -2.94811300 | 5.00008000 | 1.17663900 |
| H | -3.45519600 | 4.57838700 | 0.30398300 |
| C | -3.82507600 | 5.44245100 | 2.21452200 |
| H | -3.42330300 | 6.15864000 | 2.93465100 |
| H | -0.65777000 | 4.58049400 | -0.46479500 |
| C | -2.10593500 | 5.51447000 | -1.72428900 |
| C | -3.10277800 | 6.48918700 | -1.89051300 |
| C | -1.96226800 | 4.51579900 | -2.69558100 |
| C | -3.93501800 | 6.46649900 | -3.01114300 |
| H | -3.23267800 | 7.25813600 | -1.12460200 |
| C | -2.79109300 | 4.49449400 | -3.82310800 |
| H | -1.19750500 | 3.74445100 | -2.56670300 |
| C | -3.77924600 | 5.46987200 | -3.98296500 |
| H | -4.71159100 | 7.22693400 | -3.12658100 |
| H | -2.66751600 | 3.70983700 | -4.57382900 |
| H | -4.43175200 | 5.45184700 | -4.85958000 |
| C | -5.04017179 | 4.89007114 | 2.44901243 |
| H | -5.30231670 | 5.02814793 | 3.47717333 |
| H | -5.77241247 | 5.36204474 | 1.82775201 |
| H | -5.00516630 | 3.84388863 | 2.22725408 |

# Appendix 4: Methods, Supplementary Figures, and Coordinates/Energies of Structures from Chapter 4 (Mechanistic Studies of First-Row Earth-Abundant Transition Metal-Catalyzed Reactions)

## A4.1 Computational Methods

### *A4.1.a Computational Methods in the Study of Nickel-Catalyzed Hydroarylation of gem-Difluoroalkenes*

All optimizations of intermediates and transition states were calculated using unrestricted UB3LYP-D3/def2-SVP,[226,227] level of theory, with the "guess=mix," "nosymm," and "empiricaldispersion=gd3"[228] keywords as implemented in Gaussian16 Revision C.01.[230] These optimizations were performed using the CPCM implicit solvation model[229] with acetonitrile as the solvent by using the "SCRF=(CPCM,solvent=toluene)" keyword. Frequency calculations (at the same level of theory) were used to obtain thermal corrections (at 298K) and to characterize all optimized structures as either transition states (containing one imaginary frequency) or intermediates (no imaginary frequencies). All 3-D structures were generated using CYLview20.[234]

### *A4.1.b Computational Methods in the Study of Cobalt(I)-Catalyzed Allylic Substitution*

An initial screening of different methods for use in the calculations was performed (see **Figures A4.2.b2** and **A4.2.b3** below). Following this screening, all optimizations of intermediates and transition states were calculated using unrestricted UB3LYP-D3/def2-SVP,[226,227] level of theory, with the "guess=mix," "nosymm," and "empiricaldispersion=gd3"[266] keywords as implemented in Gaussian16 Revision C.01.[230] These optimizations were performed using the CPCM implicit solvation model[229] with acetonitrile as the solvent by using the "SCRF=(CPCM,solvent=acetonitrile)" keyword. Frequency calculations (at the same level of theory) were used to obtain thermal corrections (at 298K) and to characterize all optimized structures as either transition states (if they contain only one imaginary frequency) or intermediates

(if they contain no imaginary frequencies). All 3-D structures were generated using CYLview20.[234]

## A4.2 Supplementary Figures

### *A4.2.a Supplementary Figures in the Study of Nickel-Catalyzed Hydroarylation of gem-Difluoroalkenes*

Following formation of the Ni(0) catalyst **a-4**, the hydroarylation will proceed through 4 key steps: oxidative addition, H-atom abstraction, migratory insertion, and reductive elimination. The energetics of each of these steps are outlined in **Figures A4.2.a1** through **A4.2.a3** below.

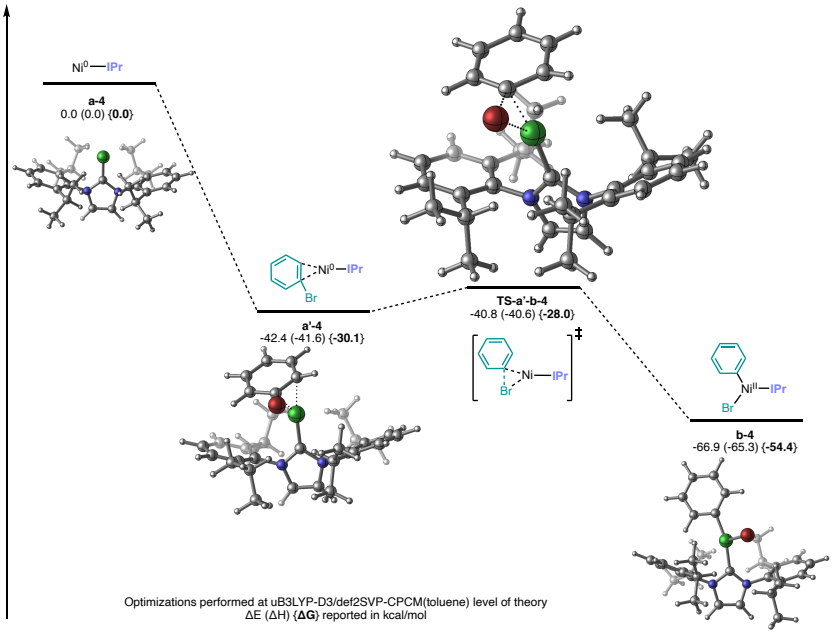



**Figure A4.2.a1.** Energetics of oxidative addition. All structures optimized at UB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔE (ΔH) {ΔG} reported in kcal/mol.

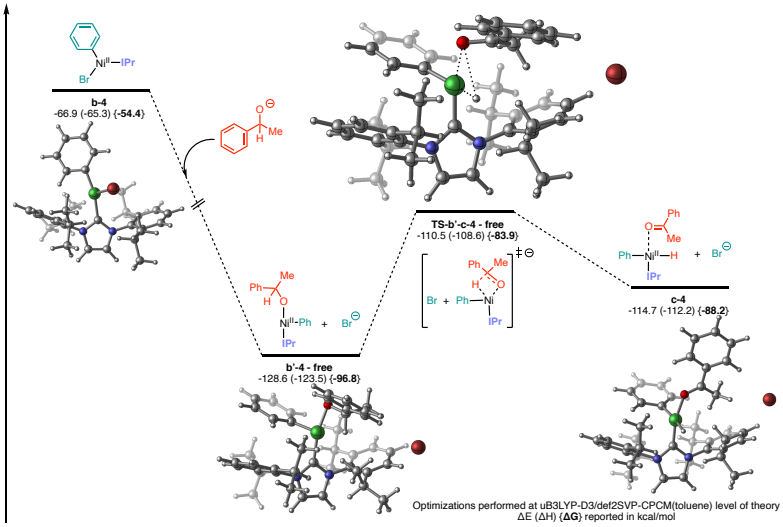



**Figure A4.2.a2.** Energetics of H-atom abstraction from alkoxide **C-4**. All structures optimized at UB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔE (ΔH) {ΔG} reported in kcal/mol.

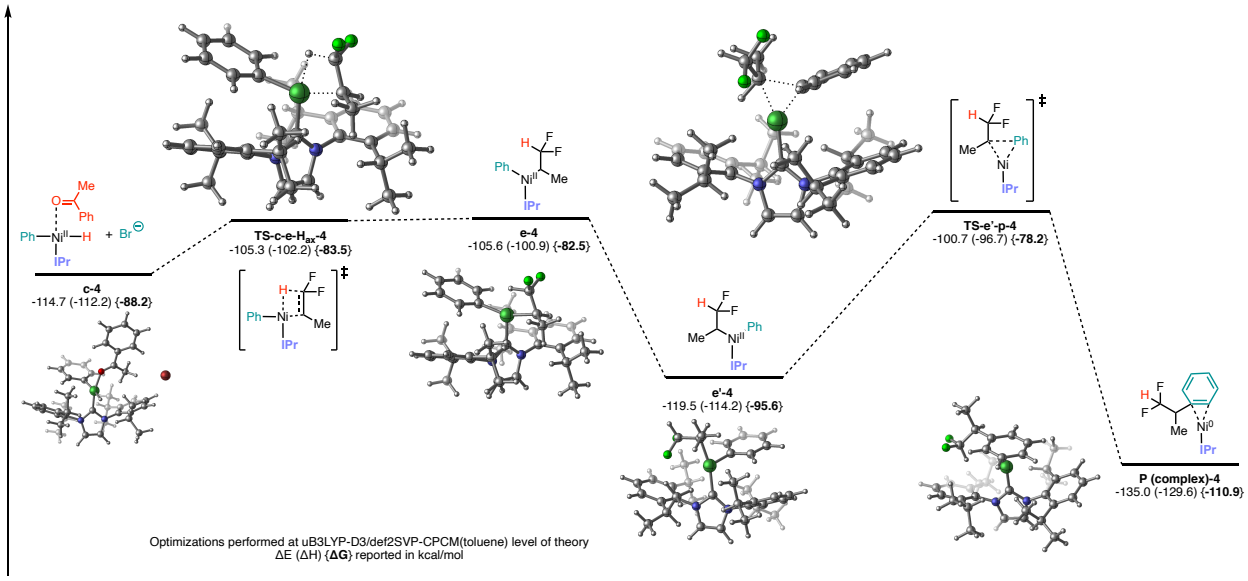



**Figure A4.2.a3.** Energetics of migratory insertion of H onto *gem*-difluoroalkene **A-5** and reductive elimination of product **P-4**. All structures optimized at UB3LYP-D3/def2-SVP-CPCM(toluene) level of theory, ΔE (ΔH) {ΔG} reported in kcal/mol.

Previous results from the Koh group showed that hydroarylation of non-fluorinated alkenes can be achieved under very similar conditions to those described in this work.[206] However, they proposed that the mechanism should proceed with C-C bond formation prior to C-H bond formation. Initially, we were interested in comparing the properties of fluorinated and non-

fluorinated alkenes to see if there were any obvious differences in the electronic properties of these substrates. Interestingly, the HOMO-LUMO gaps (as seen in **Figure A4.2.a4**) are very similar for fluorinated and non-fluorinated alkenes. This indicated that a difference in mechanism must have to do with alternative properties of these substrates. Further investigations into the mechanism of non-fluorinated alkenes are ongoing.

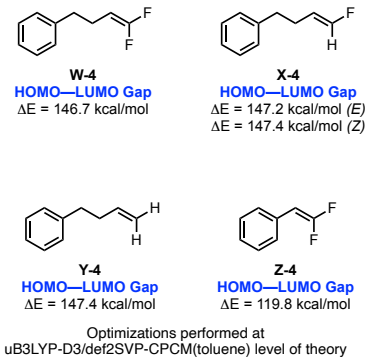



**Figure A4.2.a4.** HOMO-LUMO gaps for representative fluorinated and non-fluorinated alkenes. All structures optimized at UB3LYP-D3/def2-SVP-CPCM(toluene) level of theory

*A4.2.b Supplementary Figures in the Study of Cobalt(I)-Catalyzed Allylic Substitution*

Before starting the process of structure optimization, we found it necessary to run a screen of multiple potential methods in order to determine which would be most appropriate for modeling this reaction. To this end, we employed the results of the Casitas group's synthesis of the relevant Co(I) complexes (see **Figure A4.2.b1** below). Based on the geometries of these catalysts (as determined by X-ray Crystallography), we could determine which optimization method provided the closest geometry.

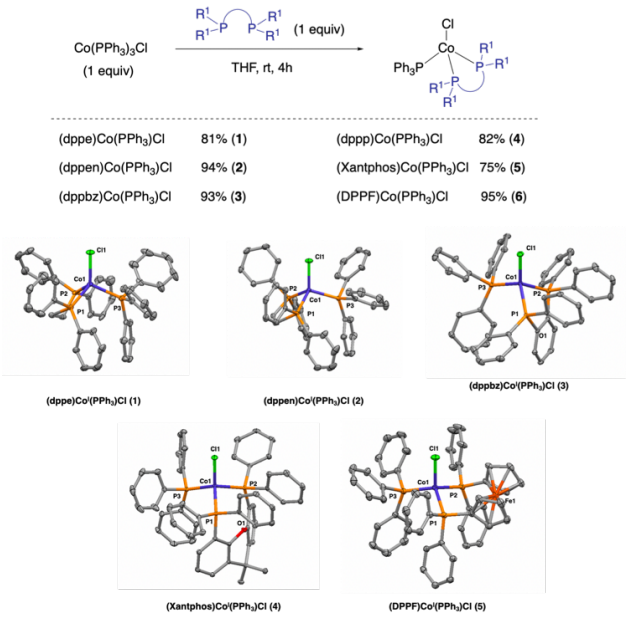



**Figure A4.2.b1** X-Ray crystallography results of the synthesis of tetrahedral Co(I) complexes by ligand substitution reactions.

For the method screen, we employed the dppen and dppp ligands and used the following methods to optimize each of the structures: UB3LYP-D3/def2-SVP-CPCM(acetonitrile),[226,227] UB3LYP-D3/6-31G(d,p)-CPCM(acetonitrile),[239] UωB97XD/def2-SVP-CPCM(acetonitrile),[239] UM06L/def2-SVP-CPCM(acetonitrile).[184] We were interested in which method provided structures with the closest geometries to the observed structures, as well as which methods were the most time efficient. The results of this screening are summarized in **Figure A4.2.b2 and Figure A4.2.b3** below.

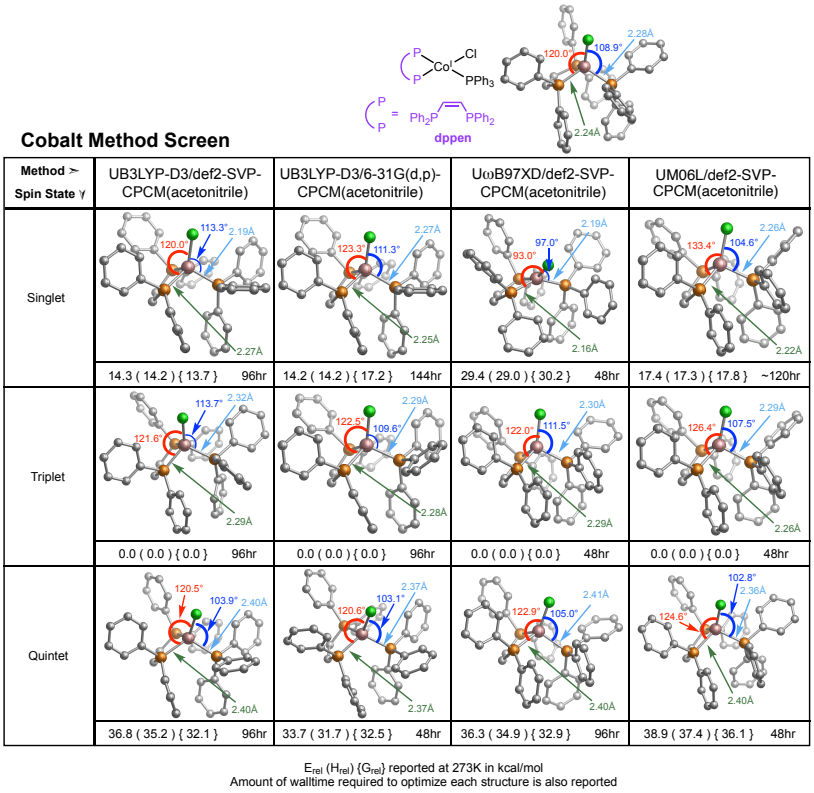
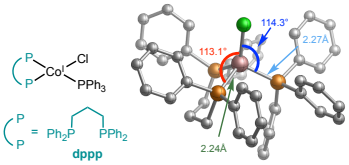
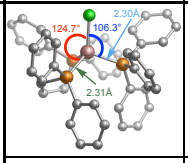
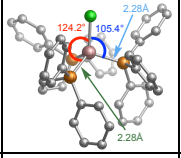
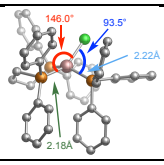
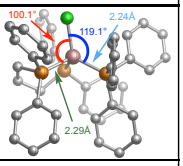
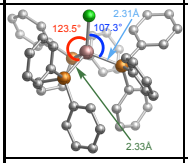
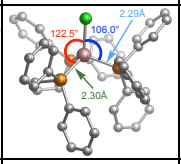
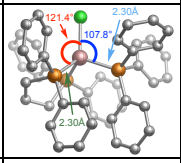
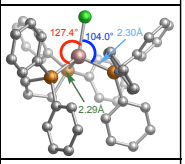
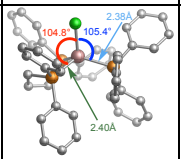
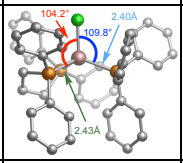



**Figure A4.2.b2.** Method screening results for cobalt(I) catalyst with dppen ligand. Optimizations performed at UωB97XD/def2-SVP-CPCM(acetonitrile) and UM06-L/def2-SVP-CPCM(acetonitrile) level of theory by Robert Martin. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) and UB3LYP-D3/6-31G(d,p)-CPCM(acetonitrile) level of theory by Zhihui Song.




**Cobalt Method Screen**

| Method ➢ Spin State ∨ | UB3LYP-D3/def2-SVP-CPCM(acetonitrile) | UB3LYP-D3/6-31G(d,p)-CPCM(acetonitrile) | UωB97XD/def2-SVP-CPCM(acetonitrile) | UM06L/def2-SVP-CPCM(acetonitrile) |
|---|---|---|---|---|
| Singlet |   |   |   |   |
| | 14.2 ( 14.3 ) { 15.4 } 48hr | 14.5 ( 14.6 ) { 15.4 } 48hr | 29.3 ( 29.2 ) { 30.3 } 144hr | 22.4 ( 21.9 ) { 23.3 } 48hr |
| Triplet |   |   |   |   |
| | 0.0 ( 0.0 ) { 0.0 } 48hr | 0.0 ( 0.0 ) { 0.0 } 48hr | 0.0 ( 0.0 ) { 0.0 } 48hr | 0.0 ( 0.0 ) { 0.0 } 60hr |
| Quintet | ——— |   |   | ——— |
| | | 48.2 ( 46.3 ) { 43.4 } 48hr | 51.8 ( 50.2 ) { 48.1 } 96hr | |

$E_{rel}$ ($H_{rel}$) {$G_{rel}$} reported at 273K in kcal/mol
Amount of walltime required to optimize each structure is also reported

**Figure A4.2.b3.** Method screening results for cobalt(I) catalyst with dppp ligand. Optimizations performed at UωB97XD/def2-SVP-CPCM(acetonitrile) and UM06-L/def2-SVP-CPCM(acetonitrile) level of theory by Robert Martin. Optimizations performed at UB3LYP-D3/def2-SVP-CPCM(acetonitrile) and UB3LYP-D3/6-31G(d,p)-CPCM(acetonitrile) level of theory by Zhihui Song.

Based on this method screening, we found that UB3LYP-D3/def2-SVP-CPCM(acetonitrile) was the most time-efficient method that also provided reasonably accurate geometries. As such, further calculations we performed would employ this level of theory. Notably, for all structures computed, the quintet state was by far the highest energy state, and often did not match the observed geometry well. The triplet state was consistently the lowest energy and had relatively accurate geometries. As such, we surmised that the triplet state of cobalt would be the primary spin state, which held up as further calculations were performed on the proposed mechanistic pathways. EPR experiments from the Casitas group suggest that the cobalt(I) catalyst complex is paramagnetic, further intimating the relevance of the triplet state.

## A4.3 Coordinates & Energies

### *A4.3.a Coordinates & Energies in the Study of Nickel-Catalyzed Hydroarylation of gem-Difluoroalkenes*

**a-4**

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

Zero-point correction= 0.570864 (Hartree/Particle)
Thermal correction to Energy= 0.601760
Thermal correction to Enthalpy= 0.602704
Thermal correction to Gibbs Free Energy= 0.510126
Sum of electronic and zero-point Energies= -2666.888251
Sum of electronic and thermal Energies= -2666.857355
Sum of electronic and thermal Enthalpies= -2666.856411
Sum of electronic and thermal Free Energies= -2666.948989

| | | | |
|---|---|---|---|
| Ni | -1.46545600 | 0.05157200 | -0.00985900 |
| C | -3.21345700 | 0.04625800 | 0.05040800 |
| C | -5.43106400 | -0.09602400 | -0.53788400 |
| C | -5.38557800 | 0.17695400 | 0.79133800 |
| N | -4.03890700 | 0.26139800 | 1.13817000 |
| N | -4.11127900 | -0.17342000 | -0.97748300 |
| H | -6.17757600 | 0.31882300 | 1.52101000 |
| H | -6.27109300 | -0.24221600 | -1.21077900 |
| C | -3.55742800 | 0.53573100 | 2.45854700 |
| C | -3.32136900 | -0.54565500 | 3.33380300 |
| C | -3.35457300 | 1.87853800 | 2.84238600 |
| C | -2.85420400 | -0.25090600 | 4.62264100 |
| C | -2.88682300 | 2.12120600 | 4.14175400 |
| C | -2.63912200 | 1.06831600 | 5.02368800 |
| H | -2.64857200 | -1.06433600 | 5.32155300 |
| H | -2.70660400 | 3.14754900 | 4.46802400 |
| C | -3.72155100 | -0.44746800 | -2.32787600 |
| C | -3.53625800 | -1.78967700 | -2.72231000 |
| C | -3.55609900 | 0.63335300 | -3.21993200 |
| C | -3.15911500 | -2.03234800 | -4.05082500 |
| C | -3.17866500 | 0.33867200 | -4.53784000 |
| C | -2.98209400 | -0.97998400 | -4.95020800 |
| H | -2.99446400 | -3.05822200 | -4.38672300 |
| H | -3.02911400 | 1.15167900 | -5.25131300 |
| C | -3.55549700 | 3.02341700 | 1.85614300 |
| C | -2.20553200 | 3.41310600 | 1.22802700 |
| H | -4.19435600 | 2.65167700 | 1.04076600 |
| H | -1.75940600 | 2.53728700 | 0.72743000 |
| H | -2.33730200 | 4.21184200 | 0.48006800 |
| H | -1.50385100 | 3.77239700 | 1.99924000 |
| C | -3.65932900 | -2.93366800 | -1.72239400 |
| C | -2.26545400 | -3.31533500 | -1.19326400 |
| H | -4.23929000 | -2.56353900 | -0.86343900 |
| H | -1.78930000 | -2.43625000 | -0.72722500 |
| H | -2.33841700 | -4.11354000 | -0.43675000 |
| H | -1.61948500 | -3.67211700 | -2.01280300 |
| C | -3.69957900 | 2.07689000 | -2.75163500 |
| C | -4.46834000 | 2.96105400 | -3.74340000 |
| H | -4.27177800 | 2.06626200 | -1.81163200 |
| H | -5.45030400 | 2.52844000 | -3.99347700 |
| H | -4.63441100 | 3.96012500 | -3.30941600 |
| H | -3.91271600 | 3.10468200 | -4.68419300 |
| C | -4.18551800 | -2.87813700 | 3.91258500 |
| H | -3.56956000 | -3.01881600 | 4.81549100 |
| H | -5.15161900 | -2.45087500 | 4.22571200 |
| H | -4.37388700 | -3.87801600 | 3.48968600 |
| C | -3.48723700 | -1.98945200 | 2.87377000 |
| H | -4.11940400 | -1.98103100 | 1.97301500 |
| H | -2.27365800 | 1.27785700 | 6.03247400 |
| H | -2.68689100 | -1.18943600 | -5.98176500 |
| C | -4.26444900 | 4.23696700 | 2.47334800 |
| H | -5.21790000 | 3.95115200 | 2.94577600 |
| H | -3.64370100 | 4.73249600 | 3.23723800 |
| H | -4.47883400 | 4.98610600 | 1.69433900 |
| C | -2.12140200 | -2.56476100 | 2.45901700 |
| H | -1.42414700 | -2.57495700 | 3.31335000 |
| H | -2.22764600 | -3.59637600 | 2.08590800 |
| H | -1.68518200 | -1.94720500 | 1.65581600 |
| C | -4.40507400 | -4.15169800 | -2.28496400 |
| H | -3.83877900 | -4.64558100 | -3.09107300 |
| H | -4.55894900 | -4.90051900 | -1.49147000 |
| H | -5.39155900 | -3.87122500 | -2.68761000 |
| C | -2.31252900 | 2.65955700 | -2.42728200 |
| H | -1.67337900 | 2.67393300 | -3.32587000 |
| H | -2.39948500 | 3.69038500 | -2.04706100 |
| H | -1.82060500 | 2.04397300 | -1.65535700 |

**a'-4**

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

Zero-point correction= 0.661332 (Hartree/Particle)
Thermal correction to Energy= 0.700017
Thermal correction to Enthalpy= 0.700962
Thermal correction to Gibbs Free Energy= 0.589252
Sum of electronic and zero-point Energies= -5472.226929
Sum of electronic and thermal Energies= -5472.188243
Sum of electronic and thermal Enthalpies= -5472.187299
Sum of electronic and thermal Free Energies= -5472.299009

| | | | |
|---|---|---|---|
| Ni | 7.28207600 | -2.41618700 | -0.38056500 |
| C | 8.41712500 | -1.12314600 | 0.39221000 |
| C | 9.79223300 | 0.67993900 | 0.64372200 |
| C | 9.70379800 | 0.06471500 | 1.85324200 |
| N | 8.85542100 | -1.02564000 | 1.68206900 |
| N | 8.99459800 | -0.05372100 | -0.23039100 |
| H | 10.15813800 | 0.30035100 | 2.81097600 |
| H | 10.33825900 | 1.56377200 | 0.32737900 |
| C | 8.47489100 | -1.94896200 | 2.71709800 |
| C | 9.34333500 | -3.01875100 | 3.00882500 |
| C | 7.23407300 | -1.76880900 | 3.37020400 |
| C | 8.96997700 | -3.89824600 | 4.03624200 |
| C | 6.91215500 | -2.67309500 | 4.39150500 |
| C | 7.77432400 | -3.71850300 | 4.72923800 |
| H | 9.61506900 | -4.74198900 | 4.28761900 |
| H | 5.96750600 | -2.57272700 | 4.92636300 |
| H | 7.49952100 | -4.41081700 | 5.52929500 |
| C | 8.78396700 | 0.25984800 | -1.61770700 |
| C | 7.57197600 | 0.87785000 | -2.00255800 |
| C | 9.79375500 | -0.08298900 | -2.53970200 |
| C | 7.43052000 | 1.21845500 | -3.35522400 |
| C | 9.60218500 | 0.28359100 | -3.87996500 |
| C | 8.43982500 | 0.94188800 | -4.27956100 |
| H | 6.51475300 | 1.70062100 | -3.69841500 |
| H | 10.36209800 | 0.03807500 | -4.62357100 |
| H | 8.30735800 | 1.22359600 | -5.32741500 |
| C | 6.51806700 | -5.33827200 | 0.86413400 |
| C | 7.06549500 | -5.71745000 | -0.38821300 |
| C | 6.88674000 | -4.90028700 | -1.49415300 |
| C | 6.14233200 | -3.68286600 | -1.41308800 |
| C | 5.62224700 | -3.29574500 | -0.12906800 |
| C | 5.80662900 | -4.15761500 | 0.99976100 |
| H | 6.67370200 | -5.97026900 | 1.74217300 |
| H | 7.63087300 | -6.64783700 | -0.47727100 |
| H | 7.28395900 | -5.20329300 | -2.46717900 |
| H | 5.78720100 | -3.20774300 | -2.33312200 |
| H | 5.39133800 | -3.86931700 | 1.96606600 |
| C | 6.26810200 | -0.66600000 | 2.94094600 |
| C | 6.70801300 | 0.72162900 | 3.44322100 |
| C | 4.81598300 | -0.92632600 | 3.35792800 |
| H | 6.28772500 | -0.66338000 | 1.83823200 |

| | | | |
|---|---|---|---|
| H | 7.71192000 | 0.99587400 | 3.09375900 |
| H | 6.00995100 | 1.49505800 | 3.08497200 |
| H | 6.71007600 | 0.74942600 | 4.54554300 |
| H | 4.46688400 | -1.91808400 | 3.03759900 |
| H | 4.68127600 | -0.84229100 | 4.44893600 |
| H | 4.15803500 | -0.18130500 | 2.88524900 |
| C | 10.57753200 | -3.28819500 | 2.15624400 |
| C | 10.20243400 | -4.26538500 | 1.02620000 |
| C | 11.78467900 | -3.79065700 | 2.95867200 |
| H | 10.87520400 | -2.34129200 | 1.68098900 |
| H | 9.36073400 | -3.87306700 | 0.43562600 |
| H | 11.05684000 | -4.42942300 | 0.34986000 |
| H | 9.89395200 | -5.23915500 | 1.43983300 |
| H | 12.02871900 | -3.11192400 | 3.79142100 |
| H | 11.61111200 | -4.79434700 | 3.37885200 |
| H | 12.66831400 | -3.86291800 | 2.30479600 |
| C | 6.45278400 | 1.11735600 | -0.99129200 |
| C | 5.06519300 | 1.23567900 | -1.63038000 |
| C | 6.73668400 | 2.33319500 | -0.09219800 |
| H | 6.42389100 | 0.21536500 | -0.35880500 |
| H | 4.84924500 | 0.37885600 | -2.28609400 |
| H | 4.29751300 | 1.24864100 | -0.84173500 |
| H | 4.95463500 | 2.16290900 | -2.21666800 |
| H | 7.68971800 | 2.23721200 | 0.44648000 |
| H | 6.77432600 | 3.25850100 | -0.69099000 |
| H | 5.93956300 | 2.44629100 | 0.66007400 |
| C | 10.97912800 | -0.94318000 | -2.11524400 |
| C | 12.27136000 | -0.64976200 | -2.88710100 |
| C | 10.58500400 | -2.42946600 | -2.22868300 |
| H | 11.18426300 | -0.74148000 | -1.05302500 |
| H | 13.10708100 | -1.22127800 | -2.45332800 |
| H | 12.19473400 | -0.94392900 | -3.94617700 |
| H | 12.53145900 | 0.42001000 | -2.85003600 |
| H | 9.67681500 | -2.64609000 | -1.64471400 |
| H | 10.38189000 | -2.69533800 | -3.27914000 |
| H | 11.39360100 | -3.07936800 | -1.85719200 |
| Br | 4.07098900 | -2.06279100 | -0.06550200 |

**TS-a'-b-4**

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

Zero-point correction= 0.661159 (Hartree/Particle)
Thermal correction to Energy= 0.699188
Thermal correction to Enthalpy= 0.700133
Thermal correction to Gibbs Free Energy= 0.590128
Sum of electronic and zero-point Energies= -5472.224582
Sum of electronic and thermal Energies= -5472.186553
Sum of electronic and thermal Enthalpies= -5472.185609
Sum of electronic and thermal Free Energies= -5472.295613

| | | | |
|---|---|---|---|
| Ni | 7.09274500 | -2.33607400 | -0.10421500 |
| C | 8.37962600 | -1.07452500 | 0.42564500 |
| C | 9.83500000 | 0.67505600 | 0.61174600 |
| C | 9.76153300 | 0.07969900 | 1.83201800 |
| N | 8.86639000 | -0.97857400 | 1.70088600 |
| N | 8.98006500 | -0.03666500 | -0.22957500 |
| H | 10.25842700 | 0.30680700 | 2.77056800 |
| H | 10.40677700 | 1.53140800 | 0.26645000 |
| C | 8.44802300 | -1.87129500 | 2.74592300 |
| C | 9.25986100 | -2.98257500 | 3.04661800 |
| C | 7.21323900 | -1.63017400 | 3.39058300 |
| C | 8.83827300 | -3.83612400 | 4.07702000 |
| C | 6.83686500 | -2.51388800 | 4.41085600 |
| C | 7.64652800 | -3.59708800 | 4.75991500 |
| H | 9.43917300 | -4.71016700 | 4.33482500 |
| H | 5.89275000 | -2.36376800 | 4.93587400 |
| H | 7.33292200 | -4.27295100 | 5.55980100 |
| C | 8.71658700 | 0.28054800 | -1.60551700 |
| C | 7.50592500 | 0.93075500 | -1.93564000 |
| C | 9.66762700 | -0.10047700 | -2.57437700 |
| C | 7.30229100 | 1.26079400 | -3.28322400 |
| C | 9.41770900 | 0.25891500 | -3.90682300 |
| C | 8.25388100 | 0.94475400 | -4.25446700 |
| H | 6.38399800 | 1.76666500 | -3.58350500 |
| H | 10.13167800 | -0.01302200 | -4.68572700 |
| H | 8.07545900 | 1.21831300 | -5.29769100 |
| C | 6.67007400 | -5.84366100 | 0.61479500 |
| C | 7.44144200 | -6.06994400 | -0.55037500 |
| C | 7.44749300 | -5.13856200 | -1.57896900 |
| C | 6.69667600 | -3.93859200 | -1.47695500 |
| C | 5.92257100 | -3.73459000 | -0.29499500 |
| C | 5.89901300 | -4.69852300 | 0.74840400 |
| H | 6.69244700 | -6.57209000 | 1.42989600 |
| H | 8.02955000 | -6.98657900 | -0.63836900 |
| H | 8.02213100 | -5.32942800 | -2.48976100 |
| H | 6.53574200 | -3.33274300 | -2.37286500 |
| H | 5.31040500 | -4.51004200 | 1.64794400 |
| C | 6.32000500 | -0.46766400 | 2.96568600 |
| C | 6.76704900 | 0.85412900 | 3.61383200 |
| C | 4.82864800 | -0.72033600 | 3.21441400 |
| H | 6.43674500 | -0.37395600 | 1.87573600 |
| H | 7.81647900 | 1.08814800 | 3.38408000 |
| H | 6.14917400 | 1.69057000 | 3.24901700 |
| H | 6.66114700 | 0.80316700 | 4.71025300 |
| H | 4.50562500 | -1.67165800 | 2.76596100 |
| H | 4.58179900 | -0.73430500 | 4.28855400 |
| H | 4.23521900 | 0.08473600 | 2.75305600 |
| C | 10.46994000 | -3.32580600 | 2.18745000 |
| C | 10.02952800 | -4.30771100 | 1.08474300 |
| C | 11.66163400 | -3.86950700 | 2.98568200 |
| H | 10.80477200 | -2.40393500 | 1.68869300 |
| H | 9.18062600 | -3.90148400 | 0.51402500 |
| H | 10.85584100 | -4.50911700 | 0.38403500 |
| H | 9.70667200 | -5.26494100 | 1.52418300 |
| H | 11.95442800 | -3.18257100 | 3.79575900 |
| H | 11.44212900 | -4.85100500 | 3.43591100 |
| H | 12.52984500 | -4.00608400 | 2.32142600 |
| C | 6.45598900 | 1.22805200 | -0.86755400 |
| C | 5.03094400 | 1.33723000 | -1.42074300 |
| C | 6.81780900 | 2.47368500 | -0.04034200 |
| H | 6.45568300 | 0.35638800 | -0.19583200 |
| H | 4.76725600 | 0.45541400 | -2.02395400 |
| H | 4.31519800 | 1.39656300 | -0.58587400 |
| H | 4.89050000 | 2.23964700 | -2.03830900 |
| H | 7.80653700 | 2.38065400 | 0.43123800 |
| H | 6.82617900 | 3.37437100 | -0.67659000 |
| H | 6.07835000 | 2.62951100 | 0.76194300 |
| C | 10.85091300 | -0.98362100 | -2.19343200 |
| C | 12.08557500 | -0.79273300 | -3.08206200 |
| C | 10.39524600 | -2.45691500 | -2.17841800 |
| H | 11.14881200 | -0.72518000 | -1.16557700 |
| H | 12.93221100 | -1.37001400 | -2.67817100 |
| H | 11.91212800 | -1.15125000 | -4.10956400 |
| H | 12.38755000 | 0.26523700 | -3.13804700 |
| H | 9.51993200 | -2.60096900 | -1.52740500 |
| H | 10.11508200 | -2.78094000 | -3.19474000 |
| H | 11.20546300 | -3.11265400 | -1.82013200 |
| Br | 4.41932000 | -2.31674000 | -0.33757200 |

**b-4**

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

Zero-point correction= 0.662568 (Hartree/Particle)
Thermal correction to Energy= 0.701444
Thermal correction to Enthalpy= 0.702388
Thermal correction to Gibbs Free Energy= 0.589669
Sum of electronic and zero-point Energies= -5472.264772
Sum of electronic and thermal Energies= -5472.225896
Sum of electronic and thermal Enthalpies= -5472.224952
Sum of electronic and thermal Free Energies= -5472.337671

| | | | |
|---|---|---|---|
| Ni | 7.29931300 | -2.58520300 | -0.12919800 |
| C | 8.35338800 | -1.01166800 | 0.43689100 |
| C | 9.53463300 | 0.90409100 | 0.72660800 |

| | | | |
|---|---|---|---|
| C | 9.48630700 | 0.27515300 | 1.93293800 |
| N | 8.76406500 | -0.89326900 | 1.72933000 |
| N | 8.82927400 | 0.10601600 | -0.16868900 |
| H | 9.89998900 | 0.54348700 | 2.90055100 |
| H | 10.00875400 | 1.83195000 | 0.42362500 |
| C | 8.44417100 | -1.89073800 | 2.71670800 |
| C | 9.43096100 | -2.83966300 | 3.05861500 |
| C | 7.13414300 | -1.91589600 | 3.24413600 |
| C | 9.08401700 | -3.81789300 | 4.00117100 |
| C | 6.84069000 | -2.91885100 | 4.17882700 |
| C | 7.80523700 | -3.85251000 | 4.55882500 |
| H | 9.81437900 | -4.57381500 | 4.29237700 |
| H | 5.84077800 | -2.97831000 | 4.60998800 |
| H | 7.55243600 | -4.62722800 | 5.28696400 |
| C | 8.62009500 | 0.41994300 | -1.55768700 |
| C | 7.62200200 | 1.35951500 | -1.89289600 |
| C | 9.40770500 | -0.23771800 | -2.52243000 |
| C | 7.44181600 | 1.64786100 | -3.25201000 |
| C | 9.17377900 | 0.07507000 | -3.86982200 |
| C | 8.20646600 | 1.01156700 | -4.23093600 |
| H | 6.68143400 | 2.37069700 | -3.55260800 |
| H | 9.75665000 | -0.42431300 | -4.64674600 |
| H | 8.04077300 | 1.24371000 | -5.28604200 |
| C | 7.03012200 | -6.40873100 | 0.89704500 |
| C | 6.58082500 | -7.13029300 | -0.21377600 |
| C | 6.16891300 | -6.44874300 | -1.36798900 |
| C | 6.21201200 | -5.05078900 | -1.41593600 |
| C | 6.68805500 | -4.31787900 | -0.31877900 |
| C | 7.06756000 | -5.00735200 | 0.85001600 |
| H | 7.33417700 | -6.93185200 | 1.80880900 |
| H | 6.53907400 | -8.22240300 | -0.17789900 |
| H | 5.81215400 | -7.01349000 | -2.23473300 |
| H | 5.88220800 | -4.51947400 | -2.31267300 |
| H | 7.39749900 | -4.46470900 | 1.74528800 |
| C | 6.08734700 | -0.89171900 | 2.81817600 |
| C | 6.18663800 | 0.37717000 | 3.68306000 |
| C | 4.66211700 | -1.45534900 | 2.80097000 |
| H | 6.30871500 | -0.61173100 | 1.77864400 |
| H | 7.19380000 | 0.81980100 | 3.63585500 |
| H | 5.46637900 | 1.13620700 | 3.33741100 |
| H | 5.96516000 | 0.15034800 | 4.73919300 |
| H | 4.61291100 | -2.37390600 | 2.19692600 |
| H | 4.28447000 | -1.67467900 | 3.81286900 |
| H | 3.98036400 | -0.72081900 | 2.34554500 |
| C | 10.78331500 | -2.86124300 | 2.35238900 |
| C | 10.68088200 | -3.66653200 | 1.04246700 |
| C | 11.92719500 | -3.38858000 | 3.22809400 |
| H | 11.03774100 | -1.82589000 | 2.07864700 |
| H | 9.91350000 | -3.25323200 | 0.37337200 |
| H | 11.63930500 | -3.65335400 | 0.49924200 |
| H | 10.40933000 | -4.71431100 | 1.24670700 |
| H | 11.97708600 | -2.85889200 | 4.19230000 |
| H | 11.82235500 | -4.46536700 | 3.43608600 |
| H | 12.88962000 | -3.25196500 | 2.71069900 |
| C | 6.78239900 | 2.05763300 | -0.82819300 |
| C | 5.30052500 | 2.17777600 | -1.21287100 |
| C | 7.36398200 | 3.44518100 | -0.49746700 |
| H | 6.82666800 | 1.44078500 | 0.08246300 |
| H | 4.88696000 | 1.19766600 | -1.48767700 |
| H | 4.72433800 | 2.56913900 | -0.35908900 |
| H | 5.14940400 | 2.87445300 | -2.05324700 |
| H | 8.41166800 | 3.38816600 | -0.16716400 |
| H | 7.33001500 | 4.09906900 | -1.38448400 |
| H | 6.78181100 | 3.92869700 | 0.30376000 |
| C | 10.45379300 | -1.28162200 | -2.14851400 |
| C | 11.82908900 | -0.97805200 | -2.76317000 |
| C | 9.96845200 | -2.69199300 | -2.52318700 |
| H | 10.57958700 | -1.26164200 | -1.05611600 |
| H | 12.57459600 | -1.70597100 | -2.40445900 |
| H | 11.80949000 | -1.04251300 | -3.86286000 |
| H | 12.17596200 | 0.03108700 | -2.48998100 |
| H | 9.00771000 | -2.91798500 | -2.03416900 |
| H | 9.81854900 | -2.78590300 | -3.61084500 |
| H | 10.69920900 | -3.45388600 | -2.20896400 |
| Br | 5.45658400 | -1.61431400 | -1.09220300 |

**b'-4-free**

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

Zero-point correction= 0.812893 (Hartree/Particle)
Thermal correction to Energy= 0.858246
Thermal correction to Enthalpy= 0.859191
Thermal correction to Gibbs Free Energy= 0.733455
Sum of electronic and zero-point Energies= -3283.461189
Sum of electronic and thermal Energies= -3283.415836
Sum of electronic and thermal Enthalpies= -3283.414892
Sum of electronic and thermal Free Energies= -3283.540628

| | | | |
|---|---|---|---|
| C | -2.53176500 | 0.16197900 | -0.25690700 |
| C | -4.74388200 | 0.39452100 | -0.76716700 |
| C | -4.61068300 | 0.58090800 | 0.57119900 |
| N | -3.25752900 | 0.43928500 | 0.86409500 |
| N | -3.46937600 | 0.13098800 | -1.25308700 |
| H | -5.34489700 | 0.79190100 | 1.34156600 |
| H | -5.61723100 | 0.40354700 | -1.41222500 |
| C | -2.74010400 | 0.47176800 | 2.20503000 |
| C | -2.37602000 | -0.74700200 | 2.81385600 |
| C | -2.64377400 | 1.71410200 | 2.86396200 |
| C | -1.87309800 | -0.68849000 | 4.12172100 |
| C | -2.15531300 | 1.71277700 | 4.17700100 |
| C | -1.76528200 | 0.52635800 | 4.79792200 |
| H | -1.56446600 | -1.61073700 | 4.61890100 |
| H | -2.06380000 | 2.65721700 | 4.71681000 |
| C | -3.18975800 | -0.32549900 | -2.58768900 |
| C | -3.50188600 | -1.66402900 | -2.90289500 |
| C | -2.59937600 | 0.56338300 | -3.51072100 |
| C | -3.21957300 | -2.10290300 | -4.20529400 |
| C | -2.35125900 | 0.07747100 | -4.80087800 |
| C | -2.65815700 | -1.24047200 | -5.14514600 |
| H | -3.43758300 | -3.13630900 | -4.48366700 |
| H | -1.89743900 | 0.73096200 | -5.54679600 |
| C | -3.06398300 | 3.01890400 | 2.19731000 |
| C | -2.00320700 | 4.11982400 | 2.33542400 |
| H | -3.17798900 | 2.82221200 | 1.12075700 |
| H | -1.02920400 | 3.77904500 | 1.96328600 |
| H | -2.30495500 | 5.00690500 | 1.75532900 |
| H | -1.88010000 | 4.44062000 | 3.38252600 |
| C | -4.09947000 | -2.62672900 | -1.88009000 |
| C | -3.08868800 | -3.70921600 | -1.47124100 |
| H | -4.33670800 | -2.05875700 | -0.97027800 |
| H | -2.17399400 | -3.26630800 | -1.05338100 |
| H | -3.52226600 | -4.37086300 | -0.70413400 |
| H | -2.79716600 | -4.33335700 | -2.33078700 |
| C | -2.27036000 | 1.99711200 | -3.11226100 |
| C | -3.50241500 | 2.90337500 | -3.28427600 |
| H | -2.01296500 | 1.97992000 | -2.04316200 |
| H | -4.36007100 | 2.53208900 | -2.70238100 |
| H | -3.27985200 | 3.92767100 | -2.94431000 |
| H | -3.80628300 | 2.95170000 | -4.34306500 |
| C | -3.36929200 | -3.08216300 | 2.88937900 |
| H | -2.91878600 | -3.34852700 | 3.85904600 |
| H | -4.36955500 | -2.66399800 | 3.08493100 |
| H | -3.49328800 | -4.01460800 | 2.31505800 |
| C | -2.49211300 | -2.09274000 | 2.10611700 |
| H | -2.98382400 | -1.92858000 | 1.13714900 |
| Ni | -0.69432100 | -0.12153700 | -0.60324900 |
| C | 0.03098300 | 1.30233400 | 0.37709100 |
| C | 0.36716700 | 2.50827500 | -0.26049300 |
| C | 0.47499700 | 1.10846600 | 1.69552900 |
| C | 1.12627900 | 3.48792300 | 0.39421300 |
| H | 0.05998500 | 2.68246200 | -1.29361900 |
| C | 1.23383300 | 2.08370800 | 2.35437800 |

| | | | |
|---|---|---|---|
| H | 0.23194400 | 0.18263700 | 2.22182800 |
| H | 1.37862500 | 4.41683500 | -0.12663400 |
| H | 1.56601700 | 1.90676500 | 3.38192900 |
| O | 0.96949000 | -0.60377900 | -1.24844200 |
| C | -4.42311000 | 3.49660100 | 2.74043700 |
| H | -4.35418900 | 3.71851200 | 3.81813200 |
| H | -4.74492400 | 4.41616900 | 2.22528700 |
| H | -5.21121600 | 2.73943700 | 2.60815400 |
| C | -1.10385600 | -2.67840700 | 1.80853100 |
| H | -0.54365100 | -2.88255700 | 2.73514900 |
| H | -1.18405600 | -3.62167800 | 1.24656800 |
| H | -0.50694000 | -1.98200800 | 1.20211600 |
| C | -5.41747900 | -3.24234000 | -2.37631800 |
| H | -5.26138600 | -3.88006600 | -3.26123300 |
| H | -5.86493700 | -3.87120000 | -1.59007300 |
| H | -6.14633300 | -2.46226800 | -2.64773300 |
| C | -1.05062600 | 2.56684000 | -3.84535700 |
| H | -1.23745700 | 2.70583600 | -4.92218400 |
| H | -0.79352300 | 3.55416200 | -3.43137400 |
| H | -0.17478100 | 1.91016300 | -3.72674200 |
| C | 1.56812000 | 3.27768700 | 1.70510100 |
| H | 2.16232800 | 4.03915600 | 2.21767000 |
| C | 0.39432200 | -1.67773900 | -1.87406400 |
| H | -0.76533100 | -1.64558800 | -1.70433900 |
| C | 0.55106800 | -1.60724500 | -3.40013500 |
| H | 0.00645600 | -2.40344100 | -3.92788700 |
| H | 0.17104600 | -0.63888000 | -3.75069900 |
| H | 1.62216600 | -1.68014100 | -3.64394400 |
| C | 0.81753000 | -3.02812600 | -1.28240100 |
| C | 1.67287300 | -3.04828700 | -0.17332500 |
| C | 0.35781700 | -4.24714400 | -1.80342000 |
| C | 2.05789600 | -4.25999900 | 0.40810700 |
| H | 2.01243100 | -2.09095600 | 0.22476300 |
| C | 0.73601900 | -5.46078800 | -1.22097800 |
| H | -0.31133500 | -4.25432300 | -2.66650700 |
| C | 1.58861300 | -5.47136200 | -0.11105900 |
| H | 2.72517700 | -4.25849200 | 1.27447600 |
| H | 0.36421800 | -6.40171100 | -1.63588100 |
| H | 1.88584600 | -6.41947000 | 0.34500000 |
| H | -1.37319900 | 0.54891100 | 5.81789200 |
| H | -2.44468700 | -1.60059100 | -6.15458600 |

**TS-b'-c-4-free**

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

Zero-point correction= 0.808764 (Hartree/Particle)
Thermal correction to Energy= 0.856414
Thermal correction to Enthalpy= 0.857358
Thermal correction to Gibbs Free Energy= 0.725397
Sum of electronic and zero-point Energies= -5857.455372
Sum of electronic and thermal Energies= -5857.407722
Sum of electronic and thermal Enthalpies= -5857.406778
Sum of electronic and thermal Free Energies= -5857.538738

| | | | |
|---|---|---|---|
| C | -2.56479500 | 0.07488400 | -0.11536800 |
| C | -4.76674800 | 0.16859500 | -0.69665900 |
| C | -4.69681000 | 0.35424200 | 0.64605900 |
| N | -3.34309800 | 0.31041500 | 0.98264400 |
| N | -3.46001000 | 0.00972300 | -1.14963300 |
| H | -5.46886100 | 0.51862900 | 1.39091100 |
| H | -5.61598400 | 0.12750600 | -1.37162800 |
| C | -2.82509700 | 0.52854300 | 2.30127500 |
| C | -2.38445900 | -0.57614500 | 3.05760200 |
| C | -2.75816700 | 1.85379800 | 2.77858100 |
| C | -1.88632200 | -0.32097600 | 4.34390200 |
| C | -2.26750600 | 2.05289800 | 4.07567600 |
| C | -1.83549500 | 0.97727900 | 4.85211600 |
| H | -1.53284000 | -1.15415900 | 4.95587600 |
| H | -2.20272400 | 3.06690900 | 4.47611900 |
| C | -3.09030000 | -0.34763600 | -2.49182200 |
| C | -3.21836700 | -1.69390700 | -2.89025200 |
| C | -2.57629000 | 0.65490100 | -3.34402900 |
| C | -2.83935500 | -2.02498500 | -4.20057900 |
| C | -2.21994200 | 0.27470500 | -4.64537800 |
| C | -2.34933600 | -1.05056600 | -5.06729700 |
| H | -2.86605200 | -3.06250700 | -4.54291900 |
| H | -1.81549000 | 1.01552900 | -5.33621400 |
| C | -3.19937600 | 3.03774200 | 1.92488500 |
| C | -2.13545100 | 4.14302300 | 1.85449700 |
| H | -3.33931900 | 2.67242100 | 0.89729100 |
| H | -1.17848100 | 3.74539100 | 1.49205100 |
| H | -2.46597400 | 4.93748400 | 1.16531700 |
| H | -1.96432600 | 4.61151700 | 2.83758100 |
| C | -3.74625500 | -2.77861400 | -1.95872600 |
| C | -2.79820100 | -3.98574600 | -1.87742600 |
| H | -3.81288600 | -2.35378600 | -0.94666900 |
| H | -1.81175700 | -3.66982300 | -1.50918400 |
| H | -3.20134400 | -4.73380600 | -1.17415500 |
| H | -2.65158700 | -4.47506300 | -2.85350100 |
| C | -2.40784400 | 2.08845300 | -2.84785000 |
| C | -3.75019000 | 2.84285900 | -2.82127900 |
| H | -2.03861400 | 2.01941300 | -1.81228900 |
| H | -4.49584700 | 2.33354100 | -2.19476000 |
| H | -3.61304900 | 3.86025600 | -2.41876500 |
| H | -4.16504600 | 2.93133400 | -3.83938700 |
| C | -3.44086400 | -2.85347100 | 3.32333000 |
| H | -3.13310000 | -2.95580800 | 4.37745600 |
| H | -4.44683200 | -2.40370600 | 3.30889100 |
| H | -3.51331700 | -3.86634200 | 2.89460600 |
| C | -2.43936300 | -2.00329400 | 2.52449100 |
| H | -2.78868200 | -1.96265800 | 1.48474100 |
| Ni | -0.79008100 | -0.32349200 | -0.19115500 |
| C | 0.05667000 | 1.33775700 | 0.38186000 |
| C | 0.48989500 | 2.38595000 | -0.45805900 |
| C | 0.43996000 | 1.45015100 | 1.73848000 |
| C | 1.24668700 | 3.47080100 | 0.01007200 |
| H | 0.24129300 | 2.35807500 | -1.52248700 |
| C | 1.20242600 | 2.51975500 | 2.22393500 |
| H | 0.12724300 | 0.67657700 | 2.44779800 |
| H | 1.55756900 | 4.26032700 | -0.68315200 |
| H | 1.47131000 | 2.56112800 | 3.28519900 |
| O | 0.99237600 | -1.28675400 | -0.41764500 |
| C | -4.54975700 | 3.59064200 | 2.41305300 |
| H | -4.46608200 | 3.97652900 | 3.44282800 |
| H | -4.88767300 | 4.41810300 | 1.76773000 |
| H | -5.33138100 | 2.81474300 | 2.40900900 |
| C | -1.04711400 | -2.65331300 | 2.48337700 |
| H | -0.60838600 | -2.74997300 | 3.49034800 |
| H | -1.11141700 | -3.66129000 | 2.04306300 |
| H | -0.36251000 | -2.06515600 | 1.85432200 |
| C | -5.16235700 | -3.20651700 | -2.38309500 |
| H | -5.15042400 | -3.65076900 | -3.39173300 |
| H | -5.56613500 | -3.95961000 | -1.68624000 |
| H | -5.85579600 | -2.34969000 | -2.40010900 |
| C | -1.37053900 | 2.89236000 | -3.64140400 |
| H | -1.72379700 | 3.12700900 | -4.65899800 |
| H | -1.16938100 | 3.84835400 | -3.13337800 |
| H | -0.41711200 | 2.34983900 | -3.73184600 |
| Br | -1.13776500 | -5.02930600 | -5.53560400 |
| C | 1.60972900 | 3.54386500 | 1.35949800 |
| H | 2.19840800 | 4.38729800 | 1.73314000 |
| C | 0.92475600 | -1.94784200 | -1.46745500 |
| H | -1.43744700 | -1.65559100 | -0.51843800 |
| C | 0.60435500 | -1.27561700 | -2.77416000 |
| H | -0.40392800 | -1.57235600 | -3.09971600 |
| H | 0.62161200 | -0.18773000 | -2.63432100 |
| H | 1.30712700 | -1.57669300 | -3.56571500 |
| C | 1.13175300 | -3.41269900 | -1.42894000 |
| C | 1.53545100 | -4.01421700 | -0.21897400 |
| C | 0.84648300 | -4.22235700 | -2.54327200 |
| C | 1.66995100 | -5.39722600 | -0.13593900 |
| H | 1.72712500 | -3.37408700 | 0.64390700 |

| | | | |
|---|---|---|---|
| C | 0.96129000 | -5.61108400 | -2.44993400 |
| H | 0.47722900 | -3.81398900 | -3.48715300 |
| C | 1.38091300 | -6.19794000 | -1.25292900 |
| H | 1.98802900 | -5.85991200 | 0.80203300 |
| H | 0.68634100 | -6.20740400 | -3.32357000 |
| H | 1.47276200 | -7.28529600 | -1.18033000 |
| H | -1.44491400 | 1.15367600 | 5.85790100 |
| H | -2.03363300 | -1.34531300 | -6.07132600 |

**c-4-free**

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

Zero-point correction= 0.808972 (Hartree/Particle)
Thermal correction to Energy= 0.855059
Thermal correction to Enthalpy= 0.856003
Thermal correction to Gibbs Free Energy= 0.727046
Sum of electronic and zero-point Energies= -3283.444186
Sum of electronic and thermal Energies= -3283.398099
Sum of electronic and thermal Enthalpies= -3283.397154
Sum of electronic and thermal Free Energies= -3283.526111

| | | | |
|---|---|---|---|
| C | -2.87917700 | -0.04165300 | -0.06330300 |
| C | -5.00513500 | 0.55977500 | -0.63729800 |
| C | -4.86820400 | 0.77805600 | 0.69436300 |
| N | -3.56052000 | 0.42335800 | 1.02503200 |
| N | -3.78161000 | 0.06850600 | -1.08787900 |
| H | -5.56441400 | 1.15735500 | 1.43539300 |
| H | -5.84839100 | 0.70607000 | -1.30478000 |
| C | -2.99458800 | 0.59513900 | 2.33265100 |
| C | -2.80285200 | -0.53364000 | 3.15309400 |
| C | -2.64658300 | 1.90034400 | 2.73856400 |
| C | -2.26812700 | -0.32022800 | 4.43218400 |
| C | -2.12733800 | 2.06061600 | 4.02992100 |
| C | -1.94098200 | 0.96295700 | 4.87048000 |
| H | -2.10624200 | -1.17360700 | 5.09467800 |
| H | -1.84862700 | 3.05780700 | 4.37698800 |
| C | -3.52671600 | -0.38892900 | -2.42388500 |
| C | -3.97726800 | -1.67302600 | -2.79042700 |
| C | -2.82552800 | 0.45567100 | -3.31245900 |
| C | -3.73811700 | -2.09441800 | -4.10705600 |
| C | -2.60932000 | -0.01472200 | -4.61511400 |
| C | -3.06527800 | -1.27395100 | -5.01075500 |
| H | -4.08014900 | -3.08094500 | -4.42676200 |
| H | -2.07377600 | 0.60541900 | -5.33460200 |
| C | -2.81933400 | 3.10514600 | 1.81967100 |
| C | -1.53714700 | 3.94265100 | 1.70399700 |
| H | -3.03809800 | 2.72698000 | 0.81045600 |
| H | -0.69079000 | 3.32445500 | 1.37809400 |
| H | -1.68205700 | 4.75008600 | 0.96767500 |
| H | -1.26929600 | 4.41695400 | 2.66211400 |
| C | -4.71493100 | -2.57784600 | -1.81118700 |
| C | -4.14238900 | -4.00252900 | -1.78369800 |
| H | -4.57113600 | -2.16231900 | -0.80418700 |
| H | -3.06522600 | -3.97845900 | -1.56145700 |
| H | -4.64125000 | -4.59421200 | -0.99908400 |
| H | -4.29534400 | -4.52992600 | -2.73919000 |
| C | -2.32971500 | 1.82633600 | -2.86154000 |
| C | -3.46843200 | 2.86365300 | -2.84858700 |
| H | -1.97269500 | 1.70635800 | -1.82666900 |
| H | -4.29864700 | 2.55600000 | -2.19787300 |
| H | -3.09746600 | 3.83424000 | -2.48103200 |
| H | -3.86873700 | 3.01359300 | -3.86503100 |
| C | -4.33009900 | -2.51591800 | 3.49405300 |
| H | -4.08116200 | -2.61171000 | 4.56398000 |
| H | -5.21801900 | -1.86857200 | 3.41237800 |
| H | -4.60154400 | -3.51714300 | 3.12120300 |
| C | -3.14955800 | -1.94408800 | 2.69250800 |
| H | -3.45160100 | -1.89153400 | 1.63835000 |
| Ni | -1.24188500 | -0.85704300 | -0.17287300 |
| C | -0.08146600 | 0.62551700 | 0.36572400 |
| C | 0.55732800 | 1.53418400 | -0.50304100 |
| C | 0.33729600 | 0.67109700 | 1.71415800 |
| C | 1.54466300 | 2.43091900 | -0.06685100 |
| H | 0.29067800 | 1.54860300 | -1.56262100 |
| C | 1.32437400 | 1.55468000 | 2.16700400 |
| H | -0.12420000 | -0.00400400 | 2.44148400 |
| H | 2.01064300 | 3.11925900 | -0.78006600 |
| H | 1.61249600 | 1.55432700 | 3.22350200 |
| O | 0.34846600 | -1.94974600 | -0.43271500 |
| C | -4.01129500 | 3.96984900 | 2.26591200 |
| H | -3.83958700 | 4.38288300 | 3.27372400 |
| H | -4.15823900 | 4.81549800 | 1.57438000 |
| H | -4.94676600 | 3.38979800 | 2.29794100 |
| C | -1.92474300 | -2.87090600 | 2.74140700 |
| H | -1.55992200 | -3.01642800 | 3.77132200 |
| H | -2.18037500 | -3.86097000 | 2.33084800 |
| H | -1.10390300 | -2.45942700 | 2.13457100 |
| C | -6.22436700 | -2.58848700 | -2.11029500 |
| H | -6.42408800 | -2.99928800 | -3.11391000 |
| H | -6.76172900 | -3.21049500 | -1.37599100 |
| H | -6.65076200 | -1.57392100 | -2.07308000 |
| C | -1.15147500 | 2.35301900 | -3.69037000 |
| H | -1.46102400 | 2.63982500 | -4.70857500 |
| H | -0.72845300 | 3.24883900 | -3.21086500 |
| H | -0.34707700 | 1.60685900 | -3.78051100 |
| C | 1.93630800 | 2.44485700 | 1.27569700 |
| H | 2.70392700 | 3.14191700 | 1.62428700 |
| C | 0.83800200 | -2.22970100 | -1.53532100 |
| H | -2.09940600 | -2.08343600 | -0.49565500 |
| C | 0.15137000 | -1.71364000 | -2.76551600 |
| H | -0.91201200 | -2.00071000 | -2.69687400 |
| H | 0.16485800 | -0.61385700 | -2.71266300 |
| H | 0.57549200 | -2.03984300 | -3.72042400 |
| C | 2.07023400 | -3.05400000 | -1.57712700 |
| C | 2.67528500 | -3.41871300 | -0.35599400 |
| C | 2.65697700 | -3.48329400 | -2.78242600 |
| C | 3.83315800 | -4.19180300 | -0.34337000 |
| H | 2.21926300 | -3.07761700 | 0.57468100 |
| C | 3.81677800 | -4.26127100 | -2.76657500 |
| H | 2.21139800 | -3.21625100 | -3.74109800 |
| C | 4.40689900 | -4.61635600 | -1.54960500 |
| H | 4.29465500 | -4.46554200 | 0.60843900 |
| H | 4.26158100 | -4.59029600 | -3.70866300 |
| H | 5.31585800 | -5.22320300 | -1.53945300 |
| H | -1.52767500 | 1.10782900 | 5.87202200 |
| H | -2.88679800 | -1.61965300 | -6.03233800 |

**TS-c-e-4**

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

Zero-point correction= 0.738123 (Hartree/Particle)
Thermal correction to Energy= 0.780136
Thermal correction to Enthalpy= 0.781080
Thermal correction to Gibbs Free Energy= 0.664571
Sum of electronic and zero-point Energies= -3215.042346
Sum of electronic and thermal Energies= -3215.000334
Sum of electronic and thermal Enthalpies= -3214.999390
Sum of electronic and thermal Free Energies= -3215.115899

| | | | |
|---|---|---|---|
| C | 0.90306800 | 0.82932400 | 0.62720800 |
| C | 2.59448500 | 2.11682100 | -0.19753900 |
| C | 2.86701200 | 1.88151800 | 1.10756900 |
| N | 1.83762400 | 1.07902300 | 1.59385200 |
| N | 1.39351600 | 1.46915200 | -0.48122500 |
| H | 3.69629900 | 2.19057800 | 1.73522100 |
| H | 3.14344200 | 2.66469000 | -0.95550300 |
| C | 1.91926000 | 0.44579600 | 2.88449500 |
| C | 1.15627400 | 0.95291200 | 3.95527700 |
| C | 2.79416200 | -0.65086100 | 3.01934500 |
| C | 1.32106000 | 0.34783200 | 5.20835400 |
| C | 2.93070000 | -1.21328100 | 4.29648200 |
| C | 2.20804500 | -0.71736100 | 5.37966200 |
| H | 0.74791300 | 0.70795500 | 6.06357500 |
| H | 3.60038400 | -2.06362900 | 4.43959900 |

| | | | |
|---|---|---|---|
| H | 2.32390500 | -1.17354900 | 6.36612800 |
| C | 0.83137100 | 1.43771700 | -1.80699200 |
| C | 0.22151400 | 2.60429200 | -2.31337000 |
| C | 0.96704800 | 0.25439700 | -2.57110800 |
| C | -0.25660600 | 2.56911300 | -3.63201000 |
| C | 0.46081100 | 0.27309100 | -3.87819300 |
| C | -0.14002500 | 1.41727500 | -4.40577600 |
| H | -0.73211700 | 3.45548500 | -4.05589800 |
| H | 0.53917300 | -0.61744000 | -4.50187300 |
| H | -0.52268700 | 1.40684400 | -5.42947200 |
| C | -1.93592300 | 1.38339500 | 0.23892900 |
| C | -2.87352600 | 0.24354000 | 0.33435000 |
| H | -2.37709800 | -0.72340000 | 0.76705000 |
| Ni | -0.71108000 | -0.06331100 | 0.79272800 |
| C | 1.66272800 | -0.98409800 | -2.00864200 |
| C | 3.19515900 | -0.81970900 | -2.00430500 |
| C | 1.28471800 | -2.28235300 | -2.73218500 |
| H | 1.33324300 | -1.09153400 | -0.96418100 |
| H | 3.52008000 | 0.06139400 | -1.43456800 |
| H | 3.66962600 | -1.70357400 | -1.54857700 |
| H | 3.57743600 | -0.71861600 | -3.03343000 |
| H | 0.19387600 | -2.40444600 | -2.81420200 |
| H | 1.70876400 | -2.32462100 | -3.74868900 |
| H | 1.68006000 | -3.14472100 | -2.17440300 |
| C | 0.08836100 | 3.87982000 | -1.48808100 |
| C | -1.30706800 | 4.51667200 | -1.59825600 |
| C | 1.16625900 | 4.90799300 | -1.87983700 |
| H | 0.24456500 | 3.60903100 | -0.43327400 |
| H | -2.10530000 | 3.78481700 | -1.41418500 |
| H | -1.41028200 | 5.32731200 | -0.85998900 |
| H | -1.47432600 | 4.95808700 | -2.59355800 |
| H | 2.18388000 | 4.50977500 | -1.75822300 |
| H | 1.04944600 | 5.20734900 | -2.93429300 |
| H | 1.08078300 | 5.81390500 | -1.25818000 |
| C | 3.57015400 | -1.22195400 | 1.83705800 |
| C | 3.41903100 | -2.74534200 | 1.71169700 |
| C | 5.05401400 | -0.82023700 | 1.90311000 |
| H | 3.14687700 | -0.79151700 | 0.91921200 |
| H | 2.36233500 | -3.03717100 | 1.66661800 |
| H | 3.91402000 | -3.09307800 | 0.79021900 |
| H | 3.88930400 | -3.27541000 | 2.55555100 |
| H | 5.18192300 | 0.27232600 | 1.93877500 |
| H | 5.53393600 | -1.24364100 | 2.80085700 |
| H | 5.59517500 | -1.19691900 | 1.01997100 |
| C | 0.19640900 | 2.11483600 | 3.73902700 |
| C | 0.93191200 | 3.46468400 | 3.81092300 |
| C | -1.00962200 | 2.09568300 | 4.68456400 |
| H | -0.19882900 | 2.00425900 | 2.72055500 |
| H | 1.75777700 | 3.51590500 | 3.08565500 |
| H | 0.23920900 | 4.29394500 | 3.59322600 |
| H | 1.35321400 | 3.62571000 | 4.81709600 |
| H | -1.53289700 | 1.12730600 | 4.64713600 |
| H | -0.72103800 | 2.28966400 | 5.73017700 |
| H | -1.72482700 | 2.88123100 | 4.39553100 |
| C | -0.21397400 | -1.85209000 | 1.37918100 |
| C | -0.19221500 | -2.93516000 | 0.47389000 |
| C | -0.11296300 | -2.18765600 | 2.74671400 |
| C | -0.04794900 | -4.26456200 | 0.89418200 |
| H | -0.30258200 | -2.74315800 | -0.59600800 |
| C | 0.02551100 | -3.51089900 | 3.18396900 |
| H | -0.13169700 | -1.39538500 | 3.49943800 |
| C | 0.06665400 | -4.55888700 | 2.25722600 |
| H | -0.02936500 | -5.07245200 | 0.15553600 |
| H | 0.11081000 | -3.72346600 | 4.25440000 |
| H | 0.18475200 | -5.59293700 | 2.59358700 |
| F | -3.36899400 | -0.18574700 | -0.86707800 |
| F | -3.93356300 | 0.41810900 | 1.18495100 |
| C | -2.23795700 | 2.56509800 | 1.14366000 |
| H | -2.42035500 | 2.24189900 | 2.17797900 |
| H | -1.39572100 | 3.27241200 | 1.16054300 |
| H | -3.13438100 | 3.12466900 | 0.81836600 |
| H | -1.80410300 | 1.66232500 | -0.81431200 |

**e-4**

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

Zero-point correction= 0.740451 (Hartree/Particle)
Thermal correction to Energy= 0.782795
Thermal correction to Enthalpy= 0.783739
Thermal correction to Gibbs Free Energy= 0.666735
Sum of electronic and zero-point Energies= -3215.040558
Sum of electronic and thermal Energies= -3214.998215
Sum of electronic and thermal Enthalpies= -3214.997271
Sum of electronic and thermal Free Energies= -3215.114275

| | | | |
|---|---|---|---|
| C | 0.89379500 | 0.82844600 | 0.62773700 |
| C | 2.58960100 | 2.10947400 | -0.19893200 |
| C | 2.86121300 | 1.87530100 | 1.10664500 |
| N | 1.82883000 | 1.07683900 | 1.59351300 |
| N | 1.38671200 | 1.46484500 | -0.48125300 |
| H | 3.69198700 | 2.18149600 | 1.73379100 |
| H | 3.14065000 | 2.65412300 | -0.95769200 |
| C | 1.90871500 | 0.44248200 | 2.88358300 |
| C | 1.14102700 | 0.94527600 | 3.95312800 |
| C | 2.78553500 | -0.65252200 | 3.01852300 |
| C | 1.30225900 | 0.33651600 | 5.20482200 |
| C | 2.91821900 | -1.21889100 | 4.29436000 |
| C | 2.19029700 | -0.72790300 | 5.37616900 |
| H | 0.72534600 | 0.69278200 | 6.05908500 |
| H | 3.58920100 | -2.06831900 | 4.43724000 |
| H | 2.30297900 | -1.18704900 | 6.36162800 |
| C | 0.82310400 | 1.43095900 | -1.80632500 |
| C | 0.21186500 | 2.59603700 | -2.31457700 |
| C | 0.95819900 | 0.24596900 | -2.56812300 |
| C | -0.26919500 | 2.55724800 | -3.63207800 |
| C | 0.44939500 | 0.26119900 | -3.87427400 |
| C | -0.15357900 | 1.40357200 | -4.40327100 |
| H | -0.74589900 | 3.44231300 | -4.05730100 |
| H | 0.52740700 | -0.63068800 | -4.49606000 |
| H | -0.53840300 | 1.39041700 | -5.42612900 |
| C | -1.95245100 | 1.40862700 | 0.24848100 |
| C | -2.83640900 | 0.24466200 | 0.39296200 |
| H | -2.27707200 | -0.71800900 | 0.80802000 |
| Ni | -0.73778000 | -0.04806200 | 0.78998000 |
| C | 1.65639700 | -0.99060200 | -2.00459500 |
| C | 3.18867200 | -0.82426900 | -2.00335100 |
| C | 1.27970200 | -2.29069900 | -2.72558900 |
| H | 1.32860500 | -1.09673700 | -0.95948700 |
| H | 3.51379500 | 0.05804500 | -1.43569200 |
| H | 3.66495300 | -1.70691600 | -1.54720300 |
| H | 3.56883800 | -0.72439200 | -3.03337300 |
| H | 0.18913900 | -2.41350900 | -2.80930100 |
| H | 1.70553200 | -2.33518800 | -3.74127200 |
| H | 1.67399500 | -3.15154900 | -2.16474800 |
| C | 0.08186900 | 3.87412300 | -1.49286400 |
| C | -1.31025700 | 4.51723100 | -1.60821200 |
| C | 1.16491900 | 4.89691300 | -1.88474100 |
| H | 0.23463800 | 3.60506000 | -0.43711100 |
| H | -2.11281900 | 3.78934900 | -1.42727700 |
| H | -1.41254200 | 5.32843300 | -0.87047400 |
| H | -1.47174900 | 4.95934500 | -2.60415300 |
| H | 2.18062800 | 4.49512800 | -1.75951700 |
| H | 1.05178100 | 5.19372300 | -2.94031600 |
| H | 1.08147500 | 5.80486900 | -1.26579100 |
| C | 3.56810300 | -1.21845300 | 1.83801900 |
| C | 3.40425600 | -2.73900300 | 1.69609600 |
| C | 5.05425200 | -0.82918100 | 1.92217900 |
| H | 3.15795600 | -0.77592200 | 0.92008500 |
| H | 2.34553200 | -3.01942900 | 1.63105300 |
| H | 3.91099700 | -3.08349100 | 0.77977300 |
| H | 3.85444500 | -3.28149600 | 2.54297900 |
| H | 5.18966100 | 0.26211600 | 1.97062600 |

| | | | |
|---|---|---|---|
| H | 5.52293800 | -1.26539900 | 2.81971600 |
| H | 5.60081700 | -1.20066900 | 1.04017100 |
| C | 0.17956300 | 2.10591700 | 3.73646500 |
| C | 0.91381200 | 3.45667100 | 3.80419800 |
| C | -1.02478200 | 2.08768200 | 4.68406100 |
| H | -0.21725200 | 1.99282900 | 2.71879700 |
| H | 1.73867200 | 3.50709300 | 3.07776000 |
| H | 0.21993900 | 4.28466700 | 3.58542500 |
| H | 1.33618300 | 3.62049500 | 4.80947200 |
| H | -1.54913600 | 1.11988000 | 4.64728600 |
| H | -0.73422100 | 2.28147400 | 5.72915100 |
| H | -1.73972200 | 2.87403800 | 4.39656700 |
| C | -0.24652000 | -1.84061800 | 1.36379500 |
| C | -0.22445200 | -2.91823900 | 0.45304900 |
| C | -0.12907000 | -2.18071700 | 2.72823000 |
| C | -0.05995700 | -4.24784700 | 0.86522500 |
| H | -0.35231300 | -2.72184600 | -0.61398000 |
| C | 0.02891800 | -3.50448600 | 3.15733300 |
| H | -0.15104300 | -1.39253900 | 3.48495100 |
| C | 0.07240400 | -4.54772400 | 2.22543900 |
| H | -0.04105500 | -5.05171400 | 0.12220900 |
| H | 0.12723600 | -3.72077400 | 4.22588500 |
| H | 0.20513400 | -5.58199200 | 2.55553400 |
| F | -3.37649100 | -0.22773900 | -0.77204400 |
| F | -3.85129400 | 0.36907700 | 1.30383500 |
| C | -2.24517700 | 2.59795500 | 1.14395600 |
| H | -2.42698500 | 2.28236900 | 2.18027000 |
| H | -1.40067800 | 3.30271600 | 1.15446300 |
| H | -3.13984900 | 3.15825700 | 0.81521600 |
| H | -1.83384500 | 1.66523400 | -0.81163900 |

**e'-4**

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

Zero-point correction= 0.741395 (Hartree/Particle)
Thermal correction to Energy= 0.783755
Thermal correction to Enthalpy= 0.784699
Thermal correction to Gibbs Free Energy= 0.667914
Sum of electronic and zero-point Energies= -3215.061717
Sum of electronic and thermal Energies= -3215.019357
Sum of electronic and thermal Enthalpies= -3215.018413
Sum of electronic and thermal Free Energies= -3215.135197

| | | | |
|---|---|---|---|
| Ni | -1.43130700 | 0.31509300 | 0.24132000 |
| N | 0.74090800 | 1.82770700 | 1.44274100 |
| N | -0.58754400 | 1.33500700 | 3.05505000 |
| C | 2.40650000 | 1.08107600 | -0.18656500 |
| C | 2.99960100 | 1.23298700 | -1.44685800 |
| C | 2.52547900 | 2.18224900 | -2.35029700 |
| C | 1.43749400 | 2.98958100 | -2.02249200 |
| C | 0.81044500 | 2.88772100 | -0.77395800 |
| C | 1.32977400 | 1.93593400 | 0.13087000 |
| C | 1.33520600 | 2.31349100 | 2.60139300 |
| C | 0.49700800 | 1.99715700 | 3.62193000 |
| C | -0.45000100 | 1.21055700 | 1.70200400 |
| C | -1.68673800 | 0.82039100 | 3.82702600 |
| C | -1.73041600 | -0.56136400 | 4.09223100 |
| C | -2.84074200 | -1.05241600 | 4.79638800 |
| C | -3.84394400 | -0.19301300 | 5.23712400 |
| C | -3.74676000 | 1.18077700 | 5.00629500 |
| C | -2.66380100 | 1.72378300 | 4.30371000 |
| H | 3.83349900 | 0.59236200 | -1.73563200 |
| H | 2.99882600 | 2.28213100 | -3.33051300 |
| H | 1.06651400 | 3.70463700 | -2.75664600 |
| H | 2.28896400 | 2.83254700 | 2.58806000 |
| H | 0.56777100 | 2.17585300 | 4.69064200 |
| H | -2.91767000 | -2.12250400 | 5.00093500 |
| H | -4.70613400 | -0.59262300 | 5.77705700 |
| H | -4.53580100 | 1.83631100 | 5.37515100 |
| C | -1.96494400 | -0.65671500 | -1.36666000 |
| H | -2.98776600 | -0.46325600 | -1.72737000 |
| C | -1.04254800 | -0.17472100 | -2.44365200 |
| C | -0.39298700 | 3.75352100 | -0.40963700 |
| C | -1.14556100 | 4.30237500 | -1.62713900 |
| C | -0.00410500 | 4.89916500 | 0.54210000 |
| H | -1.09805000 | 3.09570600 | 0.12051000 |
| H | -1.38376100 | 3.50208900 | -2.34137700 |
| H | -2.08987700 | 4.76346100 | -1.29846800 |
| H | -0.56722300 | 5.07948600 | -2.15371700 |
| H | 0.46403900 | 4.53076700 | 1.46593600 |
| H | 0.70503000 | 5.58651400 | 0.05158500 |
| H | -0.89749300 | 5.47664800 | 0.82890800 |
| C | 2.85195200 | -0.02437200 | 0.76845600 |
| C | 4.32271400 | -0.42799500 | 0.60210600 |
| C | 1.93447100 | -1.25495300 | 0.62983100 |
| H | 2.73900500 | 0.34925100 | 1.79803700 |
| H | 4.99141100 | 0.44631700 | 0.63770900 |
| H | 4.61607500 | -1.11737500 | 1.40928600 |
| H | 4.49895000 | -0.95240700 | -0.35069600 |
| H | 0.89456800 | -1.01199600 | 0.88513500 |
| H | 1.94244500 | -1.63451300 | -0.40300200 |
| H | 2.26045500 | -2.06108200 | 1.30690800 |
| C | -0.63870900 | -1.51852900 | 3.62973300 |
| C | -1.15371300 | -2.42873100 | 2.50542600 |
| C | -0.05207800 | -2.33059900 | 4.79522100 |
| H | 0.18257700 | -0.92004800 | 3.21028900 |
| H | -1.52011600 | -1.82303800 | 1.66365900 |
| H | -0.35089500 | -3.08304600 | 2.13055900 |
| H | -1.98265700 | -3.06652000 | 2.85269600 |
| H | 0.32480800 | -1.67159500 | 5.59342800 |
| H | -0.79990200 | -3.00645400 | 5.24023300 |
| H | 0.78530000 | -2.95301600 | 4.44048900 |
| C | -2.55595900 | 3.22651100 | 4.04701200 |
| C | -3.31147100 | 4.07701500 | 5.07652000 |
| C | -2.99871100 | 3.58837800 | 2.61959000 |
| H | -1.49163600 | 3.49737900 | 4.13521400 |
| H | -3.04529600 | 3.80661000 | 6.11065200 |
| H | -3.07047400 | 5.14123100 | 4.92798400 |
| H | -4.40321400 | 3.97554300 | 4.96711100 |
| H | -2.41073300 | 3.05544900 | 1.86418300 |
| H | -4.05171300 | 3.31685700 | 2.45425600 |
| H | -2.88325400 | 4.67065400 | 2.44674800 |
| C | -3.18613500 | 0.85520200 | 0.46037400 |
| C | -4.00585400 | 0.30068200 | 1.45669900 |
| C | -3.73091000 | 1.86221200 | -0.35980200 |
| C | -5.31337600 | 0.76424200 | 1.65551100 |
| H | -3.62260000 | -0.49129000 | 2.10258800 |
| C | -5.03115200 | 2.33592500 | -0.15380300 |
| H | -3.13146900 | 2.27279700 | -1.17430600 |
| C | -5.83143700 | 1.79042000 | 0.85843200 |
| H | -5.92469600 | 0.32247000 | 2.44831900 |
| H | -5.42586000 | 3.13025400 | -0.79539100 |
| H | -6.84957700 | 2.15619200 | 1.01778600 |
| F | 0.27954400 | -0.26619300 | -2.02685300 |
| F | -1.26121100 | 1.15209700 | -2.74509300 |
| C | -1.78478200 | -2.15762500 | -1.12315600 |
| H | -2.52721000 | -2.51959500 | -0.39649700 |
| H | -1.90307800 | -2.76018300 | -2.04709000 |
| H | -0.78656200 | -2.38937100 | -0.71612000 |
| H | -1.09530400 | -0.72638800 | -3.40449100 |

**TS-e'-P-4**

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

Zero-point correction= 0.739658 (Hartree/Particle)
Thermal correction to Energy= 0.781603
Thermal correction to Enthalpy= 0.782547
Thermal correction to Gibbs Free Energy= 0.665807
Sum of electronic and zero-point Energies= -3215.033559
Sum of electronic and thermal Energies= -3214.991613
Sum of electronic and thermal Enthalpies= -3214.990669
Sum of electronic and thermal Free Energies= -3215.107410

| | | | |
|---|---|---|---|
| Ni | -1.37592500 | 0.63368700 | 0.26814300 |

| | | | |
|---|---|---|---|
| N | 0.93772400 | 1.76304200 | 1.60465500 |
| N | -0.57312800 | 1.31048400 | 3.06231000 |
| C | 2.42550800 | 0.98851800 | -0.18196400 |
| C | 2.98831500 | 1.21391200 | -1.44622900 |
| C | 2.70523200 | 2.37935400 | -2.16085000 |
| C | 1.85447800 | 3.34667900 | -1.62481600 |
| C | 1.26968800 | 3.17183700 | -0.36243200 |
| C | 1.56789700 | 1.98193400 | 0.33414500 |
| C | 1.48232000 | 2.08563300 | 2.84345600 |
| C | 0.52708800 | 1.79698700 | 3.76587900 |
| C | -0.33638300 | 1.27235900 | 1.71748600 |
| C | -1.82347100 | 0.94205400 | 3.66858400 |
| C | -1.91175900 | -0.31125900 | 4.30725500 |
| C | -3.12541800 | -0.63627200 | 4.93030600 |
| C | -4.20189900 | 0.24933300 | 4.89992700 |
| C | -4.09766600 | 1.46894400 | 4.22924700 |
| C | -2.90796500 | 1.84501500 | 3.59039400 |
| H | 3.64856700 | 0.46356900 | -1.88513800 |
| H | 3.15022900 | 2.53304700 | -3.14737100 |
| H | 1.63584600 | 4.24919600 | -2.19968400 |
| H | 2.48427800 | 2.49092100 | 2.94902200 |
| H | 0.52111600 | 1.89816700 | 4.84712800 |
| H | -3.23692500 | -1.59679100 | 5.43524000 |
| H | -5.14138500 | -0.02100000 | 5.38881800 |
| H | -4.96437000 | 2.12905400 | 4.19422900 |
| C | -1.91235200 | -0.01243000 | -1.52934400 |
| H | -0.81793900 | 0.25720800 | -1.43392600 |
| C | -1.88023600 | -1.45726100 | -1.97306700 |
| C | 0.29459700 | 4.20458400 | 0.19238200 |
| C | -1.06429300 | 4.09225700 | -0.52102400 |
| C | 0.84769800 | 5.63588500 | 0.13620100 |
| H | 0.11834300 | 3.96741300 | 1.25140300 |
| H | -1.45476100 | 3.06605300 | -0.42310600 |
| H | -1.79749000 | 4.78512400 | -0.07763500 |
| H | -0.97110200 | 4.32682000 | -1.59414400 |
| H | 1.82039400 | 5.71095800 | 0.64772900 |
| H | 0.98240300 | 5.98474500 | -0.90031300 |
| H | 0.14793300 | 6.33103600 | 0.62737500 |
| C | 2.65380700 | -0.32315100 | 0.56085200 |
| C | 4.10343200 | -0.82096600 | 0.48427900 |
| C | 1.66376300 | -1.38658100 | 0.05400900 |
| H | 2.42529600 | -0.14936700 | 1.62341800 |
| H | 4.81554900 | -0.04858600 | 0.81594300 |
| H | 4.23235800 | -1.70574800 | 1.12772200 |
| H | 4.38159300 | -1.12202000 | -0.53852100 |
| H | 0.62637000 | -1.03873400 | 0.15853700 |
| H | 1.83658400 | -1.60724400 | -1.01230000 |
| H | 1.76910400 | -2.32510300 | 0.62168600 |
| C | -0.75894500 | -1.30805800 | 4.23138500 |
| C | -0.82207100 | -2.07868700 | 2.89841700 |
| C | -0.69223300 | -2.27225700 | 5.42193200 |
| H | 0.18102500 | -0.73452600 | 4.22955600 |
| H | -0.84551900 | -1.39230900 | 2.03925700 |
| H | 0.05207900 | -2.74109000 | 2.78956700 |
| H | -1.73271000 | -2.69780600 | 2.85585600 |
| H | -0.69415200 | -1.73417900 | 6.38320100 |
| H | -1.53834600 | -2.97816900 | 5.42605300 |
| H | 0.22889300 | -2.87367600 | 5.36712800 |
| C | -2.79189100 | 3.15000700 | 2.80325600 |
| C | -1.93854700 | 4.20515700 | 3.53167100 |
| C | -4.14353500 | 3.76056100 | 2.41776800 |
| H | -2.28271300 | 2.88082300 | 1.86354600 |
| H | -0.92789100 | 3.84508800 | 3.76413200 |
| H | -1.83419400 | 5.10650500 | 2.90569300 |
| H | -2.41888800 | 4.50427700 | 4.47814300 |
| H | -4.79046100 | 3.02744100 | 1.91806900 |
| H | -4.67981600 | 4.15851000 | 3.29517000 |
| H | -3.98382500 | 4.60172700 | 1.72450900 |
| C | -3.13759200 | 0.09146400 | -0.01671000 |
| C | -3.53318200 | -1.12583000 | 0.59233300 |
| C | -4.12057900 | 1.10272800 | -0.13508400 |
| C | -4.81953100 | -1.29478700 | 1.10403300 |
| H | -2.81643900 | -1.94116500 | 0.66766700 |
| C | -5.41327200 | 0.92240100 | 0.36450800 |
| H | -3.86310300 | 2.05338700 | -0.60551700 |
| C | -5.77365600 | -0.27491700 | 0.99229600 |
| H | -5.08199600 | -2.23791000 | 1.59250900 |
| H | -6.14476500 | 1.73015000 | 0.26656400 |
| H | -6.78479700 | -0.41457200 | 1.38295900 |
| F | -3.12880200 | -1.96764500 | -2.19296600 |
| F | -1.26866800 | -2.25964800 | -1.04216100 |
| C | -2.49596600 | 0.87220700 | -2.62756700 |
| H | -3.56043100 | 0.65536800 | -2.79671000 |
| H | -2.39648900 | 1.93244800 | -2.36001200 |
| H | -1.95880500 | 0.71948300 | -3.58061800 |
| H | -1.31765500 | -1.57697400 | -2.91887800 |

**P (complex)-4**

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

Zero-point correction= 0.741962 (Hartree/Particle)

Thermal correction to Energy= 0.784317

Thermal correction to Enthalpy= 0.785261

Thermal correction to Gibbs Free Energy= 0.668186

Sum of electronic and zero-point Energies= -3215.085837

Sum of electronic and thermal Energies= -3215.043482

Sum of electronic and thermal Enthalpies= -3215.042538

Sum of electronic and thermal Free Energies= -3215.159613

| | | | |
|---|---|---|---|
| C | 1.33217700 | 0.47182900 | 0.73224400 |
| C | 2.90455100 | 1.91136300 | -0.14074900 |
| C | 3.25027900 | 1.67992100 | 1.15036200 |
| N | 2.29241900 | 0.80975700 | 1.66724500 |
| N | 1.74167900 | 1.17850900 | -0.37940800 |
| H | 4.08337700 | 2.04520700 | 1.74377900 |
| H | 3.36540800 | 2.52945900 | -0.90568300 |
| C | 2.28804400 | 0.30626300 | 3.00948400 |
| C | 1.38416000 | 0.86393600 | 3.94218300 |
| C | 3.17185200 | -0.74219200 | 3.34075300 |
| C | 1.39545200 | 0.34534600 | 5.24405100 |
| C | 3.14460000 | -1.22425500 | 4.65841300 |
| C | 2.26773000 | -0.68559900 | 5.59984400 |
| H | 0.71240600 | 0.74656600 | 5.99403600 |
| H | 3.81119300 | -2.03634100 | 4.95302000 |
| H | 2.26027000 | -1.07527000 | 6.62123900 |
| C | 1.01401000 | 1.23979900 | -1.61223100 |
| C | 0.22099300 | 2.38128100 | -1.86221600 |
| C | 1.10220100 | 0.16360800 | -2.52205300 |
| C | -0.43326500 | 2.46275000 | -3.09998700 |
| C | 0.41914500 | 0.28937400 | -3.73997700 |
| C | -0.32406200 | 1.43330400 | -4.03414900 |
| H | -1.06289200 | 3.32452600 | -3.32555200 |
| H | 0.45363600 | -0.52266800 | -4.46687500 |
| H | -0.85078600 | 1.50785100 | -4.98872900 |
| C | -3.12562900 | -0.40701900 | -0.34334400 |
| C | -2.47080700 | 0.00646100 | -1.65429300 |
| H | -1.46226400 | 0.41299700 | -1.50708300 |
| Ni | -0.08558500 | -0.69637200 | 0.98911800 |
| C | 1.87863000 | -1.09695700 | -2.15746900 |
| C | 3.39107500 | -0.91881500 | -2.37250500 |
| C | 1.36416700 | -2.35212000 | -2.87170400 |
| H | 1.70173400 | -1.25582900 | -1.08236700 |
| H | 3.78381200 | -0.06247700 | -1.80466300 |
| H | 3.93509400 | -1.81909000 | -2.04220800 |
| H | 3.61900900 | -0.75452100 | -3.43910800 |
| H | 0.27270000 | -2.44921000 | -2.76642500 |
| H | 1.60351000 | -2.34900300 | -3.94796200 |
| H | 1.83321700 | -3.24859700 | -2.43600200 |
| C | -0.03653200 | 3.40775600 | -0.76337800 |
| C | -1.23106800 | 2.93604500 | 0.09120300 |
| C | -0.25105200 | 4.83501700 | -1.28061600 |
| H | 0.84327400 | 3.42985500 | -0.10319400 |

| | | | |
|---|---|---|---|
| H | -1.04911200 | 1.92530900 | 0.49011900 |
| H | -1.39871000 | 3.61965200 | 0.93978300 |
| H | -2.15012200 | 2.90555400 | -0.51705200 |
| H | 0.57568400 | 5.15859500 | -1.93285200 |
| H | -1.18974700 | 4.93015500 | -1.84982800 |
| H | -0.31442400 | 5.53673800 | -0.43384700 |
| C | 4.06687300 | -1.37889000 | 2.28061500 |
| C | 3.29445000 | -2.47137000 | 1.51754100 |
| C | 5.39002000 | -1.92208600 | 2.83499800 |
| H | 4.32208200 | -0.59827900 | 1.54804100 |
| H | 2.35726100 | -2.07300000 | 1.10256100 |
| H | 3.90447700 | -2.87307200 | 0.69159600 |
| H | 3.03780600 | -3.30542800 | 2.19208200 |
| H | 5.93015900 | -1.16053700 | 3.41975100 |
| H | 5.23573300 | -2.80040900 | 3.48253500 |
| H | 6.04077600 | -2.24331100 | 2.00632100 |
| C | 0.43531900 | 1.98503900 | 3.52904100 |
| C | 1.15479500 | 3.34537500 | 3.48706800 |
| C | -0.82979100 | 2.07911500 | 4.38939200 |
| H | 0.10406200 | 1.74063100 | 2.50913400 |
| H | 2.02981600 | 3.32543000 | 2.82214200 |
| H | 0.47227000 | 4.12928100 | 3.11933300 |
| H | 1.49805200 | 3.63703600 | 4.49379600 |
| H | -1.34785900 | 1.11082200 | 4.45878000 |
| H | -0.61371500 | 2.42427800 | 5.41388200 |
| H | -1.52870600 | 2.80397900 | 3.94278700 |
| C | -2.14603000 | -1.13176000 | 0.56034200 |
| C | -1.33999300 | -2.19950300 | 0.07986500 |
| C | -2.03065600 | -0.75775400 | 1.92736600 |
| C | -0.42452000 | -2.84971700 | 0.93997100 |
| H | -1.40750200 | -2.50191900 | -0.96430000 |
| C | -1.13801600 | -1.43175000 | 2.79322400 |
| H | -2.62865000 | 0.07302100 | 2.30844600 |
| C | -0.32886100 | -2.47560000 | 2.30031200 |
| H | 0.22074600 | -3.63597200 | 0.54398500 |
| H | -1.04029100 | -1.11573200 | 3.83239000 |
| H | 0.39607700 | -2.96134600 | 2.95473400 |
| F | -3.24256900 | 0.95009100 | -2.28002200 |
| F | -2.37574000 | -1.05304600 | -2.52385200 |
| C | -4.41966800 | -1.19590100 | -0.58626800 |
| H | -4.20166600 | -2.15708900 | -1.07466500 |
| H | -4.92763400 | -1.40006800 | 0.36766300 |
| H | -5.10408400 | -0.62585700 | -1.23325700 |
| H | -3.37606300 | 0.54846900 | 0.14473700 |

**TS-c-k-4**

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

Zero-point correction= 0.735429 (Hartree/Particle)

Thermal correction to Energy= 0.777643

Thermal correction to Enthalpy= 0.778587

Thermal correction to Gibbs Free Energy= 0.661780

Sum of electronic and zero-point Energies= -3215.012233

Sum of electronic and thermal Energies= -3214.970019

Sum of electronic and thermal Enthalpies= -3214.969075

Sum of electronic and thermal Free Energies= -3215.085882

| | | | |
|---|---|---|---|
| C | 1.09176000 | 0.60587100 | 0.58983800 |
| C | 2.75638800 | 1.85589500 | -0.34490600 |
| C | 3.09497600 | 1.63356200 | 0.95092000 |
| N | 2.08049000 | 0.84933500 | 1.49916100 |
| N | 1.54089000 | 1.20936000 | -0.55032600 |
| H | 3.95427800 | 1.95388400 | 1.53031100 |
| H | 3.26043500 | 2.40615400 | -1.13334400 |
| C | 2.09486200 | 0.30585400 | 2.83084400 |
| C | 1.27298700 | 0.88756600 | 3.81698000 |
| C | 2.92918700 | -0.80426700 | 3.09143900 |
| C | 1.27669200 | 0.30066900 | 5.09109900 |
| C | 2.89940100 | -1.34659400 | 4.38297800 |
| C | 2.07427300 | -0.80770900 | 5.37065400 |
| H | 0.65031100 | 0.72574800 | 5.87833100 |
| H | 3.52598900 | -2.20840100 | 4.61972000 |
| H | 2.05923400 | -1.25234500 | 6.36912300 |
| C | 0.79166100 | 1.22035600 | -1.77632800 |
| C | -0.01582500 | 2.33770300 | -2.06574000 |
| C | 0.87885100 | 0.09875300 | -2.63201500 |
| C | -0.72300500 | 2.33082700 | -3.27776200 |
| C | 0.14814500 | 0.14061500 | -3.82687700 |
| C | -0.63895600 | 1.24824700 | -4.15048800 |
| H | -1.35463200 | 3.18307700 | -3.53602100 |
| H | 0.18632000 | -0.70306200 | -4.51679700 |
| H | -1.19997400 | 1.25971000 | -5.08848100 |
| C | -2.30635500 | -1.21011800 | 0.37850800 |
| C | -2.62173900 | 0.15002100 | 0.78240200 |
| H | -0.95993600 | 1.56823400 | 0.90817500 |
| Ni | -0.75031600 | 0.11717300 | 0.82533600 |
| C | 1.74050800 | -1.10545200 | -2.26394300 |
| C | 3.22551600 | -0.85525500 | -2.58731800 |
| C | 1.27140600 | -2.41362200 | -2.91382900 |
| H | 1.65359600 | -1.23434500 | -1.17385700 |
| H | 3.61338500 | 0.03455800 | -2.07203200 |
| H | 3.83740000 | -1.71732700 | -2.27521600 |
| H | 3.36662800 | -0.71034600 | -3.67110000 |
| H | 0.19278800 | -2.57798500 | -2.76972600 |
| H | 1.47177400 | -2.42886900 | -3.99725600 |
| H | 1.80977100 | -3.26584300 | -2.47082400 |
| C | -0.12221700 | 3.52365100 | -1.11603400 |
| C | -1.58123300 | 3.93161800 | -0.85958200 |
| C | 0.71331800 | 4.71020600 | -1.62676600 |
| H | 0.29320200 | 3.20945200 | -0.14851400 |
| H | -2.17848700 | 3.06554600 | -0.54054500 |
| H | -1.62396000 | 4.69501400 | -0.06594800 |
| H | -2.04895000 | 4.36739900 | -1.75758800 |
| H | 1.77298200 | 4.43578200 | -1.74928700 |
| H | 0.34252200 | 5.06144900 | -2.60400400 |
| H | 0.65973000 | 5.55465300 | -0.92044600 |
| C | 3.87972800 | -1.36491500 | 2.03667200 |
| C | 3.92241500 | -2.89864200 | 2.00191500 |
| C | 5.29923900 | -0.80067700 | 2.24039300 |
| H | 3.52041600 | -1.03167000 | 1.05092400 |
| H | 2.91593400 | -3.32062100 | 1.89200300 |
| H | 4.53693600 | -3.23703800 | 1.15210200 |
| H | 4.37324700 | -3.31809500 | 2.91578000 |
| H | 5.31484900 | 0.29885700 | 2.23192000 |
| H | 5.70745500 | -1.13060800 | 3.20992500 |
| H | 5.97639900 | -1.15685300 | 1.44704400 |
| C | 0.46818000 | 2.15634500 | 3.55960800 |
| C | 1.14053100 | 3.35397300 | 4.25460300 |
| C | -1.00668800 | 2.02342000 | 3.96335800 |
| H | 0.47658300 | 2.34825500 | 2.47904800 |
| H | 2.18476300 | 3.47356900 | 3.92361300 |
| H | 0.60008600 | 4.28706600 | 4.02597900 |
| H | 1.14808400 | 3.22672700 | 5.34992000 |
| H | -1.50122300 | 1.22643900 | 3.39084900 |
| H | -1.12638400 | 1.81835300 | 5.03953400 |
| H | -1.54192200 | 2.96109800 | 3.74295400 |
| C | -0.63777800 | -1.84080700 | 1.25720300 |
| C | 0.00688000 | -2.88625600 | 0.57497400 |
| C | -0.75076400 | -1.93701600 | 2.66091000 |
| C | 0.52294300 | -3.98651600 | 1.26748100 |
| H | 0.10335400 | -2.85048100 | -0.50940100 |
| C | -0.20113300 | -3.01549200 | 3.35623700 |
| H | -1.29268900 | -1.16525700 | 3.21383000 |
| C | 0.42530300 | -4.05752100 | 2.66175100 |
| H | 1.01592800 | -4.78916400 | 0.71138400 |
| H | -0.27777800 | -3.04944400 | 4.44617300 |
| H | 0.83586300 | -4.91419600 | 3.20197300 |
| F | -3.32131900 | 0.25541000 | 1.95924000 |
| F | -3.27268500 | 0.92447300 | -0.14289500 |
| C | -2.32244200 | -1.51552700 | -1.10370200 |
| H | -1.98903100 | -2.54290000 | -1.30347600 |
| H | -3.35387700 | -1.40750400 | -1.47785500 |

| | | | |
|---|---|---|---|
| H | -1.68735900 | -0.82343600 | -1.67474700 |
| H | -2.81139500 | -1.96067000 | 0.99037700 |

**k-4**

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

Zero-point correction= 0.738399 (Hartree/Particle)
Thermal correction to Energy= 0.780692
Thermal correction to Enthalpy= 0.781636
Thermal correction to Gibbs Free Energy= 0.664029
Sum of electronic and zero-point Energies= -3215.057009
Sum of electronic and thermal Energies= -3215.014716
Sum of electronic and thermal Enthalpies= -3215.013772
Sum of electronic and thermal Free Energies= -3215.131379

| | | | |
|---|---|---|---|
| C | 1.10370600 | 0.62851000 | 0.44206100 |
| C | 2.89860100 | 1.87574500 | -0.22189300 |
| C | 3.03010200 | 1.65708000 | 1.11075700 |
| N | 1.93968500 | 0.87715900 | 1.49879100 |
| N | 1.72645800 | 1.23683700 | -0.61087200 |
| H | 3.78586100 | 1.98781100 | 1.81627300 |
| H | 3.51686200 | 2.42881200 | -0.92210900 |
| C | 1.75717600 | 0.36132200 | 2.83155300 |
| C | 0.69303500 | 0.85403900 | 3.62244000 |
| C | 2.66537400 | -0.61846600 | 3.29814000 |
| C | 0.52577800 | 0.29167700 | 4.89671400 |
| C | 2.44865700 | -1.14102600 | 4.58128200 |
| C | 1.38515000 | -0.69999100 | 5.36754900 |
| H | -0.28692600 | 0.63579600 | 5.53661500 |
| H | 3.11778900 | -1.90651700 | 4.97491700 |
| H | 1.23144200 | -1.12566000 | 6.36253900 |
| C | 1.13797700 | 1.34429300 | -1.91741200 |
| C | 0.53351700 | 2.56518500 | -2.27826600 |
| C | 1.16416900 | 0.22162000 | -2.77425400 |
| C | 0.00647300 | 2.66903100 | -3.57429500 |
| C | 0.61127200 | 0.37529400 | -4.05244200 |
| C | 0.05161000 | 1.59046700 | -4.45453900 |
| H | -0.46020600 | 3.60429900 | -3.89101400 |
| H | 0.61117500 | -0.46349900 | -4.74899000 |
| H | -0.36836300 | 1.68835800 | -5.45887700 |
| C | -2.89696100 | -0.85827400 | 1.52674400 |
| C | -2.68288800 | 0.19992900 | 0.44317000 |
| H | -0.96652200 | 1.54988400 | -0.01745600 |
| Ni | -0.78089800 | 0.18950600 | 0.37723300 |
| C | 1.76929300 | -1.10121300 | -2.31111200 |
| C | 3.30800500 | -1.05478100 | -2.33295800 |
| C | 1.26147400 | -2.31577200 | -3.09574000 |
| H | 1.44705800 | -1.24134100 | -1.26708200 |
| H | 3.70325600 | -0.23554800 | -1.71575100 |
| H | 3.72741700 | -1.99731700 | -1.94572300 |
| H | 3.67575400 | -0.91363200 | -3.36276700 |
| H | 0.16139900 | -2.36352500 | -3.10168200 |
| H | 1.60874100 | -2.30749900 | -4.14157300 |
| H | 1.64302800 | -3.24155500 | -2.63754200 |
| C | 0.42031700 | 3.73804200 | -1.30956100 |
| C | -1.03131900 | 4.22358600 | -1.15829200 |
| C | 1.35468700 | 4.88892300 | -1.71980800 |
| H | 0.73606600 | 3.38798500 | -0.31668200 |
| H | -1.68819200 | 3.40259700 | -0.83335300 |
| H | -1.08239600 | 5.02169400 | -0.39965300 |
| H | -1.42755200 | 4.63687100 | -2.09966800 |
| H | 2.40351300 | 4.55739200 | -1.77695700 |
| H | 1.07710300 | 5.29079900 | -2.70820500 |
| H | 1.29722000 | 5.71421300 | -0.99162900 |
| C | 3.83318800 | -1.10817400 | 2.43850100 |
| C | 3.37183600 | -2.11318900 | 1.37083800 |
| C | 4.99876700 | -1.68748500 | 3.25046400 |
| H | 4.23486400 | -0.23780500 | 1.90103900 |
| H | 2.51767600 | -1.73605600 | 0.79279100 |
| H | 4.19291800 | -2.33542900 | 0.67055300 |
| H | 3.06163600 | -3.05564200 | 1.84481700 |
| H | 5.33385300 | -0.99494100 | 4.03844500 |
| H | 4.73284400 | -2.64425200 | 3.72814400 |
| H | 5.85286600 | -1.88640000 | 2.58422000 |
| C | -0.22135000 | 1.97030900 | 3.12508500 |
| C | 0.50182700 | 3.32909200 | 3.11443200 |
| C | -1.55120300 | 2.07648200 | 3.87750400 |
| H | -0.48300900 | 1.73087000 | 2.08205900 |
| H | 1.41715500 | 3.30475400 | 2.50557100 |
| H | -0.15747700 | 4.10559600 | 2.69382400 |
| H | 0.78073500 | 3.63418900 | 4.13703100 |
| H | -2.05622000 | 1.10148400 | 3.95012400 |
| H | -1.42529100 | 2.47193400 | 4.89913100 |
| H | -2.22607700 | 2.75498000 | 3.33418300 |
| C | -1.69041600 | -1.78574100 | 1.44272800 |
| C | -1.27243200 | -2.29467200 | 0.19267900 |
| C | -0.99749700 | -2.19869100 | 2.60049300 |
| C | -0.22665400 | -3.23053300 | 0.12069000 |
| H | -1.82588200 | -2.03526400 | -0.71214900 |
| C | 0.04000600 | -3.12350800 | 2.52180900 |
| H | -1.28409800 | -1.78378200 | 3.56950400 |
| C | 0.41426400 | -3.65784000 | 1.27984000 |
| H | 0.06510100 | -3.63518800 | -0.84986400 |
| H | 0.56599400 | -3.42459500 | 3.43052400 |
| H | 1.21534000 | -4.39745900 | 1.22002900 |
| F | -3.38277300 | 1.34652900 | 0.80060100 |
| F | -3.31079000 | -0.21983700 | -0.74056100 |
| C | -4.24536100 | -1.58649000 | 1.47178200 |
| H | -4.34532400 | -2.14552900 | 0.53003900 |
| H | -4.34657900 | -2.29244000 | 2.31125700 |
| H | -5.06784400 | -0.85624600 | 1.52496200 |
| H | -2.82637200 | -0.30745900 | 2.47629000 |

**TS-k-p-4**

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

Zero-point correction= 0.736523 (Hartree/Particle)
Thermal correction to Energy= 0.778626
Thermal correction to Enthalpy= 0.779570
Thermal correction to Gibbs Free Energy= 0.662344
Sum of electronic and zero-point Energies= -3215.043616
Sum of electronic and thermal Energies= -3215.001513
Sum of electronic and thermal Enthalpies= -3215.000569
Sum of electronic and thermal Free Energies= -3215.117795

| | | | |
|---|---|---|---|
| C | 1.18631900 | 0.57835700 | 0.49088400 |
| C | 2.92962400 | 1.88383800 | -0.22346200 |
| C | 3.08471800 | 1.70147600 | 1.11222800 |
| N | 2.02447700 | 0.89582400 | 1.53226900 |
| N | 1.77720600 | 1.19106800 | -0.58487800 |
| H | 3.84150700 | 2.06720900 | 1.79971400 |
| H | 3.52002200 | 2.44313500 | -0.94273700 |
| C | 1.84624200 | 0.42622000 | 2.87767200 |
| C | 0.79233000 | 0.95604300 | 3.65655400 |
| C | 2.73087600 | -0.56371700 | 3.36161200 |
| C | 0.63457400 | 0.44945400 | 4.95514200 |
| C | 2.53019400 | -1.02967200 | 4.66890700 |
| C | 1.49123400 | -0.53154100 | 5.45548600 |
| H | -0.16824000 | 0.82660900 | 5.58956400 |
| H | 3.18772300 | -1.79710500 | 5.07900700 |
| H | 1.34853200 | -0.91092100 | 6.47071900 |
| C | 1.13353400 | 1.28036500 | -1.86382000 |
| C | 0.42783900 | 2.46165800 | -2.16974400 |
| C | 1.19020900 | 0.17591500 | -2.74238300 |
| C | -0.16210300 | 2.55534800 | -3.43922800 |
| C | 0.57436700 | 0.31650700 | -3.99310700 |
| C | -0.08027000 | 1.49984400 | -4.34518200 |
| H | -0.70561100 | 3.46189500 | -3.71468000 |
| H | 0.59641800 | -0.50855300 | -4.70583900 |
| H | -0.54793700 | 1.58878700 | -5.32915200 |
| C | -2.85026100 | -0.74142500 | 1.37368200 |
| C | -2.53923200 | 0.35026500 | 0.34670100 |
| H | -1.32250400 | 1.09845600 | -0.00377900 |
| Ni | -0.59289900 | -0.06537600 | 0.45312100 |

| | | | |
|---|---|---|---|
| C | 1.87230700 | -1.12032800 | -2.31338400 |
| C | 3.40617300 | -1.00568800 | -2.36985200 |
| C | 1.39915900 | -2.34893900 | -3.09783600 |
| H | 1.58067900 | -1.28266500 | -1.26318900 |
| H | 3.77854300 | -0.17368300 | -1.75565300 |
| H | 3.87462700 | -1.93167400 | -1.99825600 |
| H | 3.74571200 | -0.84327300 | -3.40637800 |
| H | 0.30154800 | -2.43479700 | -3.09194300 |
| H | 1.73364300 | -2.32366100 | -4.14788400 |
| H | 1.81520200 | -3.26282500 | -2.64569500 |
| C | 0.28097200 | 3.59942000 | -1.16412200 |
| C | -1.18793400 | 3.99748700 | -0.94450600 |
| C | 1.13332600 | 4.81274200 | -1.57265600 |
| H | 0.65303600 | 3.24106500 | -0.19405300 |
| H | -1.78876600 | 3.14100500 | -0.60487900 |
| H | -1.25153900 | 4.77988800 | -0.17048400 |
| H | -1.64771000 | 4.40202700 | -1.86047400 |
| H | 2.19560800 | 4.54139100 | -1.67669600 |
| H | 0.79644900 | 5.22489400 | -2.53822600 |
| H | 1.05794200 | 5.61293800 | -0.81847600 |
| C | 3.82694000 | -1.14273500 | 2.46786100 |
| C | 3.24267400 | -2.17977900 | 1.49228000 |
| C | 5.01308800 | -1.73211800 | 3.24042600 |
| H | 4.22714700 | -0.31932300 | 1.85825000 |
| H | 2.35622700 | -1.79542800 | 0.96921800 |
| H | 3.99393400 | -2.47214000 | 0.74059700 |
| H | 2.93385500 | -3.08409700 | 2.03808800 |
| H | 5.42728100 | -1.01358800 | 3.96528000 |
| H | 4.73325900 | -2.64594800 | 3.78915200 |
| H | 5.81480700 | -2.01047100 | 2.53837500 |
| C | -0.12795100 | 2.04319200 | 3.10712700 |
| C | 0.56851900 | 3.41550100 | 3.08416400 |
| C | -1.48098000 | 2.13572500 | 3.82008500 |
| H | -0.34951000 | 1.76841100 | 2.06368300 |
| H | 1.50213800 | 3.39150900 | 2.50357500 |
| H | -0.09159500 | 4.16955800 | 2.62522200 |
| H | 0.81104200 | 3.75002200 | 4.10677400 |
| H | -1.95949000 | 1.14848800 | 3.91026600 |
| H | -1.39275000 | 2.56318800 | 4.83259300 |
| H | -2.15969400 | 2.77962700 | 3.24054900 |
| C | -1.69942400 | -1.73665600 | 1.28007000 |
| C | -1.33854400 | -2.31055200 | 0.03471600 |
| C | -0.99536500 | -2.15272300 | 2.43492600 |
| C | -0.35217700 | -3.31077900 | -0.02559300 |
| H | -1.89768200 | -2.05138400 | -0.86677600 |
| C | -0.02513300 | -3.15070700 | 2.36449500 |
| H | -1.22703600 | -1.68575200 | 3.39524600 |
| C | 0.28568800 | -3.74745100 | 1.13444100 |
| H | -0.10090400 | -3.75600400 | -0.99026500 |
| H | 0.50326700 | -3.45324100 | 3.27166100 |
| H | 1.04545700 | -4.53037900 | 1.08036100 |
| F | -3.19113700 | 1.51590000 | 0.75661500 |
| F | -3.11425200 | 0.04206000 | -0.87573200 |
| C | -4.24768200 | -1.35809700 | 1.23437200 |
| H | -4.35670800 | -1.85891900 | 0.26145300 |
| H | -4.41883300 | -2.09976900 | 2.03019600 |
| H | -5.01998600 | -0.57703600 | 1.30853500 |
| H | -2.77816000 | -0.24087800 | 2.34991900 |

**PhBr**

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

Zero-point correction= 0.090496 (Hartree/Particle)
Thermal correction to Energy= 0.096186
Thermal correction to Enthalpy= 0.097131
Thermal correction to Gibbs Free Energy= 0.059616
Sum of electronic and zero-point Energies= -2805.271157
Sum of electronic and thermal Energies= -2805.265466
Sum of electronic and thermal Enthalpies= -2805.264522
Sum of electronic and thermal Free Energies= -2805.302037

| | | | |
|---|---|---|---|
| C | -1.01477600 | -0.42340500 | 1.90747200 |
| C | -2.40564600 | -0.42823900 | 1.76363100 |
| C | -0.41579000 | -0.42071600 | 3.17096100 |
| C | -3.20628400 | -0.43038700 | 2.91066300 |
| H | -2.85603400 | -0.43025800 | 0.76984500 |
| C | -1.23055500 | -0.42294600 | 4.30801400 |
| H | 0.67126000 | -0.41694500 | 3.26455000 |
| C | -2.62357300 | -0.42776700 | 4.18222800 |
| H | -4.29383400 | -0.43415100 | 2.80402500 |
| H | -0.76768200 | -0.42087400 | 5.29790700 |
| H | -3.25433300 | -0.42946100 | 5.07408000 |
| Br | 0.08994600 | -0.42040800 | 0.34551800 |

**Alkoxide**

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

Zero-point correction= 0.145714 (Hartree/Particle)
Thermal correction to Energy= 0.153559
Thermal correction to Enthalpy= 0.154503
Thermal correction to Gibbs Free Energy= 0.113215
Sum of electronic and zero-point Energies= -385.121575
Sum of electronic and thermal Energies= -385.113730
Sum of electronic and thermal Enthalpies= -385.112785
Sum of electronic and thermal Free Energies= -385.154073

| | | | |
|---|---|---|---|
| C | -0.96777900 | 0.12605300 | 1.98169000 |
| H | -2.06426700 | 0.02908800 | 1.90674800 |
| H | -0.74156600 | 1.18712000 | 2.19134800 |
| H | -0.51571400 | -0.15237200 | 1.01019400 |
| C | 1.06566700 | -0.63408700 | 3.26008500 |
| C | 1.91859400 | -1.10264500 | 2.24712600 |
| C | 1.64525400 | -0.04766000 | 4.39252300 |
| C | 3.30837100 | -0.97897900 | 2.35625500 |
| H | 1.48479400 | -1.58118700 | 1.36128400 |
| C | 3.03352700 | 0.08331200 | 4.51139600 |
| H | 0.93658600 | 0.27857000 | 5.16032300 |
| C | 3.87423000 | -0.38098600 | 3.49180200 |
| H | 3.95677600 | -1.35223100 | 1.55611800 |
| H | 3.46783400 | 0.54509900 | 5.40521100 |
| H | 4.96095800 | -0.28572900 | 3.58158000 |
| C | -0.49318000 | -0.73345700 | 3.21001000 |
| H | -0.65164000 | -1.81894700 | 2.84832500 |
| O | -1.10399200 | -0.40509600 | 4.33049400 |

**Br-anion**

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

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= -0.016176
Sum of electronic and zero-point Energies= -2573.992096
Sum of electronic and thermal Energies= -2573.990680
Sum of electronic and thermal Enthalpies= -2573.989736
Sum of electronic and thermal Free Energies= -2574.008272

| | | | |
|---|---|---|---|
| Br | 3.04208300 | -0.50802100 | 2.55145300 |

**AlkSM**

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

Zero-point correction= 0.064652 (Hartree/Particle)
Thermal correction to Energy= 0.069936
Thermal correction to Enthalpy= 0.070880
Thermal correction to Gibbs Free Energy= 0.036182
Sum of electronic and zero-point Energies= -316.085341
Sum of electronic and thermal Energies= -316.080057
Sum of electronic and thermal Enthalpies= -316.079113
Sum of electronic and thermal Free Energies= -316.113810

| | | | |
|---|---|---|---|
| C | 0.00150500 | -0.34773000 | 0.47090800 |
| H | -1.02371900 | -0.29846700 | 0.09681500 |
| C | 0.56024200 | 0.81543400 | 0.78666800 |
| C | 0.68717200 | -1.67528700 | 0.59922300 |
| H | 0.13158700 | -2.34338500 | 1.27898900 |
| H | 0.74422400 | -2.18719000 | -0.37641300 |
| H | 1.70992500 | -1.56658200 | 0.98788600 |

| | | | |
|---|---|---|---|
| F | -0.03076200 | 1.99465500 | 0.67947000 |
| F | 1.79071100 | 0.96733100 | 1.25541300 |

**W-4**
UB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.175199 (Hartree/Particle)
Thermal correction to Energy= 0.186023
Thermal correction to Enthalpy= 0.186967
Thermal correction to Gibbs Free Energy= 0.135824
Sum of electronic and zero-point Energies= -586.160499
Sum of electronic and thermal Energies= -586.149675
Sum of electronic and thermal Enthalpies= -586.148731
Sum of electronic and thermal Free Energies= -586.199875

| | | | |
|---|---|---|---|
| C | 1.37095100 | 0.45480500 | 2.00318600 |
| C | 1.97756100 | -0.35986700 | 1.03301900 |
| C | 1.77630200 | -0.12547200 | -0.33061700 |
| C | 0.95973400 | 0.93096800 | -0.74856600 |
| C | 0.34819700 | 1.74934600 | 0.20706500 |
| C | 0.55274800 | 1.51077000 | 1.56975000 |
| H | 2.61925800 | -1.18662900 | 1.35238700 |
| H | 2.26138000 | -0.76833500 | -1.07000500 |
| H | 0.80327800 | 1.11743300 | -1.81414200 |
| H | -0.28872200 | 2.57954700 | -0.10977600 |
| H | 0.07326000 | 2.15712400 | 2.31117700 |
| C | 1.54733500 | 0.16357900 | 3.47569700 |
| H | 2.54921800 | -0.25718400 | 3.66106500 |
| H | 1.48496600 | 1.10063400 | 4.05417000 |
| C | 0.48791800 | -0.82832600 | 4.00845500 |
| H | 0.55192200 | -1.76850000 | 3.43873700 |
| H | -0.51406700 | -0.40921100 | 3.80867500 |
| C | 0.63178400 | -1.10206000 | 5.47752400 |
| H | 0.49635500 | -0.28904500 | 6.19490600 |
| C | 0.95294300 | -2.28636600 | 5.98680500 |
| F | 1.10008900 | -2.54372000 | 7.27578100 |
| F | 1.16432700 | -3.38675000 | 5.27979000 |

**X-4-*cis***
UB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.182832 (Hartree/Particle)
Thermal correction to Energy= 0.192956
Thermal correction to Enthalpy= 0.193901
Thermal correction to Gibbs Free Energy= 0.144681
Sum of electronic and zero-point Energies= -486.986927
Sum of electronic and thermal Energies= -486.976803
Sum of electronic and thermal Enthalpies= -486.975858
Sum of electronic and thermal Free Energies= -487.025078

| | | | |
|---|---|---|---|
| C | 1.02135200 | 0.47035700 | 1.98749700 |
| C | 1.09224200 | -0.55480200 | 1.03193100 |
| C | 1.15243800 | -0.26070800 | -0.33652600 |
| C | 1.14292600 | 1.06474000 | -0.77586400 |
| C | 1.07159200 | 2.09831100 | 0.16639200 |
| C | 1.01072700 | 1.80072700 | 1.52874700 |
| H | 1.10288100 | -1.60015600 | 1.34552000 |
| H | 1.20659700 | -1.07750700 | -1.06132100 |
| H | 1.18898200 | 1.29348700 | -1.84365800 |
| H | 1.06103700 | 3.14075400 | -0.16321900 |
| H | 0.95295500 | 2.61525900 | 2.25743000 |
| C | 0.97435400 | 0.20934300 | 3.48203200 |
| H | 1.91915000 | 0.56419200 | 3.93244500 |
| H | 0.18728100 | 0.84674000 | 3.92275800 |
| C | 0.74128000 | -1.24598900 | 3.91279700 |
| H | 1.55890300 | -1.88781000 | 3.55114000 |
| H | -0.18643400 | -1.61512300 | 3.43886100 |
| C | 0.62377000 | -1.38690300 | 5.40342500 |
| H | -0.17700500 | -0.84433500 | 5.91636900 |
| C | 1.43559700 | -2.11157500 | 6.17119100 |
| F | 2.46205300 | -2.82086300 | 5.66139200 |
| H | 1.35896900 | -2.21215800 | 7.25776900 |

**X-4-*trans***
UB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.182531 (Hartree/Particle)
Thermal correction to Energy= 0.192738
Thermal correction to Enthalpy= 0.193682
Thermal correction to Gibbs Free Energy= 0.144916
Sum of electronic and zero-point Energies= -486.985953
Sum of electronic and thermal Energies= -486.975746
Sum of electronic and thermal Enthalpies= -486.974802
Sum of electronic and thermal Free Energies= -487.023568

| | | | |
|---|---|---|---|
| C | 0.98564000 | 0.46358400 | 1.99002300 |
| C | 1.01665400 | -0.55783300 | 1.02873700 |
| C | 1.10955400 | -0.25871900 | -0.33713600 |
| C | 1.17345200 | 1.06786800 | -0.76751200 |
| C | 1.14372300 | 2.09809400 | 0.18097300 |
| C | 1.05097500 | 1.79571700 | 1.54013400 |
| H | 0.96821900 | -1.60465000 | 1.33372300 |
| H | 1.13167000 | -1.07281000 | -1.06663100 |
| H | 1.24566300 | 1.30050700 | -1.83299000 |
| H | 1.19275100 | 3.14160900 | -0.14161600 |
| H | 1.02814800 | 2.60719700 | 2.27412000 |
| C | 0.89131300 | 0.20182000 | 3.48225600 |
| H | 1.77173900 | 0.65094900 | 3.97562600 |
| H | 0.02353200 | 0.75861600 | 3.87990800 |
| C | 0.78152900 | -1.26624200 | 3.91693600 |
| H | 1.66103400 | -1.83066500 | 3.56397600 |
| H | -0.09853800 | -1.72188800 | 3.42815100 |
| C | 0.64516400 | -1.40992100 | 5.40591800 |
| H | -0.22120800 | -0.95055300 | 5.89578800 |
| C | 1.52768500 | -2.04854800 | 6.17029900 |
| F | 1.37908500 | -2.15225000 | 7.50279100 |
| H | 2.43551100 | -2.54422200 | 5.80949200 |

**Y-4**
UB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.189822 (Hartree/Particle)
Thermal correction to Energy= 0.199269
Thermal correction to Enthalpy= 0.200213
Thermal correction to Gibbs Free Energy= 0.153803
Sum of electronic and zero-point Energies= -387.820070
Sum of electronic and thermal Energies= -387.810623
Sum of electronic and thermal Enthalpies= -387.809679
Sum of electronic and thermal Free Energies= -387.856090

| | | | |
|---|---|---|---|
| C | 0.99030600 | 0.46319400 | 1.98774100 |
| C | 1.02463900 | -0.55706800 | 1.02538000 |
| C | 1.11086800 | -0.25628800 | -0.34055100 |
| C | 1.16483200 | 1.07104100 | -0.77015000 |
| C | 1.13191600 | 2.10024100 | 0.17935000 |
| C | 1.04582400 | 1.79606400 | 1.53859000 |
| H | 0.98444100 | -1.60413400 | 1.33062800 |
| H | 1.13579500 | -1.06965700 | -1.07079800 |
| H | 1.23187800 | 1.30501200 | -1.83569600 |
| H | 1.17316600 | 3.14434600 | -0.14251400 |
| H | 1.02040800 | 2.60679900 | 2.27335700 |
| C | 0.90257100 | 0.19880000 | 3.48003800 |
| H | 1.78513700 | 0.64898800 | 3.96894200 |
| H | 0.03645500 | 0.75600000 | 3.88114100 |
| C | 0.79570900 | -1.26977800 | 3.91423100 |
| H | 1.67557200 | -1.83479100 | 3.56345900 |
| H | -0.08767800 | -1.72251500 | 3.42700700 |
| C | 0.65951000 | -1.41321900 | 5.40463600 |
| H | -0.21866100 | -0.92539900 | 5.84980500 |
| C | 1.51423700 | -2.05968900 | 6.20319100 |
| H | 1.35569800 | -2.12096900 | 7.28385600 |
| H | 2.40558400 | -2.55607300 | 5.80335000 |

**Z-4**
UB3LYP-D3/def2-SVP-CPCM(toluene)
Zero-point correction= 0.118764 (Hartree/Particle)
Thermal correction to Energy= 0.126776
Thermal correction to Enthalpy= 0.127720

Thermal correction to Gibbs Free Energy= 0.084915
Sum of electronic and zero-point Energies= -507.644655
Sum of electronic and thermal Energies= -507.636643
Sum of electronic and thermal Enthalpies= -507.635699
Sum of electronic and thermal Free Energies= -507.678504

| | | | |
|---|---|---|---|
| C | 0.95785500 | 0.36099300 | 1.85678400 |
| C | 1.06475500 | -0.57945000 | 0.80904000 |
| C | 1.19045100 | -0.15737500 | -0.51540700 |
| C | 1.21305600 | 1.20579900 | -0.83176100 |
| C | 1.10818800 | 2.14887600 | 0.19552700 |
| C | 0.98236700 | 1.73109500 | 1.52135900 |
| H | 1.04977000 | -1.64649300 | 1.02944100 |
| H | 1.27173000 | -0.90374600 | -1.30998000 |
| H | 1.31172300 | 1.52948300 | -1.87084700 |
| H | 1.12438000 | 3.21709400 | -0.03570100 |
| H | 0.90111000 | 2.47724300 | 2.31654900 |
| F | 0.83873500 | -2.36750100 | 3.18352300 |
| F | 0.64911200 | -1.42645500 | 5.12169700 |
| C | 0.77353100 | -1.21379900 | 3.82471100 |
| C | 0.82279600 | 0.00229000 | 3.27351700 |
| H | 0.75048600 | 0.81807400 | 3.99561300 |

## *A4.3.b Coordinates & Energies in the Study of Cobalt(I)-Catalyzed Allylic Substitution*

**Co-dppen-b3lyp-def-sing**
UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
Zero-point correction= 0.678995 (Hartree/Particle)
Thermal correction to Energy= 0.724208
Thermal correction to Enthalpy= 0.725153
Thermal correction to Gibbs Free Energy= 0.594971
Sum of electronic and zero-point Energies= -4563.802183
Sum of electronic and thermal Energies= -4563.756970
Sum of electronic and thermal Enthalpies= -4563.756026
Sum of electronic and thermal Free Energies= -4563.886207

| | | | |
|---|---|---|---|
| Co | -0.65322800 | 0.38001500 | 0.78465400 |
| Cl | 0.02627800 | 1.28706800 | 2.77597300 |
| P | 0.05232200 | -1.78687800 | 0.48464000 |
| C | 1.89475300 | -1.96563700 | 0.55750300 |
| C | 2.57815200 | -3.10605800 | 0.10159900 |
| C | 2.62936400 | -0.91231500 | 1.12604000 |
| C | 3.97052800 | -3.18051700 | 0.19364500 |
| H | 2.02599600 | -3.93713400 | -0.34241400 |
| C | 4.02261500 | -0.99123400 | 1.22514100 |
| H | 2.10482100 | -0.02647500 | 1.49365700 |
| C | 4.69677300 | -2.12159200 | 0.75276000 |
| H | 4.49118800 | -4.06871600 | -0.17346400 |
| H | 4.58212400 | -0.16215300 | 1.66592800 |
| H | 5.78608400 | -2.18024000 | 0.82074900 |
| C | -0.48466500 | -2.92617200 | 1.84272800 |
| C | -0.43160100 | -4.32685500 | 1.73878000 |
| C | -0.93580700 | -2.34754800 | 3.04000400 |
| C | -0.84074300 | -5.13133400 | 2.80550600 |
| H | -0.08302300 | -4.79674900 | 0.81659500 |
| C | -1.33816700 | -3.15385100 | 4.11024500 |
| H | -0.96904900 | -1.25892600 | 3.13253500 |
| C | -1.29810100 | -4.54665400 | 3.99319300 |
| H | -0.80319800 | -6.21949500 | 2.70931400 |
| H | -1.69083500 | -2.69017800 | 5.03510300 |
| H | -1.62057500 | -5.17759600 | 4.82541700 |
| C | -0.41403000 | -2.69245300 | -1.05176300 |
| C | -1.63109500 | -3.39374400 | -1.12632700 |
| C | 0.37464300 | -2.58786000 | -2.21174900 |
| C | -2.04073600 | -3.98401500 | -2.32480600 |
| H | -2.26951000 | -3.48261800 | -0.24667900 |
| C | -0.03729000 | -3.17934300 | -3.40887600 |
| H | 1.31804900 | -2.04148900 | -2.18774600 |
| C | -1.24546800 | -3.88133400 | -3.47080000 |
| H | -2.99193800 | -4.52029800 | -2.35857000 |
| H | 0.59094400 | -3.08143000 | -4.29730700 |
| H | -1.56669400 | -4.34372900 | -4.40760500 |
| P | -0.24591600 | 1.41121400 | -1.20146700 |
| C | -3.96634100 | 1.55877700 | 1.06982400 |
| C | -5.34661100 | 1.61932200 | 0.80883500 |
| C | -3.39785000 | 2.44723800 | 1.99583100 |
| C | -6.14441200 | 2.56311000 | 1.46047300 |
| H | -5.80163600 | 0.92371700 | 0.09845700 |
| C | -4.20065600 | 3.39050300 | 2.64775700 |
| H | -2.32997900 | 2.38110300 | 2.21886500 |
| C | -5.57178000 | 3.45193600 | 2.37986200 |
| H | -7.21674100 | 2.60507600 | 1.25262700 |
| H | -3.75205000 | 4.07642000 | 3.37116300 |
| H | -6.19781800 | 4.18844400 | 2.89021500 |
| C | -3.86730300 | -1.15944900 | 0.16958300 |
| C | -4.47567500 | -1.68581800 | -0.97966500 |
| C | -3.95686200 | -1.87472900 | 1.37791200 |
| C | -5.16153700 | -2.90459800 | -0.92034200 |
| H | -4.40299500 | -1.16544500 | -1.93628900 |
| C | -4.63447300 | -3.09326500 | 1.43453800 |
| H | -3.47431100 | -1.48519300 | 2.27728500 |
| C | -5.23813400 | -3.61332800 | 0.28184600 |
| H | -5.62563200 | -3.30689100 | -1.82422100 |
| H | -4.68128100 | -3.64373000 | 2.37746100 |
| H | -5.76288600 | -4.57100600 | 0.32181000 |
| C | 0.17742600 | 3.21056600 | -1.14306500 |
| C | 0.15275400 | 3.85854200 | 0.10180600 |
| C | 0.48419400 | 3.94620300 | -2.30134100 |
| C | 0.42396200 | 5.22917200 | 0.18529900 |
| H | -0.05788100 | 3.28035100 | 1.00515500 |
| C | 0.75280700 | 5.31447700 | -2.21417200 |
| H | 0.51954800 | 3.44844500 | -3.27425500 |
| C | 0.72090000 | 5.95860900 | -0.97029100 |
| H | 0.40734700 | 5.72657400 | 1.15861200 |
| H | 0.98991200 | 5.88077600 | -3.11857000 |
| H | 0.93321500 | 7.02880700 | -0.90385200 |
| C | 0.96827700 | 0.77257500 | -2.42579900 |
| C | 0.63720000 | 0.35644000 | -3.72397600 |
| C | 2.29354700 | 0.62188800 | -1.97779400 |
| C | 1.61418900 | -0.19910900 | -4.55831300 |
| H | -0.38734000 | 0.43868900 | -4.09084600 |
| C | 3.26525300 | 0.06115200 | -2.80759900 |
| H | 2.56288500 | 0.92640900 | -0.96377300 |
| C | 2.92628800 | -0.35380600 | -4.10239600 |
| H | 1.34168300 | -0.52507000 | -5.56514600 |
| H | 4.28635100 | -0.06326500 | -2.43858700 |
| H | 3.68367300 | -0.80022400 | -4.75139200 |
| P | -2.84967000 | 0.37190300 | 0.19473500 |
| C | -1.83982200 | 1.46853700 | -2.12286000 |
| H | -1.88136800 | 1.93017600 | -3.11645100 |
| C | -2.95452000 | 1.02158800 | -1.52535500 |
| H | -3.93010600 | 1.10796300 | -2.01798900 |

**Co-dppen-b3lyp-631-sing**
UB3LYP-D3/6-31g(d,p)-CPCM(acetonitrile)
Zero-point correction= 0.679075 (Hartree/Particle)
Thermal correction to Energy= 0.724627
Thermal correction to Enthalpy= 0.725571
Thermal correction to Gibbs Free Energy= 0.594789
Sum of electronic and zero-point Energies= -4565.457587
Sum of electronic and thermal Energies= -4565.412035
Sum of electronic and thermal Enthalpies= -4565.411091
Sum of electronic and thermal Free Energies= -4565.541872

| | | | |
|---|---|---|---|
| Co | -0.60561900 | 0.26153500 | 0.65283700 |
| Cl | 0.21591900 | 1.24123300 | 2.56051500 |
| P | 0.04535100 | -1.90745700 | 0.49224600 |

| | | | |
|---|---|---|---|
| C | 1.87257400 | -2.11086500 | 0.37608400 |
| C | 2.50688100 | -2.90677600 | -0.58562700 |
| C | 2.65707300 | -1.38849900 | 1.29205300 |
| C | 3.90157400 | -2.96950400 | -0.64102700 |
| H | 1.91751600 | -3.47112900 | -1.30008000 |
| C | 4.04822900 | -1.45504400 | 1.23624000 |
| H | 2.17351000 | -0.75810900 | 2.03358500 |
| C | 4.67505000 | -2.24360300 | 0.26552700 |
| H | 4.38156400 | -3.58417000 | -1.39678200 |
| H | 4.64405600 | -0.88840900 | 1.94572800 |
| H | 5.75886100 | -2.29014100 | 0.21776500 |
| C | -0.36713600 | -2.90548600 | 1.98418200 |
| C | 0.43044800 | -3.96980300 | 2.43256000 |
| C | -1.55647700 | -2.61129000 | 2.66737100 |
| C | 0.04255500 | -4.72249300 | 3.54204700 |
| H | 1.35409100 | -4.20963900 | 1.91529400 |
| C | -1.94872500 | -3.37009200 | 3.77063400 |
| H | -2.17928700 | -1.79082700 | 2.33042300 |
| C | -1.14836800 | -4.42648300 | 4.21117600 |
| H | 0.66862400 | -5.54218600 | 3.88201000 |
| H | -2.87664200 | -3.13408100 | 4.28300700 |
| H | -1.44879500 | -5.01566900 | 5.07246600 |
| C | -0.59565000 | -2.92694000 | -0.89803100 |
| C | -1.20742600 | -4.17492200 | -0.72578500 |
| C | -0.51316200 | -2.38248700 | -2.19029900 |
| C | -1.74029800 | -4.85626300 | -1.82278300 |
| H | -1.28571300 | -4.61171800 | 0.26362400 |
| C | -1.03979300 | -3.06483400 | -3.28488500 |
| H | -0.03160900 | -1.42328300 | -2.33674200 |
| C | -1.66403500 | -4.30299100 | -3.10186800 |
| H | -2.22239500 | -5.81783500 | -1.67379300 |
| H | -0.96793600 | -2.62765500 | -4.27634500 |
| H | -2.08559300 | -4.83216900 | -3.95110000 |
| P | -0.20825300 | 1.27889400 | -1.30378800 |
| C | -3.78771600 | 1.70186900 | 0.74204300 |
| C | -5.13041500 | 1.89100000 | 0.37429200 |
| C | -3.17146100 | 2.63079600 | 1.59136500 |
| C | -5.83975900 | 2.99460400 | 0.84572500 |
| H | -5.62246600 | 1.17102900 | -0.27316000 |
| C | -3.88433600 | 3.73581400 | 2.06324300 |
| H | -2.13413500 | 2.48530800 | 1.87762500 |
| C | -5.21632800 | 3.92009300 | 1.68960900 |
| H | -6.87680000 | 3.13455400 | 0.55552000 |
| H | -3.39748800 | 4.45010400 | 2.72046000 |
| H | -5.77025500 | 4.77973300 | 2.05492700 |
| C | -3.89663500 | -1.13245100 | 0.24783700 |
| C | -4.66231500 | -1.29799900 | 1.41448000 |
| C | -3.89988900 | -2.14688800 | -0.71991500 |
| C | -5.41451000 | -2.45597400 | 1.60770300 |
| H | -4.67096100 | -0.51942300 | 2.17164000 |
| C | -4.66067400 | -3.30141100 | -0.52669000 |
| H | -3.29680200 | -2.05033300 | -1.61719700 |
| C | -5.41611800 | -3.46119200 | 0.63618500 |
| H | -6.00021700 | -2.57248800 | 2.51473200 |
| H | -4.64771600 | -4.07995900 | -1.28272100 |
| H | -6.00154500 | -4.36325500 | 0.78650100 |
| C | -0.05105900 | 3.10976100 | -1.13675000 |
| C | -1.20047200 | 3.88606100 | -0.92041700 |
| C | 1.20796200 | 3.72647100 | -1.07994200 |
| C | -1.09227800 | 5.25184300 | -0.65777000 |
| H | -2.18134400 | 3.42530900 | -0.95321400 |
| C | 1.31230700 | 5.09361700 | -0.81777100 |
| H | 2.10851100 | 3.14319200 | -1.24438300 |
| C | 0.16395600 | 5.86048200 | -0.60535400 |
| H | -1.99149800 | 5.83787900 | -0.49172800 |
| H | 2.29278900 | 5.55934600 | -0.78055100 |
| H | 0.24782400 | 6.92349300 | -0.40055400 |
| C | 1.19064900 | 0.82444400 | -2.40268200 |
| C | 1.11860300 | 0.78838400 | -3.80440100 |
| C | 2.39679600 | 0.47538100 | -1.77490700 |
| C | 2.22816100 | 0.39917100 | -4.55639800 |
| H | 0.20217100 | 1.05345100 | -4.32002700 |
| C | 3.51029900 | 0.10335700 | -2.52871300 |
| H | 2.45959800 | 0.47449800 | -0.69194000 |
| C | 3.42550500 | 0.05839600 | -3.92139500 |
| H | 2.15704900 | 0.36457200 | -5.63941800 |
| H | 4.42931200 | -0.17366600 | -2.02301200 |
| H | 4.28548800 | -0.24564100 | -4.51048300 |
| P | -2.77725100 | 0.31052400 | 0.07748700 |
| C | -1.71992700 | 1.10287700 | -2.32992800 |
| H | -1.72778400 | 1.39461200 | -3.37725800 |
| C | -2.83488800 | 0.67005800 | -1.72734800 |
| H | -3.77618500 | 0.57601900 | -2.26604900 |

**Co-dppen-uwb-sing**

UωB97XD/def2-SVP-CPCM(acetonitrile)

Zero-point correction= 0.685912 (Hartree/Particle)
Thermal correction to Energy= 0.730433
Thermal correction to Enthalpy= 0.731378
Thermal correction to Gibbs Free Energy= 0.603327
Sum of electronic and zero-point Energies= -4563.043974
Sum of electronic and thermal Energies= -4562.999453
Sum of electronic and thermal Enthalpies= -4562.998508
Sum of electronic and thermal Free Energies= -4563.126559

| | | | |
|---|---|---|---|
| Co | -1.16957500 | 1.69285700 | 0.94108900 |
| P | -0.00519000 | -0.09439600 | 0.58132000 |
| P | 0.72843900 | 2.72889500 | 1.00691200 |
| C | 0.06014600 | -0.87922700 | -1.07421900 |
| C | 0.93539600 | -0.37826700 | -2.04720500 |
| C | -0.85688000 | -1.87575500 | -1.42991300 |
| C | 0.90664100 | -0.87910500 | -3.34794300 |
| H | 1.64548200 | 0.41308000 | -1.79184300 |
| C | -0.88537200 | -2.37443000 | -2.73181100 |
| H | -1.55457500 | -2.26570100 | -0.68529200 |
| C | -0.00344500 | -1.87903200 | -3.69291000 |
| H | 1.59840400 | -0.48429300 | -4.09530100 |
| H | -1.60219600 | -3.15481100 | -2.99686400 |
| H | -0.02619100 | -2.27172400 | -4.71181200 |
| C | -0.43089600 | -1.48771300 | 1.69672300 |
| C | -1.59050100 | -1.39599500 | 2.47485600 |
| C | 0.37947600 | -2.62631400 | 1.80381700 |
| C | -1.93125400 | -2.42185400 | 3.35650600 |
| H | -2.23374300 | -0.51905900 | 2.37693000 |
| C | 0.04021000 | -3.64849000 | 2.68774200 |
| H | 1.27916100 | -2.72330900 | 1.19040000 |
| C | -1.11466600 | -3.54625000 | 3.46716700 |
| H | -2.83913600 | -2.33664900 | 3.95820200 |
| H | 0.67891400 | -4.53069800 | 2.76815000 |
| H | -1.37800700 | -4.34891900 | 4.15955800 |
| C | 1.02424800 | 3.45612400 | -0.65686600 |
| C | 0.13254300 | 3.12509200 | -1.68458100 |
| C | 2.12876700 | 4.26960900 | -0.93984300 |
| C | 0.34082500 | 3.60164700 | -2.97862700 |
| H | -0.72430500 | 2.47872300 | -1.46876800 |
| C | 2.33649300 | 4.74334500 | -2.23376500 |
| H | 2.82903000 | 4.53947400 | -0.14518300 |
| C | 1.44305400 | 4.40999700 | -3.25410000 |
| H | -0.36047000 | 3.33818100 | -3.77313200 |
| H | 3.20045300 | 5.37613100 | -2.44780500 |
| H | 1.60798100 | 4.78322700 | -4.26721200 |
| C | 1.24185800 | 4.07015200 | 2.14032100 |
| C | 2.04495300 | 3.81405300 | 3.25652700 |
| C | 0.74951500 | 5.36641100 | 1.94057700 |
| C | 2.34936800 | 4.83443200 | 4.15606500 |
| H | 2.42714800 | 2.80831700 | 3.44363400 |
| C | 1.05004400 | 6.38464500 | 2.84192100 |
| H | 0.13106400 | 5.59073000 | 1.06907800 |
| C | 1.85161400 | 6.12024400 | 3.95273000 |
| H | 2.97220700 | 4.61770200 | 5.02625200 |
| H | 0.65736100 | 7.38967000 | 2.67308000 |

| | | | |
|---|---|---|---|
| H | 2.08718200 | 6.91751100 | 4.66100600 |
| Cl | -3.00890700 | 0.84115500 | -0.06187000 |
| P | -2.21515600 | 2.77497400 | 2.53552900 |
| C | -2.86634900 | 4.45917300 | 2.20865000 |
| C | -2.54702100 | 5.04370200 | 0.97834600 |
| C | -3.69837900 | 5.15667700 | 3.09641900 |
| C | -3.01286500 | 6.31779000 | 0.65236100 |
| H | -1.93250900 | 4.48463100 | 0.26725600 |
| C | -4.16250300 | 6.42982600 | 2.77448200 |
| H | -3.99710300 | 4.69754200 | 4.04215500 |
| C | -3.81450700 | 7.01490500 | 1.55447700 |
| H | -2.75257900 | 6.76167300 | -0.31079700 |
| H | -4.80472700 | 6.96701100 | 3.47566000 |
| H | -4.18127200 | 8.01257500 | 1.30335200 |
| C | -3.72162200 | 1.91379600 | 3.16208100 |
| C | -3.67901800 | 1.02330200 | 4.24060800 |
| C | -4.92782400 | 2.06904900 | 2.46400700 |
| C | -4.81642500 | 0.30545200 | 4.61569800 |
| H | -2.75396100 | 0.88058400 | 4.80228400 |
| C | -6.06442200 | 1.35967000 | 2.84339500 |
| H | -4.97919800 | 2.74889800 | 1.61109700 |
| C | -6.01204400 | 0.47184700 | 3.91967100 |
| H | -4.76375000 | -0.38356500 | 5.46171200 |
| H | -6.99694500 | 1.49730900 | 2.29146900 |
| H | -6.90282100 | -0.08696200 | 4.21492700 |
| C | -1.18792100 | 2.90134100 | 4.05821900 |
| C | -0.39537200 | 1.78315500 | 4.35775800 |
| C | -1.15513100 | 4.00106300 | 4.91980700 |
| C | 0.37530400 | 1.74554500 | 5.51670400 |
| H | -0.37790400 | 0.93992400 | 3.66202600 |
| C | -0.36714500 | 3.97120800 | 6.07090100 |
| H | -1.73185100 | 4.89909800 | 4.69447000 |
| C | 0.38838100 | 2.84147700 | 6.37945700 |
| H | 0.97856500 | 0.86230900 | 5.73747900 |
| H | -0.34226600 | 4.84284400 | 6.72845800 |
| H | 1.00014400 | 2.82122100 | 7.28400600 |
| C | 1.76565200 | 0.23046500 | 0.92808400 |
| C | 2.09693100 | 1.50981600 | 1.12890000 |
| H | 3.13071200 | 1.82776400 | 1.30277900 |
| H | 2.51622500 | -0.56707500 | 0.91554900 |

**Co-dppen-m06-sing**

UM06-L/def-2SVP-CPCM(acetonitrile)

Zero-point correction= 0.676747 (Hartree/Particle)

Thermal correction to Energy= 0.722207

Thermal correction to Enthalpy= 0.723152

Thermal correction to Gibbs Free Energy= 0.593625

Sum of electronic and zero-point Energies= -4563.345276

Sum of electronic and thermal Energies= -4563.299816

Sum of electronic and thermal Enthalpies= -4563.298872

Sum of electronic and thermal Free Energies= -4563.428398

| | | | |
|---|---|---|---|
| Co | -1.22262800 | 2.28939400 | 0.53726100 |
| P | -0.35513800 | 0.25548600 | 0.67701600 |
| P | 0.85426100 | 3.07648300 | 0.63322900 |
| C | -0.37345300 | -0.67939800 | -0.90662400 |
| C | -1.07958000 | -0.14570000 | -1.99183700 |
| C | 0.29851200 | -1.90172500 | -1.05662100 |
| C | -1.10850100 | -0.82116100 | -3.21301100 |
| H | -1.62119800 | 0.80005000 | -1.86863200 |
| C | 0.27253100 | -2.57095700 | -2.27820200 |
| H | 0.84098800 | -2.33747000 | -0.21182200 |
| C | -0.42982400 | -2.03051100 | -3.35824100 |
| H | -1.66657600 | -0.40097100 | -4.05299300 |
| H | 0.80046200 | -3.52099800 | -2.38881800 |
| H | -0.45062700 | -2.55859700 | -4.31436500 |
| C | -0.87911000 | -1.02669800 | 1.87229400 |
| C | -2.12424700 | -1.64588600 | 1.67659100 |
| C | -0.14082300 | -1.34044500 | 3.02152700 |
| C | -2.61814600 | -2.55433300 | 2.60793300 |
| H | -2.71392300 | -1.40958000 | 0.78478300 |
| C | -0.63989500 | -2.24801700 | 3.95749500 |
| H | 0.83540800 | -0.87761100 | 3.19433600 |
| C | -1.87844800 | -2.85532800 | 3.75438600 |
| H | -3.58980300 | -3.02581000 | 2.44177700 |
| H | -0.05202600 | -2.48349600 | 4.84798100 |
| H | -2.26815200 | -3.56470000 | 4.48807700 |
| C | 1.58642900 | 3.59496200 | -0.97364900 |
| C | 0.88376500 | 3.31000100 | -2.15131000 |
| C | 2.84474600 | 4.20998100 | -1.05666400 |
| C | 1.43169100 | 3.63060000 | -3.39364100 |
| H | -0.10945400 | 2.85490300 | -2.08539600 |
| C | 3.38802100 | 4.53211200 | -2.29875500 |
| H | 3.40342400 | 4.43958500 | -0.14394600 |
| C | 2.68345400 | 4.24082900 | -3.46908700 |
| H | 0.87384800 | 3.40803700 | -4.30633400 |
| H | 4.36823300 | 5.01137100 | -2.35464500 |
| H | 3.11152700 | 4.49443400 | -4.44167800 |
| C | 1.39606300 | 4.40227500 | 1.76187700 |
| C | 2.00050500 | 4.12623300 | 2.99563600 |
| C | 1.07293300 | 5.73277000 | 1.44741200 |
| C | 2.26321600 | 5.15453100 | 3.90158000 |
| H | 2.26809400 | 3.09872900 | 3.25690600 |
| C | 1.34969400 | 6.75963500 | 2.34580900 |
| H | 0.59114100 | 5.96457400 | 0.49158700 |
| C | 1.93798400 | 6.47235200 | 3.58022600 |
| H | 2.73088000 | 4.92221600 | 4.86167900 |
| H | 1.09589900 | 7.79017000 | 2.08605400 |
| H | 2.14580800 | 7.27705100 | 4.28897400 |
| Cl | -2.65282300 | 3.29078400 | -0.94342400 |
| P | -2.15280300 | 2.65292300 | 2.56406300 |
| C | -2.97069300 | 4.28999400 | 2.63586900 |
| C | -4.31667000 | 4.48058100 | 2.29897000 |
| C | -2.17560900 | 5.41486400 | 2.90943600 |
| C | -4.85759700 | 5.76594800 | 2.24962600 |
| H | -4.95275200 | 3.61973100 | 2.07441700 |
| C | -2.71738400 | 6.69684000 | 2.86040400 |
| H | -1.12057300 | 5.28511300 | 3.17190000 |
| C | -4.06219800 | 6.87702500 | 2.52927100 |
| H | -5.91114500 | 5.89799600 | 1.99180800 |
| H | -2.08495600 | 7.56013900 | 3.08306600 |
| H | -4.48860500 | 7.88192200 | 2.49019200 |
| C | -3.51212000 | 1.44671800 | 2.83100200 |
| C | -3.80174200 | 0.86785300 | 4.07391100 |
| C | -4.25569800 | 1.04888900 | 1.70719400 |
| C | -4.82211600 | -0.07647800 | 4.19224700 |
| H | -3.22659000 | 1.14899400 | 4.96027600 |
| C | -5.28627700 | 0.11957500 | 1.83284400 |
| H | -4.01478300 | 1.47079200 | 0.72431800 |
| C | -5.57055800 | -0.44768000 | 3.07578000 |
| H | -5.03214000 | -0.52459400 | 5.16652400 |
| H | -5.86158100 | -0.17355000 | 0.95128300 |
| H | -6.36988700 | -1.18623700 | 3.17224700 |
| C | -1.22466100 | 2.61002200 | 4.14097500 |
| C | -0.05277700 | 1.85030600 | 4.19219200 |
| C | -1.65161200 | 3.27227800 | 5.30267800 |
| C | 0.67332600 | 1.72742300 | 5.37606800 |
| H | 0.30209800 | 1.36851500 | 3.27815600 |
| C | -0.91788700 | 3.16720600 | 6.48283300 |
| H | -2.56595400 | 3.87245900 | 5.28627500 |
| C | 0.24234700 | 2.38981200 | 6.52418300 |
| H | 1.58658100 | 1.12673200 | 5.39368600 |
| H | -1.25774900 | 3.69013000 | 7.37975400 |
| H | 0.81208500 | 2.30685700 | 7.45249900 |
| C | 1.43798800 | 0.43143800 | 1.01239700 |
| C | 1.95899900 | 1.66743500 | 1.02950000 |
| H | 3.03227000 | 1.83572600 | 1.18938100 |
| H | 2.06827800 | -0.45442300 | 1.16318500 |

**Co-dppen-b3lyp-def-trip**

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

Zero-point correction= 0.679204 (Hartree/Particle)
Thermal correction to Energy= 0.724293
Thermal correction to Enthalpy= 0.725237
Thermal correction to Gibbs Free Energy= 0.595923
Sum of electronic and zero-point Energies= -4563.824688
Sum of electronic and thermal Energies= -4563.779600
Sum of electronic and thermal Enthalpies= -4563.778655
Sum of electronic and thermal Free Energies= -4563.907969

| | | | |
|---|---|---|---|
| Co | -0.58864700 | 0.39330300 | 0.77919800 |
| Cl | 0.22506800 | 1.34831200 | 2.70091500 |
| P | 0.13195400 | -1.78331700 | 0.44563700 |
| C | 1.97572800 | -1.93973500 | 0.39706500 |
| C | 2.64141400 | -3.07218400 | -0.10229000 |
| C | 2.73176200 | -0.87834300 | 0.92085500 |
| C | 4.03759100 | -3.13044300 | -0.09839800 |
| H | 2.07081000 | -3.90985400 | -0.50940600 |
| C | 4.12931900 | -0.94139500 | 0.93181600 |
| H | 2.22071000 | -0.00013600 | 1.32486100 |
| C | 4.78515300 | -2.06339800 | 0.41547900 |
| H | 4.54454700 | -4.01236500 | -0.49834700 |
| H | 4.70618800 | -0.10692200 | 1.33874600 |
| H | 5.87718500 | -2.10952300 | 0.41487000 |
| C | -0.29548000 | -2.92069500 | 1.84180000 |
| C | -0.28298200 | -4.32149000 | 1.73148400 |
| C | -0.61530000 | -2.33542400 | 3.07796500 |
| C | -0.60734500 | -5.12009700 | 2.83154200 |
| H | -0.03278800 | -4.79565600 | 0.77995500 |
| C | -0.93160900 | -3.13610800 | 4.18058700 |
| H | -0.61396300 | -1.24622300 | 3.17480300 |
| C | -0.93609000 | -4.52926900 | 4.05793200 |
| H | -0.60388100 | -6.20850400 | 2.73096300 |
| H | -1.18278700 | -2.66810700 | 5.13589400 |
| H | -1.19279200 | -5.15553900 | 4.91615500 |
| C | -0.43229700 | -2.68865000 | -1.05720600 |
| C | -1.65394800 | -3.38629000 | -1.05321600 |
| C | 0.27580800 | -2.57825800 | -2.26757000 |
| C | -2.14657800 | -3.96667600 | -2.22498600 |
| H | -2.23096400 | -3.47969700 | -0.13269900 |
| C | -0.21903700 | -3.16012300 | -3.43783600 |
| H | 1.21961600 | -2.03322500 | -2.30505000 |
| C | -1.43115900 | -3.85772100 | -3.42201800 |
| H | -3.09964100 | -4.50013300 | -2.19737700 |
| H | 0.34720600 | -3.05730700 | -4.36648100 |
| H | -1.81739800 | -4.31190400 | -4.33805500 |
| P | -0.34288900 | 1.39394700 | -1.27247300 |
| C | -3.90732500 | 1.54270300 | 1.22218500 |
| C | -5.30224200 | 1.58518000 | 1.05268500 |
| C | -3.28490500 | 2.47118400 | 2.07125400 |
| C | -6.06185900 | 2.55062600 | 1.71827200 |
| H | -5.79845800 | 0.85867800 | 0.40338500 |
| C | -4.04909400 | 3.43644600 | 2.73700400 |
| H | -2.20370500 | 2.41950300 | 2.22376500 |
| C | -5.43569600 | 3.47938000 | 2.56000700 |
| H | -7.14608300 | 2.57842800 | 1.58211100 |
| H | -3.55837400 | 4.15387900 | 3.39994700 |
| H | -6.03186900 | 4.23282900 | 3.08126400 |
| C | -3.82863600 | -1.21608400 | 0.42944600 |
| C | -4.54799900 | -1.77229500 | -0.63901900 |
| C | -3.77145200 | -1.91318400 | 1.65020200 |
| C | -5.19576500 | -3.00398300 | -0.48865600 |
| H | -4.59208600 | -1.26636800 | -1.60496200 |
| C | -4.41336600 | -3.14350100 | 1.79785700 |
| H | -3.19860200 | -1.50115500 | 2.48422900 |
| C | -5.12594100 | -3.69457100 | 0.72470700 |
| H | -5.74607300 | -3.43042400 | -1.33103700 |
| H | -4.34441500 | -3.67987500 | 2.74749000 |
| H | -5.62120800 | -4.66247700 | 0.83428600 |
| C | 0.00291400 | 3.21100300 | -1.27868700 |
| C | 0.16371500 | 3.94066800 | -2.46965300 |
| C | 0.07260600 | 3.87686300 | -0.04491500 |
| C | 0.38124000 | 5.32000900 | -2.42509200 |
| H | 0.12553500 | 3.42975400 | -3.43570500 |
| C | 0.29213700 | 5.25872500 | -0.00409700 |
| H | -0.02479900 | 3.30535900 | 0.88192100 |
| C | 0.44336300 | 5.98164100 | -1.19151100 |
| H | 0.50489000 | 5.88147000 | -3.35477900 |
| H | 0.34923100 | 5.77010100 | 0.96041100 |
| H | 0.61519200 | 7.06062300 | -1.15848600 |
| C | 0.82183900 | 0.77567400 | -2.55411500 |
| C | 0.44336800 | 0.35882500 | -3.83908300 |
| C | 2.16644100 | 0.64227400 | -2.16185900 |
| C | 1.39253600 | -0.18243600 | -4.71395000 |
| H | -0.59601600 | 0.42879400 | -4.16428700 |
| C | 3.11106000 | 0.09710800 | -3.03243200 |
| H | 2.47203200 | 0.94612900 | -1.15797800 |
| C | 2.72440500 | -0.32040800 | -4.31281700 |
| H | 1.08333800 | -0.51014100 | -5.70958500 |
| H | 4.14786500 | -0.01477800 | -2.70559000 |
| H | 3.46008200 | -0.75593200 | -4.99342900 |
| P | -2.83716100 | 0.32885800 | 0.32727200 |
| C | -1.99393400 | 1.36357400 | -2.08893600 |
| H | -2.11506900 | 1.78509000 | -3.09372500 |
| C | -3.05663200 | 0.90888500 | -1.40739000 |
| H | -4.06079900 | 0.95273700 | -1.84529100 |

**Co-dppen-b3lyp-631-trip**

UB3LYP-D3/6-31g(d,p)-CPCM(acetonitrile)
Zero-point correction= 0.679043 (Hartree/Particle)
Thermal correction to Energy= 0.724696
Thermal correction to Enthalpy= 0.725640
Thermal correction to Gibbs Free Energy= 0.592992
Sum of electronic and zero-point Energies= -4565.480325
Sum of electronic and thermal Energies= -4565.434672
Sum of electronic and thermal Enthalpies= -4565.433728
Sum of electronic and thermal Free Energies= -4565.566376

| | | | |
|---|---|---|---|
| Co | -0.54101700 | 0.21358700 | 0.67530100 |
| Cl | 0.39118300 | 1.00560300 | 2.62513700 |
| P | 0.04614400 | -1.98280800 | 0.37956200 |
| C | 1.85764400 | -2.21787900 | 0.14678600 |
| C | 2.40032400 | -3.09469700 | -0.80181000 |
| C | 2.72535600 | -1.44169500 | 0.93456800 |
| C | 3.78367000 | -3.18448500 | -0.96992200 |
| H | 1.74580100 | -3.69989100 | -1.41983900 |
| C | 4.10697500 | -1.54087000 | 0.77158800 |
| H | 2.31403800 | -0.74720000 | 1.66197400 |
| C | 4.63976700 | -2.40888300 | -0.18608400 |
| H | 4.19128400 | -3.86026900 | -1.71592400 |
| H | 4.76656600 | -0.93423100 | 1.38498000 |
| H | 5.71504000 | -2.47851900 | -0.32039700 |
| C | -0.34645400 | -2.97208800 | 1.88339000 |
| C | 0.62933100 | -3.51073800 | 2.73264900 |
| C | -1.70233100 | -3.12062900 | 2.22436000 |
| C | 0.25462800 | -4.18207100 | 3.90004900 |
| H | 1.68143800 | -3.40948200 | 2.48956200 |
| C | -2.07343800 | -3.79893000 | 3.38355900 |
| H | -2.46847700 | -2.71746000 | 1.57355300 |
| C | -1.09400300 | -4.32894600 | 4.22882700 |
| H | 1.02114400 | -4.59341100 | 4.55031400 |
| H | -3.12686400 | -3.90786700 | 3.62436600 |
| H | -1.38040300 | -4.85249300 | 5.13601500 |
| C | -0.68917000 | -2.94710800 | -1.00359900 |
| C | -1.23445200 | -4.23009300 | -0.86826500 |
| C | -0.71228700 | -2.32926400 | -2.26429700 |
| C | -1.81772600 | -4.86781100 | -1.96591900 |
| H | -1.22246000 | -4.72956900 | 0.09401000 |
| C | -1.28416900 | -2.96943400 | -3.36163000 |
| H | -0.27901200 | -1.34439200 | -2.38479700 |
| C | -1.84978800 | -4.23949300 | -3.21209000 |
| H | -2.24932000 | -5.85679400 | -1.84396400 |
| H | -1.29345600 | -2.47408400 | -4.32797200 |

| | | | |
|---|---|---|---|
| H | -2.30839200 | -4.73638700 | -4.06161200 |
| P | -0.20542600 | 1.33624100 | -1.26218300 |
| C | -3.69653800 | 1.73774700 | 1.06027400 |
| C | -5.03847700 | 2.01875100 | 0.75319400 |
| C | -3.02181400 | 2.54333900 | 1.98787800 |
| C | -5.68933100 | 3.09142500 | 1.36060700 |
| H | -5.57602400 | 1.39332000 | 0.04635100 |
| C | -3.67586000 | 3.61858500 | 2.59488800 |
| H | -1.98566400 | 2.32600800 | 2.23016100 |
| C | -5.00738000 | 3.89476100 | 2.28076400 |
| H | -6.72626200 | 3.30251800 | 1.11677300 |
| H | -3.14433400 | 4.23691900 | 3.31204300 |
| H | -5.51558600 | 4.73092900 | 2.75171700 |
| C | -3.92616300 | -1.03314400 | 0.30602900 |
| C | -3.95031100 | -1.97841100 | -0.73028000 |
| C | -4.67750000 | -1.27409100 | 1.46856600 |
| C | -4.70987300 | -3.14272000 | -0.60501800 |
| H | -3.35957500 | -1.82198100 | -1.62681400 |
| C | -5.43151500 | -2.44113700 | 1.59229400 |
| H | -4.66819800 | -0.55231800 | 2.27953500 |
| C | -5.44728800 | -3.38010700 | 0.55659100 |
| H | -4.70881600 | -3.86847400 | -1.41189600 |
| H | -6.00537500 | -2.61773500 | 2.49716500 |
| H | -6.03028200 | -4.29067200 | 0.65594500 |
| C | 0.09315700 | 3.14320900 | -1.03127700 |
| C | -0.95527000 | 3.93167600 | -0.52898200 |
| C | 1.35236900 | 3.72865100 | -1.22466000 |
| C | -0.74853800 | 5.27750500 | -0.22908800 |
| H | -1.93528200 | 3.49448900 | -0.37174300 |
| C | 1.55596800 | 5.07734000 | -0.92327700 |
| H | 2.17563000 | 3.13801600 | -1.61314000 |
| C | 0.50880800 | 5.85526000 | -0.42495400 |
| H | -1.57037100 | 5.87253600 | 0.15846900 |
| H | 2.53542100 | 5.51953900 | -1.08067500 |
| H | 0.67066400 | 6.90321400 | -0.19135600 |
| C | 1.06290900 | 0.82314600 | -2.48465400 |
| C | 0.84176300 | 0.72252200 | -3.86700100 |
| C | 2.31580400 | 0.45442700 | -1.96848000 |
| C | 1.85148100 | 0.25173600 | -4.70884500 |
| H | -0.11657200 | 0.99260200 | -4.29653800 |
| C | 3.32836000 | -0.00076100 | -2.81214800 |
| H | 2.49249800 | 0.50253200 | -0.89929000 |
| C | 3.09519800 | -0.10905700 | -4.18494300 |
| H | 1.66443500 | 0.16719200 | -5.77516000 |
| H | 4.28409700 | -0.29382000 | -2.39027800 |
| H | 3.87567700 | -0.47892700 | -4.84299600 |
| P | -2.76463200 | 0.38423000 | 0.22559000 |
| C | -1.79792000 | 1.33363900 | -2.17551500 |
| H | -1.85847700 | 1.72256700 | -3.18946200 |
| C | -2.89650300 | 0.91478000 | -1.53428200 |
| H | -3.87349100 | 0.92901900 | -2.01459300 |

**Co-dppen-uwb-trip**

UωB97XD/def2-SVP-CPCM(acetonitrile)

Zero-point correction= 0.685842 (Hartree/Particle)

Thermal correction to Energy= 0.730728

Thermal correction to Enthalpy= 0.731672

Thermal correction to Gibbs Free Energy= 0.601918

Sum of electronic and zero-point Energies= -4563.091285

Sum of electronic and thermal Energies= -4563.046400

Sum of electronic and thermal Enthalpies= -4563.045456

Sum of electronic and thermal Free Energies= -4563.175210

| | | | |
|---|---|---|---|
| Co | -1.36054100 | 2.22088000 | 0.43966900 |
| P | -0.43385000 | 0.13430800 | 0.59894400 |
| P | 0.77444000 | 3.02542100 | 0.52962500 |
| C | -0.36696600 | -0.86146500 | -0.94646200 |
| C | -0.89366700 | -0.30931900 | -2.11901900 |
| C | 0.22161800 | -2.13330300 | -0.98625400 |
| C | -0.82357300 | -1.01768100 | -3.32034200 |
| H | -1.38007900 | 0.66979900 | -2.08506600 |
| C | 0.29174100 | -2.83692500 | -2.18608200 |
| H | 0.62282300 | -2.58103200 | -0.07271900 |
| C | -0.22888600 | -2.27774000 | -3.35600400 |
| H | -1.24034400 | -0.58213200 | -4.23118900 |
| H | 0.75251900 | -3.82685900 | -2.20990100 |
| H | -0.17455100 | -2.83115800 | -4.29616800 |
| C | -0.96151400 | -1.11745700 | 1.82793300 |
| C | -2.29009300 | -1.55780800 | 1.74593900 |
| C | -0.15133100 | -1.59287400 | 2.86472900 |
| C | -2.79743900 | -2.45674800 | 2.67849800 |
| H | -2.93881000 | -1.18335000 | 0.94944300 |
| C | -0.66367800 | -2.48842500 | 3.80591400 |
| H | 0.88555800 | -1.26230700 | 2.95819900 |
| C | -1.98473000 | -2.92183300 | 3.71453400 |
| H | -3.83647300 | -2.78359900 | 2.60528100 |
| H | -0.02224600 | -2.84755000 | 4.61354200 |
| H | -2.38449700 | -3.62005600 | 4.45301700 |
| C | 1.51751300 | 3.62490500 | -1.04122400 |
| C | 0.74017600 | 3.56637000 | -2.20293800 |
| C | 2.83348700 | 4.10266600 | -1.11469000 |
| C | 1.27512300 | 3.97376400 | -3.42665500 |
| H | -0.29452600 | 3.21678500 | -2.14244900 |
| C | 3.36532700 | 4.50761200 | -2.33645600 |
| H | 3.44518900 | 4.16515500 | -0.21043700 |
| C | 2.58645300 | 4.44115600 | -3.49479300 |
| H | 0.66115900 | 3.92885200 | -4.32885900 |
| H | 4.39137100 | 4.87848600 | -2.38698300 |
| H | 3.00454400 | 4.76061500 | -4.45202900 |
| C | 1.30821000 | 4.30380500 | 1.72570300 |
| C | 2.04250000 | 4.00395800 | 2.87686500 |
| C | 0.88396300 | 5.62325300 | 1.51262400 |
| C | 2.35273200 | 5.00646300 | 3.79609700 |
| H | 2.36537200 | 2.98017400 | 3.07620700 |
| C | 1.19072800 | 6.62259800 | 2.43233200 |
| H | 0.31277800 | 5.87632800 | 0.61473300 |
| C | 1.92813900 | 6.31535000 | 3.57774400 |
| H | 2.92222400 | 4.75615000 | 4.69336800 |
| H | 0.85312200 | 7.64588100 | 2.25404800 |
| H | 2.16792200 | 7.09775400 | 4.30101900 |
| Cl | -2.87372400 | 2.75251200 | -1.18581800 |
| P | -2.17602700 | 2.69653100 | 2.53600500 |
| C | -3.08288300 | 4.29197800 | 2.58025300 |
| C | -2.74270800 | 5.26908500 | 1.63829400 |
| C | -4.08161300 | 4.57024900 | 3.52285300 |
| C | -3.37035400 | 6.51467400 | 1.65173100 |
| H | -1.99098400 | 5.04469200 | 0.87868800 |
| C | -4.71337700 | 5.81221300 | 3.53319900 |
| H | -4.36576000 | 3.81184300 | 4.25690300 |
| C | -4.35470400 | 6.78796900 | 2.60062800 |
| H | -3.09361100 | 7.27015700 | 0.91324600 |
| H | -5.48973800 | 6.02026100 | 4.27264000 |
| H | -4.85029000 | 7.76128600 | 2.61057300 |
| C | -3.46169700 | 1.49886200 | 3.07137300 |
| C | -3.54986900 | 0.95957000 | 4.35821800 |
| C | -4.39418500 | 1.10671100 | 2.09969900 |
| C | -4.55552700 | 0.04280100 | 4.66927700 |
| H | -2.83004800 | 1.25046600 | 5.12632500 |
| C | -5.40562500 | 0.20388900 | 2.41641300 |
| H | -4.31492100 | 1.50355100 | 1.08260900 |
| C | -5.48624500 | -0.33302500 | 3.70256100 |
| H | -4.61087200 | -0.37753400 | 5.67586900 |
| H | -6.12686200 | -0.09296800 | 1.65176900 |
| H | -6.27238800 | -1.05028000 | 3.94853500 |
| C | -1.06213400 | 2.81292600 | 3.98953700 |
| C | -0.20805200 | 1.72946600 | 4.23356000 |
| C | -1.00064200 | 3.92367200 | 4.83677600 |
| C | 0.66916800 | 1.74059300 | 5.31380700 |
| H | -0.23787500 | 0.85987000 | 3.57636300 |
| C | -0.11195200 | 3.94150600 | 5.91254800 |
| H | -1.64364800 | 4.78770000 | 4.66065700 |

| | | | |
|---|---|---|---|
| C | 0.71957900 | 2.85082000 | 6.15805400 |
| H | 1.31970200 | 0.88134900 | 5.49149300 |
| H | -0.06978500 | 4.81909200 | 6.56122100 |
| H | 1.41223300 | 2.86789200 | 7.00229300 |
| C | 1.35420000 | 0.36734000 | 0.93085900 |
| C | 1.86807500 | 1.60241900 | 0.90486800 |
| H | 2.94440800 | 1.76199700 | 1.04020900 |
| H | 2.00579200 | -0.50157300 | 1.07976400 |

**Co-dppen-m06-trip**

UM06-L/def-2SVP-CPCM(acetonitrile)

Zero-point correction= 0.676884 (Hartree/Particle)
Thermal correction to Energy= 0.722378
Thermal correction to Enthalpy= 0.723322
Thermal correction to Gibbs Free Energy= 0.592934
Sum of electronic and zero-point Energies= -4563.372825
Sum of electronic and thermal Energies= -4563.327332
Sum of electronic and thermal Enthalpies= -4563.326388
Sum of electronic and thermal Free Energies= -4563.456776

| | | | |
|---|---|---|---|
| Co | -1.26425100 | 2.32992100 | 0.52568800 |
| P | -0.38482300 | 0.24572500 | 0.63373300 |
| P | 0.86265600 | 3.09144600 | 0.63064600 |
| C | -0.33425300 | -0.69715000 | -0.94438100 |
| C | -0.95800300 | -0.14725900 | -2.07103000 |
| C | 0.31912800 | -1.93401100 | -1.05383900 |
| C | -0.92234100 | -0.82072800 | -3.29325600 |
| H | -1.48880000 | 0.80733900 | -1.97892500 |
| C | 0.35608700 | -2.60202900 | -2.27563900 |
| H | 0.79769800 | -2.38141100 | -0.17698000 |
| C | -0.26277100 | -2.04466800 | -3.39756200 |
| H | -1.41614200 | -0.38787000 | -4.16645300 |
| H | 0.86835700 | -3.56379200 | -2.35414700 |
| H | -0.23385400 | -2.57137300 | -4.35426100 |
| C | -0.92607600 | -1.03656600 | 1.82143300 |
| C | -2.17026900 | -1.65169800 | 1.60855300 |
| C | -0.20335000 | -1.35609800 | 2.97883700 |
| C | -2.67889100 | -2.56108900 | 2.53124200 |
| H | -2.74861300 | -1.41063500 | 0.71061800 |
| C | -0.71697500 | -2.26449200 | 3.90621700 |
| H | 0.77188800 | -0.89664000 | 3.16573500 |
| C | -1.95459400 | -2.86757400 | 3.68587700 |
| H | -3.65048300 | -3.02802300 | 2.35227700 |
| H | -0.14121700 | -2.50360700 | 4.80359000 |
| H | -2.35578400 | -3.57742900 | 4.41288500 |
| C | 1.60433100 | 3.58838000 | -0.97750100 |
| C | 0.85586400 | 3.38757700 | -2.14380300 |
| C | 2.90445800 | 4.10633800 | -1.07481800 |
| C | 1.40068200 | 3.69400500 | -3.39139500 |
| H | -0.16871000 | 3.00853900 | -2.06383700 |
| C | 3.44494000 | 4.41412300 | -2.32159700 |
| H | 3.49700700 | 4.27179800 | -0.16948300 |
| C | 2.69484200 | 4.20548000 | -3.48159600 |
| H | 0.80805800 | 3.53781600 | -4.29592000 |
| H | 4.45793700 | 4.81756700 | -2.38999600 |
| H | 3.12122500 | 4.44736900 | -4.45791900 |
| C | 1.43853200 | 4.40566800 | 1.75765600 |
| C | 2.00188100 | 4.11164500 | 3.00635800 |
| C | 1.17967100 | 5.74660700 | 1.42941300 |
| C | 2.28403700 | 5.13257000 | 3.91478400 |
| H | 2.22026000 | 3.07534900 | 3.27824400 |
| C | 1.47344900 | 6.76560500 | 2.33184600 |
| H | 0.73410100 | 5.99418800 | 0.46027300 |
| C | 2.01842400 | 6.46062700 | 3.58162100 |
| H | 2.71677700 | 4.88506300 | 4.88746500 |
| H | 1.26795900 | 7.80428000 | 2.06201800 |
| H | 2.23948800 | 7.25951800 | 4.29291900 |
| Cl | -2.76384000 | 3.10174500 | -1.04726000 |
| P | -2.19918200 | 2.66267300 | 2.59071600 |
| C | -3.02586500 | 4.29672000 | 2.65271000 |
| C | -4.40355400 | 4.47310600 | 2.47850200 |
| C | -2.20504600 | 5.43057800 | 2.76829900 |
| C | -4.94887400 | 5.75759300 | 2.42844700 |
| H | -5.06073800 | 3.60389600 | 2.38401700 |
| C | -2.75126800 | 6.71018300 | 2.72266800 |
| H | -1.12499900 | 5.30812900 | 2.90334000 |
| C | -4.12749300 | 6.87768800 | 2.54998600 |
| H | -6.02637900 | 5.88108600 | 2.29617200 |
| H | -2.09850600 | 7.58152500 | 2.82053300 |
| H | -4.55785000 | 7.88087600 | 2.51088100 |
| C | -3.54638100 | 1.45498700 | 2.89544200 |
| C | -3.82806400 | 0.90747000 | 4.15421100 |
| C | -4.29645600 | 1.03162700 | 1.78607400 |
| C | -4.84773200 | -0.03369000 | 4.30115800 |
| H | -3.24627600 | 1.21038200 | 5.02917100 |
| C | -5.32664000 | 0.10627600 | 1.94008000 |
| H | -4.06004400 | 1.42981000 | 0.79218300 |
| C | -5.60322100 | -0.43059100 | 3.19812400 |
| H | -5.05280400 | -0.45804000 | 5.28702000 |
| H | -5.90713400 | -0.20843300 | 1.06939800 |
| H | -6.40244100 | -1.16595000 | 3.31736100 |
| C | -1.24883400 | 2.64726700 | 4.15486900 |
| C | -0.10085900 | 1.85125700 | 4.20824200 |
| C | -1.63203400 | 3.36110800 | 5.30037700 |
| C | 0.64275500 | 1.74191800 | 5.38213800 |
| H | 0.21988500 | 1.33105400 | 3.30211000 |
| C | -0.87883900 | 3.26979900 | 6.46987800 |
| H | -2.52676000 | 3.99019700 | 5.28020600 |
| C | 0.25541900 | 2.45554200 | 6.51556000 |
| H | 1.53627200 | 1.11232900 | 5.40340600 |
| H | -1.18326300 | 3.83297000 | 7.35510900 |
| H | 0.83996300 | 2.38378100 | 7.43559200 |
| C | 1.39976200 | 0.42936300 | 1.00906300 |
| C | 1.93274200 | 1.66003000 | 1.03630400 |
| H | 3.00520200 | 1.81250200 | 1.21709500 |
| H | 2.02383100 | -0.45973400 | 1.16836600 |

**Co-dppen-b3lyp-def-quint**

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

Zero-point correction= 0.675536 (Hartree/Particle)
Thermal correction to Energy= 0.721674
Thermal correction to Enthalpy= 0.722618
Thermal correction to Gibbs Free Energy= 0.588406
Sum of electronic and zero-point Energies= -4563.769686
Sum of electronic and thermal Energies= -4563.723549
Sum of electronic and thermal Enthalpies= -4563.722604
Sum of electronic and thermal Free Energies= -4563.856816

| | | | |
|---|---|---|---|
| Co | -0.72996100 | 0.20283700 | 0.63498000 |
| Cl | 0.08051900 | 0.75659700 | 2.68079100 |
| P | 0.02657000 | -2.04733800 | 0.30508900 |
| C | 1.83135500 | -2.08519300 | -0.00753400 |
| C | 2.42043200 | -2.93434200 | -0.95652800 |
| C | 2.63888100 | -1.20481200 | 0.73565800 |
| C | 3.80473600 | -2.90841300 | -1.15351500 |
| H | 1.80167500 | -3.61328000 | -1.54685300 |
| C | 4.02160500 | -1.19341500 | 0.54307400 |
| H | 2.17980600 | -0.52108700 | 1.45495800 |
| C | 4.60654800 | -2.04368300 | -0.40226500 |
| H | 4.25680600 | -3.56686900 | -1.89920000 |
| H | 4.64328700 | -0.50722300 | 1.12338500 |
| H | 5.68770500 | -2.02510100 | -0.56024500 |
| C | -0.24640700 | -3.06488400 | 1.80347800 |
| C | 0.74282500 | -3.87996600 | 2.37319400 |
| C | -1.52580300 | -3.01362300 | 2.38461000 |
| C | 0.45026800 | -4.64023900 | 3.51138900 |
| H | 1.74061200 | -3.92416800 | 1.93126900 |
| C | -1.81537400 | -3.78018400 | 3.51434200 |
| H | -2.29916600 | -2.37573100 | 1.95176100 |
| C | -0.82642800 | -4.59412500 | 4.08104800 |
| H | 1.22444600 | -5.27328700 | 3.95200900 |
| H | -2.81501200 | -3.73663400 | 3.95382800 |

| | | | |
|---|---|---|---|
| H | -1.05083200 | -5.19044700 | 4.96893900 |
| C | -0.74906600 | -3.00419600 | -1.04954600 |
| C | -0.93757500 | -4.39463400 | -0.97241900 |
| C | -1.17548200 | -2.30996700 | -2.19277300 |
| C | -1.53967500 | -5.07883200 | -2.03212900 |
| H | -0.62078700 | -4.94413200 | -0.08329000 |
| C | -1.76664500 | -2.99931800 | -3.25441600 |
| H | -1.07403700 | -1.22577700 | -2.24941500 |
| C | -1.95212100 | -4.38345700 | -3.17535700 |
| H | -1.68783200 | -6.15932100 | -1.96424300 |
| H | -2.09744500 | -2.44741000 | -4.13767800 |
| H | -2.42430200 | -4.92120000 | -4.00127300 |
| P | -0.30464500 | 1.45711500 | -1.37122500 |
| C | -3.91569200 | 1.79042200 | 1.11073000 |
| C | -5.28131000 | 2.07154400 | 0.91444100 |
| C | -3.16604900 | 2.60477100 | 1.97704100 |
| C | -5.88231600 | 3.14755500 | 1.56989200 |
| H | -5.87725500 | 1.44269400 | 0.24651300 |
| C | -3.77092600 | 3.68566600 | 2.62943800 |
| H | -2.11080900 | 2.38331400 | 2.15626900 |
| C | -5.12688300 | 3.96107200 | 2.42703200 |
| H | -6.94442400 | 3.35495300 | 1.41393400 |
| H | -3.17903500 | 4.31123000 | 3.30306800 |
| H | -5.59822800 | 4.80512400 | 2.93706000 |
| C | -4.11301400 | -1.00715300 | 0.39796100 |
| C | -4.25447500 | -1.96562700 | -0.61832000 |
| C | -4.65751900 | -1.27251900 | 1.66837100 |
| C | -4.91634900 | -3.17178400 | -0.36724900 |
| H | -3.83080600 | -1.76771200 | -1.60440600 |
| C | -5.32024200 | -2.47740800 | 1.91633800 |
| H | -4.55353700 | -0.53812200 | 2.47111800 |
| C | -5.44647300 | -3.43344400 | 0.90060200 |
| H | -5.01121800 | -3.91130300 | -1.16650600 |
| H | -5.73487600 | -2.67341600 | 2.90848700 |
| H | -5.95827500 | -4.37864800 | 1.09816300 |
| C | 0.21792900 | 3.20643800 | -1.06878400 |
| C | 0.24446700 | 4.14389500 | -2.11708900 |
| C | 0.54221700 | 3.62011900 | 0.23363300 |
| C | 0.59012500 | 5.47298700 | -1.86559900 |
| H | -0.00744200 | 3.83219000 | -3.13519800 |
| C | 0.88722700 | 4.95458200 | 0.48292600 |
| H | 0.53161300 | 2.89605200 | 1.05296300 |
| C | 0.91066000 | 5.88199400 | -0.56284000 |
| H | 0.61141200 | 6.19485900 | -2.68644800 |
| H | 1.13937600 | 5.26815000 | 1.49954400 |
| H | 1.17851800 | 6.92350300 | -0.36713600 |
| C | 1.03424200 | 0.84255900 | -2.47497700 |
| C | 0.76571000 | 0.27196300 | -3.72838500 |
| C | 2.35941100 | 0.86911300 | -2.00436000 |
| C | 1.80565200 | -0.25993100 | -4.50007800 |
| H | -0.26184400 | 0.23512200 | -4.09764300 |
| C | 3.39436000 | 0.33367900 | -2.77234400 |
| H | 2.58052300 | 1.29717700 | -1.02324700 |
| C | 3.11984500 | -0.23281400 | -4.02355900 |
| H | 1.58467200 | -0.70006400 | -5.47603400 |
| H | 4.41565000 | 0.34199700 | -2.38551700 |
| H | 3.92967800 | -0.65838700 | -4.62159100 |
| P | -3.06024200 | 0.47383300 | 0.13525700 |
| C | -1.84807800 | 1.37158900 | -2.22154900 |
| H | -1.92368700 | 1.79160900 | -3.23049200 |
| C | -3.03551100 | 0.89021100 | -1.58079700 |
| H | -3.98954000 | 0.94834100 | -2.11679700 |

**Co-dppen-b3lyp-631-quint**

UB3LYP-D3/6-31g(d,p)-CPCM(acetonitrile)

Zero-point correction= 0.676015 (Hartree/Particle)

Thermal correction to Energy= 0.721424

Thermal correction to Enthalpy= 0.722368

Thermal correction to Gibbs Free Energy= 0.591081

Sum of electronic and zero-point Energies= -4565.429591

Sum of electronic and thermal Energies= -4565.384182

Sum of electronic and thermal Enthalpies= -4565.383237

Sum of electronic and thermal Free Energies= -4565.514525

| | | | |
|---|---|---|---|
| Co | -0.70035400 | 0.18234600 | 0.48790400 |
| Cl | 0.12830700 | 0.84876800 | 2.51816000 |
| P | 0.04782200 | -2.06314400 | 0.31411400 |
| C | 1.85659500 | -2.18653600 | 0.07225300 |
| C | 2.42821300 | -3.01780100 | -0.89991300 |
| C | 2.68639500 | -1.39205400 | 0.88156900 |
| C | 3.81411900 | -3.05341700 | -1.06091100 |
| H | 1.79566700 | -3.62961600 | -1.53422200 |
| C | 4.07069400 | -1.44035300 | 0.72302300 |
| H | 2.24669200 | -0.73661400 | 1.62799400 |
| C | 4.63645500 | -2.26875000 | -0.25023300 |
| H | 4.25008900 | -3.69462800 | -1.82078700 |
| H | 4.70618000 | -0.82551600 | 1.35293200 |
| H | 5.71413500 | -2.29857200 | -0.37875600 |
| C | -0.33675500 | -3.00871200 | 1.83389400 |
| C | 0.64536500 | -3.62614900 | 2.61883800 |
| C | -1.68371800 | -3.07626800 | 2.22979900 |
| C | 0.28242400 | -4.30147100 | 3.78686300 |
| H | 1.68853000 | -3.58223000 | 2.32466500 |
| C | -2.04044900 | -3.75794400 | 3.39138600 |
| H | -2.45347800 | -2.60908900 | 1.62659600 |
| C | -1.05696800 | -4.36920300 | 4.17488000 |
| H | 1.04930000 | -4.77664200 | 4.39100300 |
| H | -3.08566800 | -3.80654600 | 3.68100100 |
| H | -1.33383600 | -4.89571000 | 5.08314600 |
| C | -0.71099500 | -3.00702100 | -1.05571300 |
| C | -1.17396800 | -4.32154900 | -0.90668700 |
| C | -0.85239200 | -2.36043500 | -2.29349500 |
| C | -1.78144500 | -4.97432900 | -1.98033600 |
| H | -1.07688300 | -4.82980500 | 0.04641400 |
| C | -1.45133100 | -3.01918500 | -3.36578800 |
| H | -0.51350400 | -1.33841500 | -2.41793700 |
| C | -1.92346300 | -4.32517100 | -3.20909500 |
| H | -2.14606300 | -5.98916900 | -1.85487000 |
| H | -1.55983200 | -2.50673300 | -4.31676000 |
| H | -2.40147500 | -4.83447300 | -4.04026700 |
| P | -0.29647600 | 1.44724400 | -1.47757200 |
| C | -3.79096100 | 1.78402600 | 0.95677200 |
| C | -4.62251900 | 2.71947900 | 0.32490400 |
| C | -3.46251500 | 1.96212100 | 2.31021200 |
| C | -5.13520200 | 3.80345400 | 1.03889700 |
| H | -4.84877400 | 2.60353400 | -0.73176600 |
| C | -3.97907800 | 3.04492500 | 3.02465300 |
| H | -2.78498500 | 1.26609800 | 2.79714100 |
| C | -4.81578900 | 3.96691500 | 2.39031600 |
| H | -5.77901100 | 4.52307500 | 0.54137500 |
| H | -3.71908000 | 3.17522400 | 4.07115700 |
| H | -5.20838800 | 4.81526400 | 2.94297200 |
| C | -4.06525800 | -1.05334300 | 0.30847900 |
| C | -4.04419400 | -2.11267900 | -0.61284500 |
| C | -4.76704200 | -1.21335200 | 1.51482800 |
| C | -4.70064100 | -3.31063600 | -0.32761300 |
| H | -3.49875500 | -2.00049200 | -1.54343000 |
| C | -5.42183100 | -2.41333900 | 1.79642000 |
| H | -4.79675100 | -0.40612700 | 2.23936000 |
| C | -5.38547000 | -3.46778700 | 0.87941600 |
| H | -4.66163400 | -4.12362400 | -1.04586000 |
| H | -5.95807000 | -2.52520800 | 2.73424000 |
| H | -5.88820600 | -4.40340900 | 1.10492500 |
| C | 0.06389700 | 3.22604700 | -1.11926900 |
| C | -0.93900900 | 3.93471300 | -0.43314000 |
| C | 1.24796400 | 3.89075700 | -1.46645500 |
| C | -0.75790600 | 5.27516700 | -0.09804800 |
| H | -1.86880400 | 3.43779100 | -0.17134000 |
| C | 1.42447700 | 5.23732800 | -1.13460200 |
| H | 2.03309600 | 3.36460000 | -1.99913200 |
| C | 0.42668200 | 5.93170700 | -0.44839000 |

| | | | |
|---|---|---|---|
| H | -1.54177600 | 5.80691900 | 0.43371200 |
| H | 2.34426800 | 5.74269100 | -1.41513900 |
| H | 0.56832900 | 6.97688900 | -0.19008500 |
| C | 1.11270700 | 0.86820300 | -2.49651000 |
| C | 0.95024200 | 0.48762500 | -3.83619400 |
| C | 2.36910100 | 0.70807000 | -1.88876200 |
| C | 2.02642400 | -0.03510000 | -4.55629400 |
| H | -0.02434400 | 0.57819900 | -4.30546400 |
| C | 3.44345400 | 0.18825000 | -2.60971400 |
| H | 2.50377800 | 0.97346300 | -0.84459500 |
| C | 3.27354700 | -0.18558200 | -3.94528900 |
| H | 1.88819500 | -0.32979000 | -5.59242800 |
| H | 4.40180500 | 0.05153600 | -2.12032100 |
| H | 4.10656400 | -0.60237000 | -4.50343900 |
| P | -3.00797400 | 0.41156700 | -0.00776000 |
| C | -1.80716600 | 1.28683200 | -2.36155000 |
| H | -1.89391800 | 1.72226800 | -3.35416600 |
| C | -2.98004900 | 0.74839100 | -1.73228800 |
| H | -3.91065000 | 0.71084200 | -2.29324700 |

**Co-dppen-uwb-quint**

UωB97XD/def2-SVP-CPCM(acetonitrile)

Zero-point correction= 0.682869 (Hartree/Particle)

Thermal correction to Energy= 0.728510

Thermal correction to Enthalpy= 0.729454

Thermal correction to Gibbs Free Energy= 0.596473

Sum of electronic and zero-point Energies= -4563.036440

Sum of electronic and thermal Energies= -4562.990799

Sum of electronic and thermal Enthalpies= -4562.989855

Sum of electronic and thermal Free Energies= -4563.122836

| | | | |
|---|---|---|---|
| Co | -1.19557000 | 2.21318600 | 0.60076000 |
| P | -0.21029900 | 0.02463700 | 0.65954600 |
| P | 1.04606900 | 3.04951500 | 0.49996000 |
| C | -0.26300000 | -0.90769600 | -0.92764500 |
| C | -0.92840100 | -0.36631700 | -2.03300500 |
| C | 0.40520900 | -2.13341800 | -1.06043800 |
| C | -0.92244900 | -1.03995000 | -3.25695000 |
| H | -1.46658700 | 0.58062400 | -1.93526200 |
| C | 0.40975500 | -2.80382800 | -2.28080800 |
| H | 0.92550600 | -2.56797300 | -0.20176600 |
| C | -0.25327500 | -2.25584200 | -3.38286600 |
| H | -1.44627100 | -0.61101200 | -4.11423000 |
| H | 0.93137700 | -3.75893300 | -2.37554400 |
| H | -0.24841800 | -2.78203800 | -4.34008900 |
| C | -0.96666300 | -1.17075700 | 1.82530500 |
| C | -2.29004900 | -1.57561500 | 1.60145800 |
| C | -0.29470900 | -1.63368800 | 2.96024300 |
| C | -2.92806700 | -2.42878100 | 2.49677400 |
| H | -2.83053300 | -1.20889600 | 0.72409400 |
| C | -0.93546700 | -2.48895400 | 3.85905100 |
| H | 0.73411500 | -1.31583300 | 3.14691300 |
| C | -2.25154300 | -2.88636700 | 3.62975000 |
| H | -3.96324300 | -2.72637000 | 2.31833700 |
| H | -0.40103600 | -2.84420800 | 4.74295400 |
| H | -2.75493500 | -3.54963000 | 4.33661200 |
| C | 1.63161700 | 3.54116300 | -1.17532300 |
| C | 0.73713500 | 3.55789500 | -2.25104500 |
| C | 2.98425400 | 3.83363900 | -1.40252400 |
| C | 1.18870400 | 3.86477700 | -3.53717200 |
| H | -0.32121200 | 3.33778300 | -2.08438000 |
| C | 3.43250200 | 4.14157500 | -2.68408100 |
| H | 3.69306900 | 3.81920300 | -0.56942900 |
| C | 2.53395900 | 4.15565800 | -3.75506600 |
| H | 0.48317000 | 3.87644800 | -4.37104600 |
| H | 4.48731300 | 4.37067000 | -2.85186500 |
| H | 2.88686700 | 4.39453600 | -4.76083000 |
| C | 1.37036900 | 4.54515000 | 1.50374600 |
| C | 1.67770900 | 4.42532200 | 2.86355100 |
| C | 1.16376500 | 5.82169300 | 0.96058800 |
| C | 1.76025400 | 5.55940600 | 3.67164000 |
| H | 1.84038500 | 3.43411300 | 3.29168800 |
| C | 1.24958200 | 6.95404600 | 1.76854300 |
| H | 0.92293000 | 5.93245200 | -0.09987200 |
| C | 1.54051100 | 6.82484700 | 3.12822300 |
| H | 1.99281800 | 5.44875200 | 4.73312700 |
| H | 1.08271900 | 7.94262500 | 1.33519400 |
| H | 1.59940100 | 7.71229000 | 3.76206800 |
| Cl | -2.79672000 | 2.80428200 | -0.89380900 |
| P | -2.16533500 | 2.65642700 | 2.76629200 |
| C | -2.95727200 | 4.29895900 | 2.81292600 |
| C | -2.19936700 | 5.38676500 | 2.35774600 |
| C | -4.25113200 | 4.51187700 | 3.29793700 |
| C | -2.72610200 | 6.67452400 | 2.39978300 |
| H | -1.18756400 | 5.23097300 | 1.97517600 |
| C | -4.77923100 | 5.80339900 | 3.32974000 |
| H | -4.85057100 | 3.67132900 | 3.65459200 |
| C | -4.01866900 | 6.88415800 | 2.88458300 |
| H | -2.12444800 | 7.51546200 | 2.04824300 |
| H | -5.79059100 | 5.96415200 | 3.70873600 |
| H | -4.43470300 | 7.89345500 | 2.91345900 |
| C | -3.48658400 | 1.45745700 | 3.14521500 |
| C | -3.63057200 | 0.86480800 | 4.40347600 |
| C | -4.37908900 | 1.12650700 | 2.11553200 |
| C | -4.66491200 | -0.04272800 | 4.63203300 |
| H | -2.93488800 | 1.10762800 | 5.20960900 |
| C | -5.41912700 | 0.23236600 | 2.35404600 |
| H | -4.25178100 | 1.56397400 | 1.12095300 |
| C | -5.56287100 | -0.35365000 | 3.61237200 |
| H | -4.76877000 | -0.50682500 | 5.61492100 |
| H | -6.11300600 | -0.01821300 | 1.54903500 |
| H | -6.37276200 | -1.06303100 | 3.79551800 |
| C | -1.05600700 | 2.65040100 | 4.21344300 |
| C | -0.02806400 | 1.70184900 | 4.25534400 |
| C | -1.19576700 | 3.56371700 | 5.26497600 |
| C | 0.84334300 | 1.65783700 | 5.34107500 |
| H | 0.11875500 | 1.01153200 | 3.42292000 |
| C | -0.31445800 | 3.52565100 | 6.34424600 |
| H | -1.98866000 | 4.31427800 | 5.24122900 |
| C | 0.70408700 | 2.57277200 | 6.38498800 |
| H | 1.64434800 | 0.91581900 | 5.36072300 |
| H | -0.42453800 | 4.24567800 | 7.15764300 |
| H | 1.39390700 | 2.54680100 | 7.23125400 |
| C | 1.44109700 | 0.36564600 | 1.14853800 |
| C | 1.97202200 | 1.69806300 | 1.13133800 |
| H | 3.03211700 | 1.84705200 | 1.36372900 |
| H | 2.11854100 | -0.46761800 | 1.36469000 |

**Co-dppen-m06-quint**

UM06-L/def-2SVP-CPCM(acetonitrile)

Zero-point correction= 0.673788 (Hartree/Particle)

Thermal correction to Energy= 0.719904

Thermal correction to Enthalpy= 0.720848

Thermal correction to Gibbs Free Energy= 0.588330

Sum of electronic and zero-point Energies= -4563.313851

Sum of electronic and thermal Energies= -4563.267735

Sum of electronic and thermal Enthalpies= -4563.266791

Sum of electronic and thermal Free Energies= -4563.399309

| | | | |
|---|---|---|---|
| Co | -1.23324300 | 2.10423100 | 0.46739700 |
| P | -0.25184700 | -0.07148900 | 0.68574000 |
| P | 1.02372900 | 2.94775000 | 0.57410900 |
| C | -0.33134000 | -0.98291800 | -0.90593800 |
| C | -0.06301600 | -0.25241500 | -2.07782800 |
| C | -0.55174400 | -2.36543600 | -1.00970100 |
| C | -0.01829600 | -0.88481300 | -3.31633800 |
| H | 0.12296800 | 0.82612200 | -2.01659400 |
| C | -0.50476700 | -2.99682700 | -2.25278200 |
| H | -0.76088800 | -2.95578100 | -0.11326600 |
| C | -0.24092700 | -2.26171300 | -3.40907900 |
| H | 0.18747700 | -0.29943700 | -4.21587800 |
| H | -0.67790400 | -4.07395200 | -2.31740100 |

| | | | |
|---|---|---|---|
| H | -0.20864500 | -2.75901100 | -4.38106100 |
| C | -1.00206400 | -1.21058400 | 1.89220900 |
| C | -2.33717500 | -1.60954000 | 1.71743200 |
| C | -0.30417300 | -1.64319000 | 3.02674300 |
| C | -2.95263900 | -2.43953400 | 2.64984700 |
| H | -2.89859100 | -1.26477700 | 0.84217000 |
| C | -0.92579500 | -2.46939900 | 3.96425600 |
| H | 0.73219100 | -1.32302800 | 3.17410300 |
| C | -2.24783300 | -2.87110800 | 3.77602200 |
| H | -3.99218000 | -2.74233100 | 2.50396600 |
| H | -0.37066900 | -2.80426200 | 4.84375800 |
| H | -2.73452200 | -3.51627700 | 4.51138700 |
| C | 1.59288200 | 3.61440800 | -1.04111900 |
| C | 0.72039700 | 3.62466100 | -2.14039000 |
| C | 2.91982200 | 4.04172600 | -1.22082800 |
| C | 1.16838200 | 4.04248400 | -3.39483600 |
| H | -0.32395100 | 3.31916000 | -2.00700800 |
| C | 3.36275400 | 4.45951700 | -2.47213000 |
| H | 3.61036500 | 4.04731400 | -0.37090200 |
| C | 2.48881400 | 4.45777600 | -3.56492600 |
| H | 0.47778500 | 4.05091200 | -4.24178900 |
| H | 4.39568000 | 4.79310100 | -2.59907100 |
| H | 2.83931100 | 4.78513100 | -4.54640200 |
| C | 1.40140500 | 4.33454000 | 1.70346000 |
| C | 2.11985400 | 4.13621300 | 2.88825600 |
| C | 0.90340800 | 5.61482100 | 1.41412300 |
| C | 2.33121500 | 5.19561900 | 3.77081200 |
| H | 2.50787100 | 3.13964500 | 3.11769000 |
| C | 1.10324500 | 6.66890500 | 2.30290300 |
| H | 0.35701000 | 5.78968300 | 0.48114200 |
| C | 1.81746400 | 6.46073300 | 3.48535100 |
| H | 2.89633200 | 5.02801700 | 4.69123400 |
| H | 0.70168500 | 7.65856400 | 2.07110800 |
| H | 1.97531900 | 7.28733700 | 4.18213500 |
| Cl | -2.88964400 | 2.62991100 | -0.99257200 |
| P | -2.16395400 | 2.71102700 | 2.55410000 |
| C | -3.07623100 | 4.29336800 | 2.54142900 |
| C | -2.73209500 | 5.27083700 | 1.59794900 |
| C | -4.09414500 | 4.56584400 | 3.46769500 |
| C | -3.37516000 | 6.50794000 | 1.59625300 |
| H | -1.96462300 | 5.06099100 | 0.84843200 |
| C | -4.73995400 | 5.80063800 | 3.46026200 |
| H | -4.38062200 | 3.80796400 | 4.20322500 |
| C | -4.37805200 | 6.77475100 | 2.52796200 |
| H | -3.09640700 | 7.26262600 | 0.85737600 |
| H | -5.52948000 | 6.00369200 | 4.18721800 |
| H | -4.88531100 | 7.74213800 | 2.52396400 |
| C | -3.41984300 | 1.50519700 | 3.11358300 |
| C | -3.40022200 | 0.89515500 | 4.37354300 |
| C | -4.44436000 | 1.18274400 | 2.20880600 |
| C | -4.39912200 | -0.01267200 | 4.72743700 |
| H | -2.60545300 | 1.12930500 | 5.08735900 |
| C | -5.44400100 | 0.28400300 | 2.57131300 |
| H | -4.45181700 | 1.64204700 | 1.21412800 |
| C | -5.42407600 | -0.31471500 | 3.83261200 |
| H | -4.37414700 | -0.48525100 | 5.71228400 |
| H | -6.24030600 | 0.04434400 | 1.86265800 |
| H | -6.20525300 | -1.02477800 | 4.11400600 |
| C | -1.00715300 | 2.84054000 | 3.95684200 |
| C | -0.04249600 | 1.83024900 | 4.07974000 |
| C | -1.04233100 | 3.87133600 | 4.90427000 |
| C | 0.84432300 | 1.82553900 | 5.15321000 |
| H | 0.01711700 | 1.03898900 | 3.32560200 |
| C | -0.13970100 | 3.87441500 | 5.96788900 |
| H | -1.77578500 | 4.67751200 | 4.81687900 |
| C | 0.79713600 | 2.84910700 | 6.10040700 |
| H | 1.58513500 | 1.02593300 | 5.23845900 |
| H | -0.17134700 | 4.68481800 | 6.69993600 |
| H | 1.49834000 | 2.85380900 | 6.93819100 |
| C | 1.42600800 | 0.23893000 | 1.10178800 |
| C | 1.97392000 | 1.54727200 | 1.04548700 |
| H | 3.05811100 | 1.67284400 | 1.16055900 |
| H | 2.10183400 | -0.61952200 | 1.20077000 |

**Co-dppp-b3lyp-def-sing**

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

Zero-point correction= 0.731313 (Hartree/Particle)

Thermal correction to Energy= 0.778125

Thermal correction to Enthalpy= 0.779069

Thermal correction to Gibbs Free Energy= 0.647433

Sum of electronic and zero-point Energies= -4604.274012

Sum of electronic and thermal Energies= -4604.227200

Sum of electronic and thermal Enthalpies= -4604.226256

Sum of electronic and thermal Free Energies= -4604.357891

| | | | |
|---|---|---|---|
| Co | -0.86618000 | 2.26116700 | 0.40880300 |
| P | -0.13838800 | 0.07252300 | 0.38676600 |
| P | 1.18235800 | 3.10568400 | 0.88492400 |
| C | -0.78744000 | -0.92205200 | -1.03233900 |
| C | -1.51557700 | -0.27468000 | -2.04251400 |
| C | -0.54815800 | -2.30442500 | -1.13565100 |
| C | -1.99399600 | -0.99904400 | -3.14127300 |
| H | -1.71154600 | 0.79792700 | -1.96542900 |
| C | -1.02718900 | -3.02466500 | -2.23242200 |
| H | 0.00892700 | -2.82384100 | -0.35136500 |
| C | -1.75212400 | -2.37242400 | -3.23847900 |
| H | -2.56224500 | -0.48567800 | -3.92150300 |
| H | -0.83702200 | -4.09887600 | -2.30237400 |
| H | -2.12934500 | -2.93757000 | -4.09477200 |
| C | -0.39514400 | -1.10069900 | 1.78405300 |
| C | -1.71866400 | -1.45678400 | 2.10659200 |
| C | 0.64766700 | -1.58052000 | 2.59442800 |
| C | -1.99122300 | -2.25676200 | 3.21700300 |
| H | -2.54601300 | -1.09429600 | 1.49337200 |
| C | 0.37207300 | -2.37529000 | 3.71366700 |
| H | 1.68478800 | -1.33335800 | 2.37057300 |
| C | -0.94675700 | -2.71191000 | 4.03119200 |
| H | -3.02674800 | -2.51121100 | 3.45408700 |
| H | 1.19578400 | -2.73138800 | 4.33746400 |
| H | -1.16126900 | -3.32769300 | 4.90808700 |
| C | 2.26080700 | 3.50311900 | -0.55851600 |
| C | 1.73491100 | 3.34971800 | -1.85094100 |
| C | 3.59665400 | 3.91440800 | -0.40339000 |
| C | 2.53428300 | 3.60008400 | -2.97303500 |
| H | 0.69169600 | 3.04490400 | -1.97221900 |
| C | 4.39353500 | 4.16175500 | -1.52350200 |
| H | 4.01595900 | 4.04638000 | 0.59783700 |
| C | 3.86293800 | 4.00331600 | -2.81097600 |
| H | 2.11561700 | 3.48036700 | -3.97561500 |
| H | 5.43149600 | 4.47910400 | -1.39419500 |
| H | 4.48772400 | 4.19738500 | -3.68663700 |
| C | 1.30118400 | 4.62534200 | 1.91270000 |
| C | 1.25610300 | 5.89050400 | 1.29694900 |
| C | 1.28521300 | 4.55472500 | 3.31627900 |
| C | 1.19859700 | 7.05491700 | 2.06613500 |
| H | 1.25973800 | 5.96552600 | 0.20654700 |
| C | 1.22824100 | 5.72245700 | 4.08408600 |
| H | 1.29599400 | 3.58936900 | 3.82551600 |
| C | 1.18327300 | 6.97482200 | 3.46405800 |
| H | 1.16298600 | 8.02914800 | 1.57175800 |
| H | 1.20786800 | 5.64616600 | 5.17385700 |
| H | 1.13423500 | 7.88537900 | 4.06636800 |
| Cl | -2.00936300 | 3.27534700 | -1.30745700 |
| P | -2.12152200 | 2.59057600 | 2.30461200 |
| C | -2.95278500 | 4.23750900 | 2.30728000 |
| C | -4.19575000 | 4.46782200 | 2.91998900 |
| C | -2.28352000 | 5.30665100 | 1.69161100 |
| C | -4.75043900 | 5.75148800 | 2.92777800 |
| H | -4.73134100 | 3.64373000 | 3.39758100 |
| C | -2.83229200 | 6.59186400 | 1.71001600 |
| H | -1.33136700 | 5.12371600 | 1.19376900 |

| | | | |
|---|---|---|---|
| C | -4.06746500 | 6.81658700 | 2.32775800 |
| H | -5.71829000 | 5.92161500 | 3.40653700 |
| H | -2.29419000 | 7.41670700 | 1.23593800 |
| H | -4.50122300 | 7.81987000 | 2.33832900 |
| C | -3.54388300 | 1.41717400 | 2.35588600 |
| C | -4.00817000 | 0.79168600 | 3.52169300 |
| C | -4.14431800 | 1.10424100 | 1.12130800 |
| C | -5.04877600 | -0.14216600 | 3.45485100 |
| H | -3.54690200 | 1.01762800 | 4.48529000 |
| C | -5.18631200 | 0.17695900 | 1.05841300 |
| H | -3.77513200 | 1.57832400 | 0.20685600 |
| C | -5.63710600 | -0.45421100 | 2.22548800 |
| H | -5.39535700 | -0.63225100 | 4.36828800 |
| H | -5.64074800 | -0.06401100 | 0.09397300 |
| H | -6.44398200 | -1.18960100 | 2.17455000 |
| C | -1.40245900 | 2.50189900 | 4.00249300 |
| C | -0.64163900 | 1.36542400 | 4.33257900 |
| C | -1.49734900 | 3.54433800 | 4.93798200 |
| C | 0.01182800 | 1.27435900 | 5.56281300 |
| H | -0.55692800 | 0.54504200 | 3.62158200 |
| C | -0.83724000 | 3.45556300 | 6.16887100 |
| H | -2.07253700 | 4.44145800 | 4.70542100 |
| C | -0.07795700 | 2.32505100 | 6.48452700 |
| H | 0.59762600 | 0.38154500 | 5.79567200 |
| H | -0.91302200 | 4.28118800 | 6.88107000 |
| H | 0.44145300 | 2.26140400 | 7.44394000 |
| C | 2.20511900 | 1.86468700 | 1.82105900 |
| H | 1.55185600 | 1.50528800 | 2.63178800 |
| H | 3.06761300 | 2.35855000 | 2.29497600 |
| C | 1.68842200 | 0.00496300 | 0.00516900 |
| H | 1.71761700 | 0.50620400 | -0.97571300 |
| H | 1.98378900 | -1.04121400 | -0.17046300 |
| C | 2.69613500 | 0.68638400 | 0.96256800 |
| H | 3.11694100 | -0.06373800 | 1.65015700 |
| H | 3.54432600 | 1.02952600 | 0.34897900 |

**Co-dppp-b3lyp-631-sing**

UB3LYP-D3/6-31g(d,p)-CPCM(acetonitrile)

Zero-point correction= 0.732273 (Hartree/Particle)

Thermal correction to Energy= 0.779168

Thermal correction to Enthalpy= 0.780112

Thermal correction to Gibbs Free Energy= 0.648768

Sum of electronic and zero-point Energies= -4605.961628

Sum of electronic and thermal Energies= -4605.914734

Sum of electronic and thermal Enthalpies= -4605.913790

Sum of electronic and thermal Free Energies= -4606.045134

| | | | |
|---|---|---|---|
| Co | -0.81535000 | 2.28983900 | 0.45576000 |
| P | -0.14311500 | 0.11478000 | 0.37449300 |
| P | 1.23735100 | 3.07704900 | 0.87798900 |
| C | -0.93374100 | -0.88389500 | -0.96057400 |
| C | -1.81057600 | -0.26012700 | -1.85782300 |
| C | -0.67893600 | -2.25862800 | -1.09784800 |
| C | -2.41936200 | -0.99590900 | -2.87835100 |
| H | -2.01498000 | 0.80099300 | -1.75587200 |
| C | -1.28569700 | -2.99148100 | -2.11673800 |
| H | -0.01589800 | -2.75970300 | -0.39815500 |
| C | -2.15853300 | -2.36044900 | -3.00949500 |
| H | -3.09965300 | -0.50170500 | -3.56585800 |
| H | -1.08265600 | -4.05407600 | -2.21287500 |
| H | -2.63423300 | -2.93315800 | -3.80017200 |
| C | -0.31707100 | -1.02354400 | 1.80900300 |
| C | -1.61578500 | -1.40952700 | 2.18503100 |
| C | 0.76355900 | -1.44060000 | 2.60089600 |
| C | -1.82825400 | -2.16831400 | 3.33361500 |
| H | -2.46526900 | -1.10370200 | 1.58425100 |
| C | 0.54815200 | -2.19660300 | 3.75672800 |
| H | 1.77867100 | -1.17676600 | 2.33315000 |
| C | -0.74718000 | -2.55675100 | 4.13026400 |
| H | -2.84114500 | -2.44227000 | 3.61129900 |
| H | 1.39628800 | -2.50363700 | 4.36147700 |
| H | -0.91375500 | -3.13794000 | 5.03210300 |
| C | 2.28029500 | 3.53578300 | -0.56968300 |
| C | 1.78711200 | 3.30685200 | -1.86143300 |
| C | 3.58007600 | 4.04631300 | -0.41559900 |
| C | 2.57938500 | 3.57731700 | -2.98059000 |
| H | 0.77666500 | 2.92892700 | -1.98580900 |
| C | 4.37002400 | 4.31726300 | -1.53203800 |
| H | 3.97159900 | 4.23851700 | 0.57945700 |
| C | 3.87071000 | 4.08050100 | -2.81726900 |
| H | 2.18563100 | 3.39721300 | -3.97654300 |
| H | 5.37362500 | 4.71136600 | -1.40192400 |
| H | 4.48714900 | 4.29113500 | -3.68617900 |
| C | 1.38133900 | 4.53993500 | 1.97510100 |
| C | 1.34335600 | 5.83427200 | 1.42850500 |
| C | 1.36062700 | 4.39201500 | 3.37078400 |
| C | 1.28475100 | 6.95335000 | 2.25917300 |
| H | 1.35645400 | 5.96570200 | 0.35078600 |
| C | 1.30313600 | 5.51421400 | 4.19930000 |
| H | 1.36155300 | 3.40552600 | 3.82105300 |
| C | 1.26115200 | 6.79645500 | 3.64823300 |
| H | 1.25399800 | 7.94711700 | 1.82224300 |
| H | 1.27464000 | 5.37943600 | 5.27593700 |
| H | 1.20831300 | 7.66724900 | 4.29457200 |
| Cl | -1.91123500 | 3.38358700 | -1.27862300 |
| P | -2.11685900 | 2.61186300 | 2.29370000 |
| C | -2.95931300 | 4.24891300 | 2.23661400 |
| C | -4.34251700 | 4.39837700 | 2.07131000 |
| C | -2.15273900 | 5.39859800 | 2.29671300 |
| C | -4.90647900 | 5.67299800 | 1.96518200 |
| H | -4.98339300 | 3.52454000 | 2.02263800 |
| C | -2.71842500 | 6.66843600 | 2.20132800 |
| H | -1.08209500 | 5.29962000 | 2.42820600 |
| C | -4.09897100 | 6.80976000 | 2.03050800 |
| H | -5.97995400 | 5.77468300 | 1.83465600 |
| H | -2.07794000 | 7.54385300 | 2.25628900 |
| H | -4.54099600 | 7.79829700 | 1.94910600 |
| C | -3.50451600 | 1.40233000 | 2.32539400 |
| C | -3.96771600 | 0.78719900 | 3.49488300 |
| C | -4.06698200 | 1.03375400 | 1.09031900 |
| C | -4.95899200 | -0.19494600 | 3.43039800 |
| H | -3.54038800 | 1.05643600 | 4.45502900 |
| C | -5.06155800 | 0.05876100 | 1.02837000 |
| H | -3.70837000 | 1.49748500 | 0.17528000 |
| C | -5.50376500 | -0.56515500 | 2.19936500 |
| H | -5.30010400 | -0.67488300 | 4.34292900 |
| H | -5.48088000 | -0.22301800 | 0.06713400 |
| H | -6.26751900 | -1.33542100 | 2.15108000 |
| C | -1.42249300 | 2.53576500 | 3.99750800 |
| C | -0.59716900 | 1.44080400 | 4.30136400 |
| C | -1.62556700 | 3.51849000 | 4.97515500 |
| C | 0.02934300 | 1.34044000 | 5.54186400 |
| H | -0.44628900 | 0.66405900 | 3.56403100 |
| C | -0.98965000 | 3.42321200 | 6.21580000 |
| H | -2.26265300 | 4.37095900 | 4.76912500 |
| C | -0.15629200 | 2.34040700 | 6.50146800 |
| H | 0.66365500 | 0.48445200 | 5.75204300 |
| H | -1.14604600 | 4.20020500 | 6.95828200 |
| H | 0.34077100 | 2.27333200 | 7.46449600 |
| C | 2.29701900 | 1.79292400 | 1.70614500 |
| H | 1.69825300 | 1.38817600 | 2.52893100 |
| H | 3.18506600 | 2.25874100 | 2.14481200 |
| C | 1.64737800 | 0.00020100 | -0.13915000 |
| H | 1.63083200 | 0.49343200 | -1.11704100 |
| H | 1.90703300 | -1.04726600 | -0.32075200 |
| C | 2.73212600 | 0.66567500 | 0.75054300 |
| H | 3.22529900 | -0.10107300 | 1.35577900 |
| H | 3.50564900 | 1.05886300 | 0.08317200 |

**Co-dppp-uwb-sing**

UωB97XD/def2-SVP-CPCM(acetonitrile)

Zero-point correction= 0.738700 (Hartree/Particle)
Thermal correction to Energy= 0.784690
Thermal correction to Enthalpy= 0.785635
Thermal correction to Gibbs Free Energy= 0.656128
Sum of electronic and zero-point Energies= -4603.505008
Sum of electronic and thermal Energies= -4603.459018
Sum of electronic and thermal Enthalpies= -4603.458074
Sum of electronic and thermal Free Energies= -4603.587580

| | | | |
|---|---|---|---|
| Co | -0.48335500 | 2.34953000 | 0.76788400 |
| P | 0.14838300 | 0.26594300 | 0.94091600 |
| P | 1.55676500 | 3.05535100 | 0.62895000 |
| C | -0.95451400 | -0.69939400 | -0.17061000 |
| C | -1.83916900 | -0.00617900 | -1.00387200 |
| C | -0.91430700 | -2.09919000 | -0.22908000 |
| C | -2.68077400 | -0.70047300 | -1.87325900 |
| H | -1.87874400 | 1.08641200 | -0.96581900 |
| C | -1.75424200 | -2.79191500 | -1.09794500 |
| H | -0.23211100 | -2.65545700 | 0.41908700 |
| C | -2.64181300 | -2.09275300 | -1.91931100 |
| H | -3.37538900 | -0.14776200 | -2.50920500 |
| H | -1.71920900 | -3.88298400 | -1.13234700 |
| H | -3.30455300 | -2.63742100 | -2.59549100 |
| C | 0.16189000 | -0.75746800 | 2.46584400 |
| C | -1.04804300 | -1.26286200 | 2.95874600 |
| C | 1.32456000 | -0.95240300 | 3.21955100 |
| C | -1.09997300 | -1.93432500 | 4.17639900 |
| H | -1.96357100 | -1.13134900 | 2.37871500 |
| C | 1.27519800 | -1.62360400 | 4.44202300 |
| H | 2.28731700 | -0.58123100 | 2.86603100 |
| C | 0.06326700 | -2.11085200 | 4.92666300 |
| H | -2.05490200 | -2.31732700 | 4.54307500 |
| H | 2.19295400 | -1.76381600 | 5.01708500 |
| H | 0.02475700 | -2.63151800 | 5.88586600 |
| C | 2.38316700 | 3.43187900 | -0.96413700 |
| C | 1.76875800 | 2.99793100 | -2.14325500 |
| C | 3.62562700 | 4.07611800 | -1.03411200 |
| C | 2.38887400 | 3.19817200 | -3.37739100 |
| H | 0.78893300 | 2.51765000 | -2.08238900 |
| C | 4.24398900 | 4.27874900 | -2.26601100 |
| H | 4.11290300 | 4.42757900 | -0.12020500 |
| C | 3.62632700 | 3.83746900 | -3.43899500 |
| H | 1.90150300 | 2.85674300 | -4.29322700 |
| H | 5.21206600 | 4.78227500 | -2.31313900 |
| H | 4.11237900 | 3.99651200 | -4.40422700 |
| C | 1.66517900 | 4.62462800 | 1.56708600 |
| C | 1.35374600 | 5.83258600 | 0.92872400 |
| C | 1.88163000 | 4.62642700 | 2.95124400 |
| C | 1.26878900 | 7.01668900 | 1.65730600 |
| H | 1.15610000 | 5.84149100 | -0.14524500 |
| C | 1.79406200 | 5.81243300 | 3.68053200 |
| H | 2.11038000 | 3.69886700 | 3.48044000 |
| C | 1.48605600 | 7.00998100 | 3.03621800 |
| H | 1.02308300 | 7.95019400 | 1.14631300 |
| H | 1.96338800 | 5.79684900 | 4.75927000 |
| H | 1.41267300 | 7.93765500 | 3.60786700 |
| Cl | -1.33347700 | 3.96138100 | -0.60460900 |
| P | -2.24503500 | 2.37497000 | 2.11728200 |
| C | -2.88697700 | 4.07222900 | 2.44894200 |
| C | -4.24123800 | 4.36349000 | 2.63794500 |
| C | -1.94208500 | 5.09536400 | 2.60106000 |
| C | -4.64484700 | 5.65854600 | 2.97011700 |
| H | -4.99403800 | 3.57998000 | 2.52433000 |
| C | -2.34367500 | 6.38445700 | 2.94165700 |
| H | -0.88306900 | 4.88205500 | 2.43982000 |
| C | -3.69828600 | 6.67043300 | 3.12437400 |
| H | -5.70644300 | 5.87451400 | 3.11042900 |
| H | -1.59219700 | 7.16924900 | 3.05515700 |
| H | -4.01530900 | 7.68279200 | 3.38489000 |
| C | -3.73520200 | 1.46569400 | 1.54905500 |
| C | -4.22613500 | 0.29544400 | 2.13665000 |
| C | -4.31035300 | 1.91036800 | 0.34720100 |
| C | -5.26964500 | -0.41511000 | 1.53875600 |
| H | -3.79935200 | -0.07482300 | 3.07021700 |
| C | -5.36061100 | 1.21113800 | -0.23878300 |
| H | -3.90853500 | 2.80297400 | -0.14098400 |
| C | -5.84138900 | 0.04126900 | 0.35336600 |
| H | -5.63726700 | -1.32945600 | 2.00961900 |
| H | -5.79755600 | 1.57290800 | -1.17214900 |
| H | -6.65869400 | -0.51417400 | -0.11167300 |
| C | -1.94252600 | 1.87410400 | 3.86086800 |
| C | -0.61070200 | 1.77182500 | 4.27269300 |
| C | -2.96182800 | 1.71189300 | 4.80809100 |
| C | -0.29447700 | 1.48197600 | 5.59817200 |
| H | 0.17544300 | 1.91666800 | 3.52880400 |
| C | -2.64871700 | 1.41231300 | 6.13263700 |
| H | -4.00891100 | 1.82796300 | 4.51753200 |
| C | -1.31478200 | 1.29272600 | 6.52875600 |
| H | 0.75135700 | 1.39618700 | 5.89999600 |
| H | -3.45050100 | 1.27892600 | 6.86222000 |
| H | -1.07264600 | 1.05769300 | 7.56763100 |
| C | 2.79467200 | 1.96275600 | 1.44864900 |
| H | 2.38725100 | 1.73529200 | 2.44772300 |
| H | 3.74670600 | 2.49294100 | 1.60237700 |
| C | 1.78787500 | -0.06839600 | 0.13887300 |
| H | 1.59490500 | 0.24323500 | -0.90005000 |
| H | 1.96286900 | -1.15450200 | 0.10985200 |
| C | 3.03679400 | 0.66356400 | 0.67242300 |
| H | 3.61843800 | -0.01293000 | 1.31647900 |
| H | 3.68914000 | 0.88244400 | -0.18719700 |

**Co-dppp-m06-sing**

UM06-L/def-2SVP-CPCM(acetonitrile)
Zero-point correction= 0.729133 (Hartree/Particle)
Thermal correction to Energy= 0.775334
Thermal correction to Enthalpy= 0.776278
Thermal correction to Gibbs Free Energy= 0.645645
Sum of electronic and zero-point Energies= -4603.795749
Sum of electronic and thermal Energies= -4603.749548
Sum of electronic and thermal Enthalpies= -4603.748604
Sum of electronic and thermal Free Energies= -4603.879237

| | | | |
|---|---|---|---|
| Co | -0.90197000 | 2.05575300 | 0.39651400 |
| P | -0.03379000 | -0.02025600 | 0.44727400 |
| P | 1.08735600 | 3.05665900 | 0.65608900 |
| C | -1.13401300 | -1.21121400 | -0.40831000 |
| C | -0.90358900 | -1.66892900 | -1.71225400 |
| C | -2.31758000 | -1.59687200 | 0.24161000 |
| C | -1.82639200 | -2.50589400 | -2.34221300 |
| H | -0.00281600 | -1.37455200 | -2.25529000 |
| C | -3.23409000 | -2.43649400 | -0.38617400 |
| H | -2.53409300 | -1.22813300 | 1.25076300 |
| C | -2.99111200 | -2.89523300 | -1.68268300 |
| H | -1.62942700 | -2.85529900 | -3.35864400 |
| H | -4.14712800 | -2.72795100 | 0.13900500 |
| H | -3.71107600 | -3.55030500 | -2.17838700 |
| C | 0.47597700 | -0.98618800 | 1.91955500 |
| C | -0.33952700 | -0.93379600 | 3.05828300 |
| C | 1.63445600 | -1.77645300 | 1.95726200 |
| C | -0.01510700 | -1.65218900 | 4.20692900 |
| H | -1.23718100 | -0.30797900 | 3.04438600 |
| C | 1.96971500 | -2.48285400 | 3.11253700 |
| H | 2.28126800 | -1.85441300 | 1.07932800 |
| C | 1.14694400 | -2.42357500 | 4.23867700 |
| H | -0.66513100 | -1.59418700 | 5.08405400 |
| H | 2.87840100 | -3.08910600 | 3.13044000 |
| H | 1.41325900 | -2.97841200 | 5.14111200 |
| C | 1.82582500 | 3.96204700 | -0.76887900 |
| C | 1.18179300 | 3.94073100 | -2.01144700 |
| C | 3.04152600 | 4.65152000 | -0.63919000 |
| C | 1.74835500 | 4.59266100 | -3.10929300 |

| | | | |
|---|---|---|---|
| H | 0.22747100 | 3.41233500 | -2.11156700 |
| C | 3.60553800 | 5.29938600 | -1.73560400 |
| H | 3.54956300 | 4.68769300 | 0.33025600 |
| C | 2.95920700 | 5.26971200 | -2.97414400 |
| H | 1.23771000 | 4.57226300 | -4.07516600 |
| H | 4.55262700 | 5.83280300 | -1.62443500 |
| H | 3.40135400 | 5.77999300 | -3.83312500 |
| C | 1.27450400 | 4.29716400 | 1.99480500 |
| C | 2.15127400 | 4.15370400 | 3.07883900 |
| C | 0.42588000 | 5.41571500 | 1.95973600 |
| C | 2.17191100 | 5.09904200 | 4.10508100 |
| H | 2.81676300 | 3.28960400 | 3.14762200 |
| C | 0.45302200 | 6.36315600 | 2.97995500 |
| H | -0.27297300 | 5.54009400 | 1.12504400 |
| C | 1.32269200 | 6.20367000 | 4.06114700 |
| H | 2.85497500 | 4.96537400 | 4.94756700 |
| H | -0.21602000 | 7.22598500 | 2.93476900 |
| H | 1.33777600 | 6.94101600 | 4.86700300 |
| Cl | -1.93780800 | 2.00943200 | -1.66150200 |
| P | -2.11634600 | 2.53135400 | 2.21543500 |
| C | -2.80450800 | 4.23559900 | 2.04372500 |
| C | -3.10448200 | 4.66360000 | 0.73813000 |
| C | -2.94934000 | 5.15036800 | 3.09558700 |
| C | -3.57362000 | 5.95394400 | 0.50029500 |
| H | -2.93280900 | 3.98705200 | -0.10719300 |
| C | -3.40693100 | 6.44614200 | 2.85313700 |
| H | -2.68226000 | 4.87012100 | 4.11632800 |
| C | -3.72710000 | 6.85124700 | 1.55820600 |
| H | -3.80320700 | 6.26523100 | -0.52160900 |
| H | -3.50493200 | 7.14604900 | 3.68662500 |
| H | -4.08301100 | 7.86707100 | 1.37156400 |
| C | -3.60413800 | 1.44503200 | 2.22217100 |
| C | -3.82634000 | 0.46305300 | 3.20008100 |
| C | -4.46360100 | 1.48831300 | 1.11118000 |
| C | -4.88254700 | -0.44128800 | 3.07483600 |
| H | -3.17312100 | 0.39469100 | 4.07395100 |
| C | -5.52383800 | 0.59323800 | 0.99493300 |
| H | -4.28743700 | 2.21743800 | 0.31495600 |
| C | -5.73731700 | -0.37780000 | 1.97589700 |
| H | -5.03697300 | -1.19791600 | 3.84786200 |
| H | -6.18335600 | 0.64832000 | 0.12545400 |
| H | -6.56450000 | -1.08478700 | 1.87981700 |
| C | -1.51393400 | 2.43002700 | 3.93989900 |
| C | -0.17216900 | 2.09084200 | 4.13933100 |
| C | -2.33328300 | 2.63050900 | 5.06402800 |
| C | 0.35858300 | 1.98171100 | 5.42407000 |
| H | 0.44658200 | 1.88554900 | 3.26097600 |
| C | -1.80779700 | 2.51936400 | 6.34895700 |
| H | -3.39501600 | 2.85949300 | 4.93431200 |
| C | -0.45875300 | 2.20148900 | 6.53070000 |
| H | 1.41076900 | 1.71682800 | 5.55659800 |
| H | -2.45454300 | 2.67702200 | 7.21498900 |
| H | -0.04991800 | 2.11543700 | 7.54009700 |
| C | 2.42334700 | 1.83888500 | 1.03700000 |
| H | 2.13243200 | 1.34516900 | 1.98169300 |
| H | 3.36720400 | 2.36703800 | 1.24560900 |
| C | 1.46091700 | 0.04969600 | -0.62484800 |
| H | 1.08683900 | 0.57030300 | -1.52259500 |
| H | 1.76374800 | -0.95414800 | -0.96315600 |
| C | 2.67316800 | 0.79315100 | -0.04597300 |
| H | 3.38111000 | 0.06156400 | 0.37270500 |
| H | 3.21508800 | 1.26497400 | -0.88134100 |

**Co-dppp-b3lyp-def-trip**

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

Zero-point correction= 0.731088 (Hartree/Particle)

Thermal correction to Energy= 0.777981

Thermal correction to Enthalpy= 0.778925

Thermal correction to Gibbs Free Energy= 0.645644

Sum of electronic and zero-point Energies= -4604.296910

Sum of electronic and thermal Energies= -4604.250017

Sum of electronic and thermal Enthalpies= -4604.249073

Sum of electronic and thermal Free Energies= -4604.382354

| | | | |
|---|---|---|---|
| Co | -0.97924800 | 2.24719500 | 0.41738100 |
| P | -0.10869600 | 0.08681200 | 0.34731400 |
| P | 1.06237200 | 3.21515200 | 0.76452700 |
| C | -0.77405500 | -0.96141600 | -1.02438300 |
| C | -1.59720300 | -0.36801300 | -1.99402100 |
| C | -0.45814800 | -2.32781500 | -1.13354700 |
| C | -2.09329800 | -1.12961900 | -3.05927600 |
| H | -1.85351500 | 0.69139300 | -1.91052500 |
| C | -0.95530700 | -3.08541700 | -2.19659900 |
| H | 0.17330900 | -2.80576800 | -0.37980000 |
| C | -1.77482700 | -2.48685500 | -3.16268400 |
| H | -2.73567000 | -0.65847100 | -3.80802400 |
| H | -0.70533200 | -4.14698700 | -2.27136900 |
| H | -2.16594800 | -3.08140300 | -3.99243300 |
| C | -0.20250800 | -1.08613600 | 1.76482000 |
| C | -1.48003100 | -1.51021900 | 2.17827100 |
| C | 0.91701000 | -1.50154200 | 2.50527300 |
| C | -1.63357600 | -2.31348900 | 3.30892300 |
| H | -2.36534400 | -1.19803700 | 1.62076500 |
| C | 0.76080000 | -2.29986900 | 3.64496100 |
| H | 1.92192700 | -1.20135200 | 2.21028900 |
| C | -0.51336100 | -2.70410800 | 4.05301200 |
| H | -2.63552700 | -2.62085300 | 3.61701100 |
| H | 1.64270900 | -2.60541000 | 4.21357200 |
| H | -0.63445400 | -3.32226900 | 4.94596000 |
| C | 2.01917300 | 3.66433700 | -0.74734400 |
| C | 1.41689500 | 3.47328400 | -2.00099600 |
| C | 3.33713700 | 4.15057000 | -0.68406600 |
| C | 2.12379400 | 3.75999500 | -3.17526400 |
| H | 0.38673600 | 3.10924800 | -2.05152600 |
| C | 4.04189400 | 4.43418200 | -1.85617200 |
| H | 3.81451700 | 4.31262200 | 0.28625500 |
| C | 3.43576400 | 4.23747000 | -3.10441100 |
| H | 1.64612900 | 3.61024200 | -4.14696900 |
| H | 5.06678900 | 4.80971000 | -1.79818600 |
| H | 3.98851500 | 4.45981300 | -4.02083900 |
| C | 1.16053100 | 4.74376900 | 1.78129300 |
| C | 1.24580800 | 4.67964100 | 3.18254800 |
| C | 0.99446300 | 6.00037700 | 1.16889200 |
| C | 1.16912900 | 5.84566200 | 3.95140600 |
| H | 1.35207000 | 3.71950900 | 3.69079900 |
| C | 0.91768700 | 7.16306600 | 1.93905100 |
| H | 0.91845200 | 6.06985600 | 0.08071500 |
| C | 1.00348100 | 7.08948000 | 3.33475000 |
| H | 1.22860900 | 5.77403000 | 5.04007400 |
| H | 0.78754800 | 8.13061300 | 1.44739900 |
| H | 0.93930200 | 7.99839000 | 3.93813100 |
| Cl | -2.29707900 | 3.13940800 | -1.24273700 |
| P | -2.11626900 | 2.51007000 | 2.41577200 |
| C | -3.03546000 | 4.10816000 | 2.47271100 |
| C | -4.24120900 | 4.27647000 | 3.17371700 |
| C | -2.47522600 | 5.20511500 | 1.79944300 |
| C | -4.86581100 | 5.52702200 | 3.21112600 |
| H | -4.69299600 | 3.42980700 | 3.69647300 |
| C | -3.09337000 | 6.45772400 | 1.84692400 |
| H | -1.55223400 | 5.07072300 | 1.23509600 |
| C | -4.29051800 | 6.62077100 | 2.55252300 |
| H | -5.80398700 | 5.64896200 | 3.75868600 |
| H | -2.63926700 | 7.30521000 | 1.32712100 |
| H | -4.77874700 | 7.59817500 | 2.58629600 |
| C | -3.46050800 | 1.25674800 | 2.56453700 |
| C | -3.81699300 | 0.62043900 | 3.76200100 |
| C | -4.11182100 | 0.89230800 | 1.37066500 |
| C | -4.80206800 | -0.37398500 | 3.76614900 |
| H | -3.31382600 | 0.88607800 | 4.69406200 |
| C | -5.09881600 | -0.09540500 | 1.37884700 |
| H | -3.82383400 | 1.37387300 | 0.43106700 |

| | | | |
|---|---|---|---|
| C | -5.44205700 | -0.73610500 | 2.57684400 |
| H | -5.06472000 | -0.87164600 | 4.70318100 |
| H | -5.59353900 | -0.37612400 | 0.44548200 |
| H | -6.20531700 | -1.51832700 | 2.58116500 |
| C | -1.27464000 | 2.46814400 | 4.05806000 |
| C | -0.43171200 | 1.37548600 | 4.33240800 |
| C | -1.35672700 | 3.50858500 | 4.99683800 |
| C | 0.31310300 | 1.32515900 | 5.51203000 |
| H | -0.35392800 | 0.55804900 | 3.61692100 |
| C | -0.60524600 | 3.46086200 | 6.17661000 |
| H | -1.99400200 | 4.37300600 | 4.80569100 |
| C | 0.23413600 | 2.37382500 | 6.43710600 |
| H | 0.96160600 | 0.46622400 | 5.70221400 |
| H | -0.67297000 | 4.28468600 | 6.89170300 |
| H | 0.82445400 | 2.34243700 | 7.35626900 |
| C | 2.20989500 | 2.03561500 | 1.63363500 |
| H | 1.62890200 | 1.64190000 | 2.48257900 |
| H | 3.07104400 | 2.57803200 | 2.05414900 |
| C | 1.69159600 | 0.14017600 | -0.14740900 |
| H | 1.62609100 | 0.64217300 | -1.12625500 |
| H | 2.04335700 | -0.88419300 | -0.34645400 |
| C | 2.71342000 | 0.88438900 | 0.74608600 |
| H | 3.21920100 | 0.16310300 | 1.40669500 |
| H | 3.50056500 | 1.27370100 | 0.08078100 |

**Co-dppp-b3lyp-631-trip**

UB3LYP-D3/6-31g(d,p)-CPCM(acetonitrile)

Zero-point correction= 0.732092 (Hartree/Particle)

Thermal correction to Energy= 0.779030

Thermal correction to Enthalpy= 0.779974

Thermal correction to Gibbs Free Energy= 0.647248

Sum of electronic and zero-point Energies= -4605.984878

Sum of electronic and thermal Energies= -4605.937940

Sum of electronic and thermal Enthalpies= -4605.936996

Sum of electronic and thermal Free Energies= -4606.069723

| | | | |
|---|---|---|---|
| Co | -0.93220800 | 2.27556100 | 0.45481100 |
| P | -0.12141500 | 0.12409800 | 0.32380400 |
| P | 1.11448600 | 3.18818700 | 0.74457400 |
| C | -0.92636100 | -0.95036500 | -0.94160100 |
| C | -1.91921200 | -0.40809600 | -1.76781100 |
| C | -0.57303300 | -2.30161900 | -1.09353200 |
| C | -2.54498000 | -1.20021600 | -2.73465300 |
| H | -2.19948800 | 0.63396600 | -1.65179600 |
| C | -1.19665200 | -3.09066700 | -2.05881000 |
| H | 0.18099500 | -2.74109300 | -0.44629400 |
| C | -2.18515900 | -2.54034700 | -2.88189000 |
| H | -3.31528500 | -0.76924000 | -3.36762000 |
| H | -0.91681800 | -4.13448900 | -2.16721500 |
| H | -2.67336600 | -3.15704400 | -3.63078500 |
| C | -0.12027600 | -1.00033800 | 1.77947800 |
| C | -1.36534400 | -1.44214400 | 2.26133100 |
| C | 1.03826400 | -1.35436900 | 2.48695600 |
| C | -1.44960000 | -2.19437900 | 3.43048100 |
| H | -2.27368300 | -1.18367700 | 1.72776700 |
| C | 0.95151500 | -2.10380600 | 3.66388300 |
| H | 2.01481700 | -1.04660200 | 2.13562400 |
| C | -0.29133400 | -2.52007900 | 4.14249900 |
| H | -2.42302400 | -2.51174100 | 3.79084700 |
| H | 1.85851000 | -2.36178600 | 4.20254500 |
| H | -0.35790900 | -3.09591200 | 5.06055600 |
| C | 2.02073700 | 3.70670700 | -0.77273600 |
| C | 1.44338900 | 3.45806100 | -2.02557000 |
| C | 3.29928600 | 4.28592100 | -0.71313400 |
| C | 2.13220900 | 3.77723900 | -3.19908000 |
| H | 0.44833200 | 3.02561100 | -2.07829600 |
| C | 3.98591000 | 4.60548200 | -1.88374600 |
| H | 3.75477400 | 4.49348000 | 0.25114100 |
| C | 3.40322000 | 4.34914400 | -3.12952800 |
| H | 1.67383000 | 3.58136500 | -4.16392200 |
| H | 4.97388500 | 5.05279400 | -1.82652700 |
| H | 3.93917100 | 4.59788200 | -4.04070600 |
| C | 1.25625300 | 4.65459200 | 1.83794900 |
| C | 1.35021900 | 4.50276200 | 3.23012900 |
| C | 1.09982800 | 5.94535400 | 1.30448200 |
| C | 1.28678700 | 5.61745800 | 4.06838300 |
| H | 1.44662000 | 3.51734300 | 3.67233200 |
| C | 1.03669200 | 7.05709400 | 2.14472200 |
| H | 1.02342200 | 6.07940000 | 0.22968100 |
| C | 1.12604900 | 6.89594500 | 3.53061700 |
| H | 1.34727500 | 5.47873900 | 5.14323100 |
| H | 0.91379700 | 8.04817500 | 1.71799200 |
| H | 1.06897900 | 7.76049400 | 4.18494200 |
| Cl | -2.24481100 | 3.21582500 | -1.21247500 |
| P | -2.11048200 | 2.53276000 | 2.40490200 |
| C | -3.03644400 | 4.12509200 | 2.40564800 |
| C | -4.43304900 | 4.20408200 | 2.32848300 |
| C | -2.28644200 | 5.31404500 | 2.41506300 |
| C | -5.06630700 | 5.44838000 | 2.25989200 |
| H | -5.03058000 | 3.29873200 | 2.31962900 |
| C | -2.92063500 | 6.55349200 | 2.35669100 |
| H | -1.20596400 | 5.26993300 | 2.47916800 |
| C | -4.31462200 | 6.62453800 | 2.27465900 |
| H | -6.14967600 | 5.49555400 | 2.19828500 |
| H | -2.32296300 | 7.46021900 | 2.37135800 |
| H | -4.81027100 | 7.58934900 | 2.22270400 |
| C | -3.42522400 | 1.25118900 | 2.53327600 |
| C | -3.76778000 | 0.61271100 | 3.73148800 |
| C | -4.05217700 | 0.84947300 | 1.34027900 |
| C | -4.70407300 | -0.42395000 | 3.73551400 |
| H | -3.28842900 | 0.90706000 | 4.65918500 |
| C | -4.99183600 | -0.18049900 | 1.34735400 |
| H | -3.78484300 | 1.33163800 | 0.40355600 |
| C | -5.31349300 | -0.82629300 | 2.54546100 |
| H | -4.95173500 | -0.92085300 | 4.66888600 |
| H | -5.46214000 | -0.48739200 | 0.41790300 |
| H | -6.03407500 | -1.63853200 | 2.54998700 |
| C | -1.29257600 | 2.49990600 | 4.05446200 |
| C | -0.37482300 | 1.46332000 | 4.29047600 |
| C | -1.49289900 | 3.46336000 | 5.05172200 |
| C | 0.34158600 | 1.40136700 | 5.48404500 |
| H | -0.22145400 | 0.70232200 | 3.53708900 |
| C | -0.76677700 | 3.40758600 | 6.24431300 |
| H | -2.19955700 | 4.27080800 | 4.89720800 |
| C | 0.15564100 | 2.38274600 | 6.46249900 |
| H | 1.04591200 | 0.59020000 | 5.64262200 |
| H | -0.92306700 | 4.16949300 | 7.00228200 |
| H | 0.72194100 | 2.34619400 | 7.38823500 |
| C | 2.30064200 | 1.96338200 | 1.48843200 |
| H | 1.78313900 | 1.52310700 | 2.34712200 |
| H | 3.18882700 | 2.47782100 | 1.86883500 |
| C | 1.63278200 | 0.13112000 | -0.31342300 |
| H | 1.51426500 | 0.62440100 | -1.28437600 |
| H | 1.94833200 | -0.89584900 | -0.52137100 |
| C | 2.73365400 | 0.86387100 | 0.50038500 |
| H | 3.31409500 | 0.12958500 | 1.06743500 |
| H | 3.43326400 | 1.30206300 | -0.21863000 |

**Co-dppp-uwb-trip**

UωB97XD/def2-SVP-CPCM(acetonitrile)

Zero-point correction= 0.738339 (Hartree/Particle)

Thermal correction to Energy= 0.784741

Thermal correction to Enthalpy= 0.785685

Thermal correction to Gibbs Free Energy= 0.654551

Sum of electronic and zero-point Energies= -4603.552003

Sum of electronic and thermal Energies= -4603.505602

Sum of electronic and thermal Enthalpies= -4603.504658

Sum of electronic and thermal Free Energies= -4603.635792

| | | | |
|---|---|---|---|
| Co | -0.98010900 | 2.08390900 | 0.31729100 |
| P | -0.01482500 | -0.00418500 | 0.44159800 |
| P | 1.02657300 | 3.16584100 | 0.52258300 |

| | | | |
|---|---|---|---|
| C | -0.85258600 | -1.34209100 | -0.50976700 |
| C | -1.80539500 | -0.98585700 | -1.47208200 |
| C | -0.54992700 | -2.69744200 | -0.31723200 |
| C | -2.44494800 | -1.96964000 | -2.22893200 |
| H | -2.05255500 | 0.06892300 | -1.62577300 |
| C | -1.19002800 | -3.67776800 | -1.07244300 |
| H | 0.18704600 | -2.99140700 | 0.43472500 |
| C | -2.14018500 | -3.31518900 | -2.02972600 |
| H | -3.18886300 | -1.68030000 | -2.97462500 |
| H | -0.94841500 | -4.73082600 | -0.91182600 |
| H | -2.64452700 | -4.08489800 | -2.61826900 |
| C | 0.29525000 | -0.85015400 | 2.03865400 |
| C | -0.81725400 | -1.14314700 | 2.84103900 |
| C | 1.56753600 | -1.19690600 | 2.50370100 |
| C | -0.66337000 | -1.76921500 | 4.07266200 |
| H | -1.82058900 | -0.87371800 | 2.50050500 |
| C | 1.72537200 | -1.81189800 | 3.74814900 |
| H | 2.45403000 | -0.99780000 | 1.90009300 |
| C | 0.61235800 | -2.10001300 | 4.53348000 |
| H | -1.54176200 | -1.98492000 | 4.68400300 |
| H | 2.72698100 | -2.07060100 | 4.09841000 |
| H | 0.73646200 | -2.57986500 | 5.50665500 |
| C | 1.76147300 | 3.83333100 | -1.02511700 |
| C | 1.18418300 | 3.48627200 | -2.25125700 |
| C | 2.91624400 | 4.62837100 | -1.01136500 |
| C | 1.75892800 | 3.91990700 | -3.44815900 |
| H | 0.26787000 | 2.88950400 | -2.26743300 |
| C | 3.48701300 | 5.06261200 | -2.20510100 |
| H | 3.37110500 | 4.91465400 | -0.05885600 |
| C | 2.90949900 | 4.70582100 | -3.42657200 |
| H | 1.30051600 | 3.64492800 | -4.40067700 |
| H | 4.38608500 | 5.68249700 | -2.18468800 |
| H | 3.35768300 | 5.04673200 | -4.36257800 |
| C | 1.12522800 | 4.60452200 | 1.65135000 |
| C | 1.84877900 | 4.61084300 | 2.84842700 |
| C | 0.36048400 | 5.73167200 | 1.31544000 |
| C | 1.80894400 | 5.72346100 | 3.69251700 |
| H | 2.45195900 | 3.74950200 | 3.14205100 |
| C | 0.33271600 | 6.84440600 | 2.14870200 |
| H | -0.22683400 | 5.73322000 | 0.39286500 |
| C | 1.05571300 | 6.84172300 | 3.34353200 |
| H | 2.37578600 | 5.71230100 | 4.62604400 |
| H | -0.27097000 | 7.71137100 | 1.87373100 |
| H | 1.02552700 | 7.71086900 | 4.00416200 |
| Cl | -2.35570200 | 2.66404300 | -1.43102500 |
| P | -2.13771600 | 2.44660600 | 2.27592700 |
| C | -2.49857300 | 4.22094900 | 2.59206800 |
| C | -2.98492300 | 4.97635100 | 1.51469900 |
| C | -2.29600800 | 4.84602000 | 3.82566600 |
| C | -3.28369600 | 6.32608200 | 1.67827500 |
| H | -3.12089000 | 4.49995400 | 0.53907000 |
| C | -2.58459800 | 6.20268700 | 3.98376300 |
| H | -1.90928400 | 4.27601900 | 4.67305600 |
| C | -3.08404400 | 6.94316600 | 2.91482500 |
| H | -3.66607000 | 6.90293600 | 0.83313000 |
| H | -2.41690900 | 6.68107100 | 4.95124800 |
| H | -3.31087600 | 8.00413700 | 3.04124400 |
| C | -3.82929400 | 1.73312000 | 2.15770200 |
| C | -4.93378500 | 2.26610400 | 2.83529000 |
| C | -4.01339200 | 0.61192900 | 1.33863600 |
| C | -6.18971700 | 1.67259500 | 2.71576700 |
| H | -4.81378800 | 3.15497300 | 3.45984400 |
| C | -5.26798200 | 0.01486100 | 1.22166700 |
| H | -3.17035500 | 0.21084500 | 0.77098300 |
| C | -6.35802700 | 0.54331700 | 1.91261900 |
| H | -7.04255800 | 2.09629400 | 3.25054100 |
| H | -5.39347500 | -0.85954000 | 0.57938400 |
| H | -7.34298700 | 0.08074800 | 1.81866500 |
| C | -1.53579900 | 1.85896200 | 3.90725600 |
| C | -0.15346200 | 1.88622900 | 4.11994300 |
| C | -2.36625000 | 1.38701300 | 4.92919900 |
| C | 0.39418200 | 1.47241500 | 5.33032100 |
| H | 0.49905500 | 2.23010800 | 3.31819300 |
| C | -1.82018900 | 0.96108600 | 6.14018100 |
| H | -3.44734600 | 1.34212300 | 4.78470100 |
| C | -0.44159900 | 1.00542400 | 6.34466600 |
| H | 1.47626000 | 1.50031800 | 5.47462600 |
| H | -2.47871200 | 0.58912700 | 6.92817000 |
| H | -0.01734100 | 0.66696800 | 7.29246600 |
| C | 2.38660100 | 2.05134300 | 1.09210200 |
| H | 2.06398500 | 1.60417800 | 2.04636200 |
| H | 3.29214800 | 2.64130300 | 1.30214500 |
| C | 1.61766900 | 0.03023000 | -0.43774000 |
| H | 1.31569900 | 0.35497700 | -1.44669100 |
| H | 1.99128600 | -0.99928700 | -0.54942000 |
| C | 2.74507200 | 0.94661900 | 0.09089400 |
| H | 3.51762600 | 0.32539500 | 0.56839300 |
| H | 3.24054200 | 1.40905000 | -0.77694900 |

**Co-dppp-m06-trip**

UM06-L/def-2SVP-CPCM(acetonitrile)

Zero-point correction= 0.728982 (Hartree/Particle)

Thermal correction to Energy= 0.776027

Thermal correction to Enthalpy= 0.776971

Thermal correction to Gibbs Free Energy= 0.644129

Sum of electronic and zero-point Energies= -4603.831566

Sum of electronic and thermal Energies= -4603.784521

Sum of electronic and thermal Enthalpies= -4603.783577

Sum of electronic and thermal Free Energies= -4603.916419

| | | | |
|---|---|---|---|
| Co | -0.94239200 | 2.25502300 | 0.41119900 |
| P | -0.13337600 | 0.10846300 | 0.37850400 |
| P | 1.10415600 | 3.16701300 | 0.70886900 |
| C | -0.97970100 | -0.98127100 | -0.84066000 |
| C | -1.82464500 | -0.39710500 | -1.79348800 |
| C | -0.78867100 | -2.37107900 | -0.85842500 |
| C | -2.46673800 | -1.18858200 | -2.74719900 |
| H | -1.98260700 | 0.68786300 | -1.78172100 |
| C | -1.43290200 | -3.15977100 | -1.80964900 |
| H | -0.13350700 | -2.84247500 | -0.11909700 |
| C | -2.27456200 | -2.56973200 | -2.75519900 |
| H | -3.12519800 | -0.72261200 | -3.48427200 |
| H | -1.27867700 | -4.24145000 | -1.81289300 |
| H | -2.78214800 | -3.18990100 | -3.49778100 |
| C | -0.06156200 | -0.98719600 | 1.84339600 |
| C | -1.27063500 | -1.42747500 | 2.40872200 |
| C | 1.13928600 | -1.32786700 | 2.48176400 |
| C | -1.27611600 | -2.17811100 | 3.58119500 |
| H | -2.22020000 | -1.18440500 | 1.92115100 |
| C | 1.13184200 | -2.07374700 | 3.66207500 |
| H | 2.09770800 | -1.01611000 | 2.06102200 |
| C | -0.07424300 | -2.49688200 | 4.21792800 |
| H | -2.22676000 | -2.51467700 | 4.00247700 |
| H | 2.07830000 | -2.32786100 | 4.14508200 |
| H | -0.07937400 | -3.07935700 | 5.14195000 |
| C | 1.96885100 | 3.72975400 | -0.81147600 |
| C | 1.39119100 | 3.45704100 | -2.05782900 |
| C | 3.21680800 | 4.36975100 | -0.76254500 |
| C | 2.05172300 | 3.81066800 | -3.23608800 |
| H | 0.40740700 | 2.97583700 | -2.09972600 |
| C | 3.87398100 | 4.72448200 | -1.93839400 |
| H | 3.67820400 | 4.59475200 | 0.20453500 |
| C | 3.29264800 | 4.44297100 | -3.17750700 |
| H | 1.59163800 | 3.59455700 | -4.20315400 |
| H | 4.84539700 | 5.22223300 | -1.89010300 |
| H | 3.80961500 | 4.72141300 | -4.09879600 |
| C | 1.27147400 | 4.60613700 | 1.81943200 |
| C | 1.54015500 | 4.45034300 | 3.18746300 |
| C | 0.97958200 | 5.89041400 | 1.33103700 |
| C | 1.50934400 | 5.55015800 | 4.04600600 |

| | | | |
|---|---|---|---|
| H | 1.77155600 | 3.46300700 | 3.59592400 |
| C | 0.96233600 | 6.98874500 | 2.18729300 |
| H | 0.75877700 | 6.02971800 | 0.26774200 |
| C | 1.21983100 | 6.82163200 | 3.54989300 |
| H | 1.71709400 | 5.40921300 | 5.10982200 |
| H | 0.73758400 | 7.98161600 | 1.79004300 |
| H | 1.19772600 | 7.68200000 | 4.22255000 |
| Cl | -2.28974400 | 3.27729200 | -1.17681800 |
| P | -2.08480500 | 2.54888100 | 2.38447000 |
| C | -2.97525600 | 4.15074800 | 2.40139300 |
| C | -4.31635600 | 4.27252400 | 2.01686100 |
| C | -2.24775700 | 5.31540500 | 2.69515800 |
| C | -4.91810800 | 5.52914800 | 1.93500100 |
| H | -4.90114700 | 3.37993400 | 1.77750700 |
| C | -2.85149100 | 6.56824200 | 2.61846000 |
| H | -1.19839000 | 5.24028900 | 2.99876200 |
| C | -4.18980200 | 6.67976300 | 2.23543500 |
| H | -5.96632000 | 5.60679300 | 1.63658000 |
| H | -2.27099600 | 7.46271100 | 2.85892900 |
| H | -4.66332400 | 7.66215400 | 2.17244700 |
| C | -3.42170500 | 1.29366300 | 2.47182800 |
| C | -3.84994700 | 0.69809400 | 3.66474600 |
| C | -3.96526000 | 0.84902200 | 1.25482200 |
| C | -4.79643500 | -0.32738600 | 3.64032100 |
| H | -3.43096600 | 1.02229600 | 4.62165200 |
| C | -4.91628900 | -0.16895600 | 1.23368300 |
| H | -3.62981800 | 1.30590000 | 0.31600000 |
| C | -5.32807200 | -0.76573100 | 2.42749600 |
| H | -5.11472600 | -0.79177200 | 4.57682500 |
| H | -5.32862100 | -0.50647800 | 0.27943000 |
| H | -6.06291600 | -1.57391300 | 2.41160200 |
| C | -1.32862100 | 2.48538200 | 4.05275800 |
| C | -0.24741300 | 1.61377900 | 4.23366700 |
| C | -1.77276700 | 3.24529600 | 5.14415400 |
| C | 0.38226600 | 1.49865800 | 5.47124700 |
| H | 0.10379900 | 1.02740700 | 3.38098400 |
| C | -1.13453700 | 3.14254600 | 6.38016000 |
| H | -2.62188000 | 3.92483700 | 5.03149400 |
| C | -0.05654500 | 2.27139800 | 6.54712200 |
| H | 1.22487500 | 0.81248100 | 5.58973700 |
| H | -1.48538600 | 3.74523000 | 7.22119900 |
| H | 0.44061400 | 2.19529800 | 7.51684900 |
| C | 2.32710300 | 1.95207100 | 1.38063900 |
| H | 1.86896500 | 1.50776900 | 2.28160300 |
| H | 3.23587200 | 2.47413400 | 1.72150100 |
| C | 1.58559600 | 0.08717900 | -0.32052300 |
| H | 1.42027100 | 0.51065200 | -1.32536300 |
| H | 1.88982300 | -0.95804000 | -0.49234700 |
| C | 2.71163500 | 0.85848100 | 0.38924800 |
| H | 3.36447600 | 0.14909700 | 0.92059100 |
| H | 3.35888200 | 1.29878400 | -0.38661800 |

**Co-dppp-b3lyp-631-quint**

UB3LYP-D3/6-31g(d,p)-CPCM(acetonitrile)

Zero-point correction= 0.728226 (Hartree/Particle)

Thermal correction to Energy= 0.775895

Thermal correction to Enthalpy= 0.776839

Thermal correction to Gibbs Free Energy= 0.639613

Sum of electronic and zero-point Energies= -4605.911883

Sum of electronic and thermal Energies= -4605.864215

Sum of electronic and thermal Enthalpies= -4605.863271

Sum of electronic and thermal Free Energies= -4606.000496

| | | | |
|---|---|---|---|
| Co | -0.85354300 | 2.27404800 | 0.64299500 |
| P | -0.08391100 | 0.01750700 | 0.36935100 |
| P | 1.40005500 | 3.20160700 | 0.64693200 |
| C | -1.17670600 | -0.97462300 | -0.70300800 |
| C | -0.88933900 | -1.25358100 | -2.04624200 |
| C | -2.39797400 | -1.39877100 | -0.15315800 |
| C | -1.80974200 | -1.96154300 | -2.82365100 |
| H | 0.04109900 | -0.92604900 | -2.49696900 |
| C | -3.30970800 | -2.10647700 | -0.93265600 |
| H | -2.63748800 | -1.17484200 | 0.88117800 |
| C | -3.01739400 | -2.39026100 | -2.27016300 |
| H | -1.57913400 | -2.17693100 | -3.86251600 |
| H | -4.24989100 | -2.42577900 | -0.49408900 |
| H | -3.72950200 | -2.93929200 | -2.87869100 |
| C | 0.25452000 | -1.02635900 | 1.82801100 |
| C | 0.16987500 | -0.46126100 | 3.10767400 |
| C | 0.62434900 | -2.37393800 | 1.68871600 |
| C | 0.45933100 | -1.23030100 | 4.23684900 |
| H | -0.14949200 | 0.56623800 | 3.23330500 |
| C | 0.91149400 | -3.13917200 | 2.81811700 |
| H | 0.67838900 | -2.82552500 | 0.70226500 |
| C | 0.83120900 | -2.56737300 | 4.09309900 |
| H | 0.38747000 | -0.78018000 | 5.22231200 |
| H | 1.19617800 | -4.18076600 | 2.70569400 |
| H | 1.05497700 | -3.16712800 | 4.97009300 |
| C | 2.17433800 | 3.68107200 | -0.93868600 |
| C | 1.44294000 | 3.55261100 | -2.12813600 |
| C | 3.49776900 | 4.14853000 | -0.98325900 |
| C | 2.03472100 | 3.87855500 | -3.35093800 |
| H | 0.41512500 | 3.20326800 | -2.09727400 |
| C | 4.08302100 | 4.47322900 | -2.20590600 |
| H | 4.06910000 | 4.26538900 | -0.06684900 |
| C | 3.35246000 | 4.33646900 | -3.39082500 |
| H | 1.46401800 | 3.77611100 | -4.26875200 |
| H | 5.10681400 | 4.83316100 | -2.23518500 |
| H | 3.81109500 | 4.58985200 | -4.34175800 |
| C | 1.62414200 | 4.60893400 | 1.79368000 |
| C | 2.74693800 | 4.78355800 | 2.61586400 |
| C | 0.56715000 | 5.53081500 | 1.87204100 |
| C | 2.80468600 | 5.86020600 | 3.50343100 |
| H | 3.57477400 | 4.08394700 | 2.58650300 |
| C | 0.62926200 | 6.60632100 | 2.75575300 |
| H | -0.31712600 | 5.39328500 | 1.25974800 |
| C | 1.74772500 | 6.77014800 | 3.57674200 |
| H | 3.67481300 | 5.98300900 | 4.14076400 |
| H | -0.20080600 | 7.30380900 | 2.81116200 |
| H | 1.79361100 | 7.60021200 | 4.27493600 |
| Cl | -2.12479700 | 2.69072600 | -1.21894100 |
| P | -2.30252900 | 2.64124900 | 2.48999700 |
| C | -3.41542500 | 4.07791900 | 2.27966500 |
| C | -3.08475100 | 5.11618400 | 1.37463100 |
| C | -4.46166100 | 4.32206000 | 3.20987300 |
| C | -3.75021600 | 6.33556200 | 1.40312700 |
| H | -2.32297900 | 4.94095500 | 0.62082800 |
| C | -5.11427400 | 5.55117100 | 3.24193900 |
| H | -4.77124300 | 3.53494800 | 3.89083600 |
| C | -4.76394800 | 6.57291800 | 2.34894400 |
| H | -3.49136800 | 7.10433100 | 0.67928600 |
| H | -5.91362700 | 5.71307300 | 3.96145800 |
| H | -5.27557600 | 7.53004400 | 2.37923900 |
| C | -3.48835400 | 1.21375900 | 2.46073400 |
| C | -3.29229700 | 0.07262200 | 3.25455100 |
| C | -4.51775900 | 1.20192300 | 1.50510800 |
| C | -4.12818800 | -1.03777800 | 3.12154000 |
| H | -2.49007700 | 0.05783000 | 3.98371300 |
| C | -5.34543200 | 0.08723200 | 1.36369700 |
| H | -4.66818400 | 2.07434400 | 0.87624600 |
| C | -5.15766200 | -1.03522300 | 2.17448200 |
| H | -3.97306100 | -1.90648600 | 3.75500700 |
| H | -6.13600400 | 0.09335800 | 0.61872900 |
| H | -5.80199700 | -1.90251500 | 2.06524100 |
| C | -1.55538600 | 2.58264500 | 4.12492400 |
| C | -0.17450200 | 2.89416100 | 4.29907500 |
| C | -2.35233400 | 2.49529000 | 5.31258700 |
| C | 0.37869700 | 3.07614400 | 5.55416300 |
| H | 0.46131300 | 2.99817400 | 3.42835900 |
| C | -1.78739000 | 2.69151300 | 6.56691200 |
| H | -3.40291600 | 2.23256700 | 5.23627100 |

| | | | |
|---|---|---|---|
| C | -0.42217500 | 2.98438700 | 6.71490100 |
| H | 1.44076800 | 3.29365000 | 5.63824000 |
| H | -2.41738900 | 2.60479500 | 7.44989300 |
| H | 0.00823300 | 3.13982000 | 7.69910200 |
| C | 2.47874600 | 1.84134400 | 1.29809100 |
| H | 1.99448400 | 1.49651900 | 2.21799000 |
| H | 3.45470000 | 2.23977800 | 1.58647200 |
| C | 1.53249600 | 0.14769600 | -0.52482700 |
| H | 1.35427900 | 0.82385100 | -1.36809300 |
| H | 1.79750500 | -0.82784100 | -0.94359900 |
| C | 2.71327300 | 0.65908900 | 0.32955900 |
| H | 3.09592800 | -0.17088400 | 0.93149300 |
| H | 3.51037000 | 0.93355400 | -0.36819100 |

**Co-dppp-uwb-quint**

UωB97XD/def2-SVP-CPCM(acetonitrile)

Zero-point correction= 0.735309 (Hartree/Particle)
Thermal correction to Energy= 0.782229
Thermal correction to Enthalpy= 0.783173
Thermal correction to Gibbs Free Energy= 0.648693
Sum of electronic and zero-point Energies= -4603.472509
Sum of electronic and thermal Energies= -4603.425589
Sum of electronic and thermal Enthalpies= -4603.424645
Sum of electronic and thermal Free Energies= -4603.559124

| | | | |
|---|---|---|---|
| Co | -0.92355800 | 2.18004000 | 0.62996200 |
| P | -0.02143700 | -0.06718600 | 0.44318700 |
| P | 1.28002000 | 3.21863200 | 0.62230200 |
| C | -1.05975100 | -1.14747300 | -0.59668300 |
| C | -0.55755200 | -2.00554400 | -1.58190200 |
| C | -2.44047400 | -1.11388400 | -0.35425300 |
| C | -1.42469700 | -2.82436300 | -2.30610300 |
| H | 0.51110500 | -2.04652700 | -1.80044800 |
| C | -3.30199900 | -1.93976300 | -1.07123100 |
| H | -2.84818300 | -0.43475500 | 0.39768600 |
| C | -2.79511200 | -2.79595600 | -2.04978000 |
| H | -1.02373300 | -3.48852100 | -3.07442000 |
| H | -4.37429600 | -1.90485200 | -0.86710400 |
| H | -3.47059900 | -3.43920100 | -2.61778500 |
| C | 0.40392400 | -1.06902000 | 1.90595000 |
| C | 0.16127200 | -0.53988200 | 3.17680400 |
| C | 0.97938600 | -2.34150700 | 1.78172800 |
| C | 0.49652100 | -1.27016600 | 4.31823400 |
| H | -0.29982500 | 0.44385300 | 3.28749100 |
| C | 1.31056600 | -3.06905000 | 2.92188400 |
| H | 1.16566500 | -2.77203600 | 0.79416900 |
| C | 1.07053900 | -2.53321700 | 4.19095800 |
| H | 0.30696500 | -0.83739600 | 5.30362900 |
| H | 1.75796300 | -4.06007900 | 2.82172200 |
| H | 1.33349700 | -3.10768700 | 5.08192000 |
| C | 2.03434500 | 3.75782700 | -0.94671700 |
| C | 1.25329300 | 3.78427900 | -2.10752500 |
| C | 3.38070300 | 4.14434400 | -1.00307600 |
| C | 1.81868600 | 4.19043400 | -3.31745800 |
| H | 0.20173200 | 3.48699900 | -2.06329100 |
| C | 3.94021000 | 4.54630400 | -2.21286000 |
| H | 3.99830600 | 4.13637300 | -0.10111100 |
| C | 3.15901000 | 4.56862500 | -3.37092800 |
| H | 1.20652500 | 4.20974900 | -4.22139200 |
| H | 4.98973500 | 4.84458500 | -2.25319200 |
| H | 3.60018500 | 4.88411300 | -4.31885400 |
| C | 1.34706500 | 4.65598600 | 1.74070200 |
| C | 2.38644000 | 4.90571700 | 2.64323600 |
| C | 0.23459800 | 5.50862400 | 1.71575700 |
| C | 2.30514800 | 5.99076800 | 3.51596300 |
| H | 3.25950900 | 4.25222100 | 2.68999300 |
| C | 0.15702600 | 6.59236200 | 2.58612400 |
| H | -0.58814600 | 5.31468000 | 1.02256500 |
| C | 1.19166700 | 6.83062400 | 3.49204500 |
| H | 3.11533700 | 6.17516900 | 4.22421600 |
| H | -0.72164600 | 7.24074500 | 2.56440300 |
| H | 1.12845200 | 7.67207500 | 4.18515700 |
| Cl | -2.14394000 | 2.44642600 | -1.26024000 |
| P | -2.28198200 | 2.65225500 | 2.54510600 |
| C | -3.14701500 | 4.28752600 | 2.43112800 |
| C | -3.32388500 | 4.92601000 | 1.19524100 |
| C | -3.50370400 | 4.96864900 | 3.60298600 |
| C | -3.86010400 | 6.21291700 | 1.13360300 |
| H | -3.02776700 | 4.41903300 | 0.27216500 |
| C | -4.04202500 | 6.25312400 | 3.53976900 |
| H | -3.34170900 | 4.49488600 | 4.57442600 |
| C | -4.22063200 | 6.87967200 | 2.30472600 |
| H | -3.98926500 | 6.69962700 | 0.16407600 |
| H | -4.31684200 | 6.77169200 | 4.46120300 |
| H | -4.63442000 | 7.88941800 | 2.25649900 |
| C | -3.63718000 | 1.42007200 | 2.33582800 |
| C | -3.53344200 | 0.17039200 | 2.96253300 |
| C | -4.68644900 | 1.64192900 | 1.43486700 |
| C | -4.46766700 | -0.83177100 | 2.70243000 |
| H | -2.71169000 | -0.01784100 | 3.65650600 |
| C | -5.61317100 | 0.63455800 | 1.16688000 |
| H | -4.77768000 | 2.60369500 | 0.92565400 |
| C | -5.50782800 | -0.60402900 | 1.80111600 |
| H | -4.37599600 | -1.79906100 | 3.20123500 |
| H | -6.42168500 | 0.81884100 | 0.45602600 |
| H | -6.23448700 | -1.39173000 | 1.59035700 |
| C | -1.56328200 | 2.42089600 | 4.12347700 |
| C | -0.14922600 | 2.64464100 | 4.31980800 |
| C | -2.33343400 | 2.10704900 | 5.31448900 |
| C | 0.44828800 | 2.46135300 | 5.54400100 |
| H | 0.46193100 | 2.96114500 | 3.47323800 |
| C | -1.71052000 | 1.92773100 | 6.53211600 |
| H | -3.41781400 | 1.98234000 | 5.24181300 |
| C | -0.30891000 | 2.07092100 | 6.68549100 |
| H | 1.52657100 | 2.62748600 | 5.63565300 |
| H | -2.32216400 | 1.66993100 | 7.40337800 |
| H | 0.16741500 | 1.93598600 | 7.65853900 |
| C | 2.42130200 | 1.94824600 | 1.30608500 |
| H | 1.94387600 | 1.60167900 | 2.23817700 |
| H | 3.37902300 | 2.40205400 | 1.59961800 |
| C | 1.56582300 | 0.16624100 | -0.46125900 |
| H | 1.31323300 | 0.81121700 | -1.32009000 |
| H | 1.91276100 | -0.78973700 | -0.87931400 |
| C | 2.71530100 | 0.76631000 | 0.36582900 |
| H | 3.15896600 | -0.02932500 | 0.98367100 |
| H | 3.49602000 | 1.06868100 | -0.34875900 |

**i-4-dppen-trip**

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

Zero-point correction= 0.587464 (Hartree/Particle)
Thermal correction to Energy= 0.626138
Thermal correction to Enthalpy= 0.627082
Thermal correction to Gibbs Free Energy= 0.513225
Sum of electronic and zero-point Energies= -3567.165400
Sum of electronic and thermal Energies= -3567.126725
Sum of electronic and thermal Enthalpies= -3567.125781
Sum of electronic and thermal Free Energies= -3567.239639

| | | | |
|---|---|---|---|
| C | -3.91920400 | 2.39329000 | 0.47392100 |
| O | -2.80001400 | 1.42908600 | 0.22297500 |
| C | -4.87392200 | 2.35184700 | -0.71386600 |
| C | -3.13136400 | 3.70437600 | 0.58580700 |
| C | -4.60504100 | 2.05226300 | 1.78933200 |
| C | -2.95452900 | 0.09657700 | 0.13825500 |
| H | -5.39666000 | 1.38751300 | -0.74636800 |
| H | -5.61315100 | 3.15949900 | -0.61184100 |
| H | -4.33471800 | 2.48896600 | -1.66139600 |
| C | -2.60778000 | 4.36913500 | -0.50198100 |
| H | -3.12741700 | 4.18104300 | 1.57004000 |
| H | -5.35878400 | 2.82456200 | 2.00327200 |
| H | -5.10515500 | 1.07795500 | 1.72923400 |
| H | -3.88049400 | 2.03615400 | 2.61348200 |

| | | | |
|---|---|---|---|
| O | -1.73617300 | -0.43207900 | 0.06341300 |
| O | -3.99808100 | -0.50424400 | 0.12901400 |
| H | -2.18399100 | 5.37142300 | -0.38319800 |
| H | -2.81608700 | 4.05249300 | -1.53015600 |
| C | -1.65094900 | -1.84532200 | -0.16798500 |
| H | -2.13909100 | -2.10458300 | -1.11827200 |
| H | -0.57995700 | -2.07014500 | -0.22119500 |
| H | -2.12254100 | -2.39840800 | 0.65692300 |
| Co | -1.17617500 | 2.93106800 | 0.07504500 |
| P | -0.28679900 | 2.46451400 | 2.19717300 |
| P | 0.65845100 | 1.79847200 | -0.80123900 |
| C | 0.63838200 | 3.78043800 | 3.07738500 |
| C | -1.32593600 | 1.65865800 | 3.47011100 |
| C | 1.01129700 | 1.19668300 | 1.87684300 |
| C | 2.04324000 | 2.85813300 | -1.38525000 |
| C | 0.40836500 | 0.53285100 | -2.09471000 |
| C | 1.40005200 | 0.91144800 | 0.62443700 |
| C | 0.69031400 | 5.05644600 | 2.49391900 |
| C | 1.32811500 | 3.53846300 | 4.27905900 |
| C | -1.65936100 | 0.30083600 | 3.32083700 |
| C | -1.92005100 | 2.40395500 | 4.50270700 |
| H | 1.46714300 | 0.68595600 | 2.73330300 |
| C | 2.65208900 | 3.72370700 | -0.45756200 |
| C | 2.43527000 | 2.90746900 | -2.73248600 |
| C | 1.40100800 | -0.39452600 | -2.45406700 |
| C | -0.84677500 | 0.48298400 | -2.72173600 |
| H | 2.18532500 | 0.17048200 | 0.43629100 |
| C | 1.42774300 | 6.07897000 | 3.10043700 |
| H | 0.15388000 | 5.25022400 | 1.56232000 |
| C | 2.06184300 | 4.56165800 | 4.88261700 |
| H | 1.28881900 | 2.55145700 | 4.74690100 |
| C | -2.57268300 | -0.30054800 | 4.19053200 |
| H | -1.21433500 | -0.28543500 | 2.51448400 |
| C | -2.83246300 | 1.79739900 | 5.37107200 |
| H | -1.67403500 | 3.46081000 | 4.62965500 |
| C | 3.64489100 | 4.61427400 | -0.87083100 |
| H | 2.35246600 | 3.70559600 | 0.59297400 |
| C | 3.42924100 | 3.80350000 | -3.14171200 |
| H | 1.96949700 | 2.24721500 | -3.46699200 |
| C | 1.13333200 | -1.36413800 | -3.42432200 |
| H | 2.38741800 | -0.36108200 | -1.98477200 |
| C | -1.11028800 | -0.48432700 | -3.69513000 |
| H | -1.62269900 | 1.19541700 | -2.43151300 |
| C | 2.11404500 | 5.83168600 | 4.29305000 |
| H | 1.46340800 | 7.06910700 | 2.63994800 |
| H | 2.59662200 | 4.36850800 | 5.81575100 |
| C | -3.16335500 | 0.44649300 | 5.21571700 |
| H | -2.82566300 | -1.35586000 | 4.06285300 |
| H | -3.28871300 | 2.38474400 | 6.17162800 |
| C | 4.03629600 | 4.65631000 | -2.21459500 |
| H | 4.11183700 | 5.27901800 | -0.13987700 |
| H | 3.72954900 | 3.83222000 | -4.19209900 |
| C | -0.12143200 | -1.41055200 | -4.04396600 |
| H | 1.90707900 | -2.08525500 | -3.69835900 |
| H | -2.09072600 | -0.51837300 | -4.17593000 |
| H | 2.69045900 | 6.62973300 | 4.76746800 |
| H | -3.88009600 | -0.02331600 | 5.89346800 |
| H | 4.81274400 | 5.35394300 | -2.53784600 |
| H | -0.32788000 | -2.17125000 | -4.80082900 |

**TS-i-ii-4-dppen-trip**

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

Zero-point correction= 0.584626 (Hartree/Particle)

Thermal correction to Energy= 0.623513

Thermal correction to Enthalpy= 0.624457

Thermal correction to Gibbs Free Energy= 0.507564

Sum of electronic and zero-point Energies= -3567.149459

Sum of electronic and thermal Energies= -3567.110572

Sum of electronic and thermal Enthalpies= -3567.109628

Sum of electronic and thermal Free Energies= -3567.226521

| | | | |
|---|---|---|---|
| C | -3.10462800 | 4.36675400 | 0.73497100 |
| O | -3.05017500 | 2.35064700 | 0.94331700 |
| C | -4.04233400 | 4.42135000 | -0.42582900 |
| C | -1.67994200 | 4.57068000 | 0.54570300 |
| C | -3.66718900 | 4.69038400 | 2.07786000 |
| C | -4.04000400 | 1.53557800 | 0.73647100 |
| H | -5.00434200 | 3.95837800 | -0.17582000 |
| H | -4.21011700 | 5.49009000 | -0.64895200 |
| H | -3.62914100 | 3.94951600 | -1.32577200 |
| C | -1.00854600 | 4.41088900 | -0.67498200 |
| H | -1.13371000 | 4.95304100 | 1.41245200 |
| H | -3.84482200 | 5.78096400 | 2.10737000 |
| H | -4.62352200 | 4.17548600 | 2.23363300 |
| H | -2.96164600 | 4.43880900 | 2.88102400 |
| O | -3.59346300 | 0.33360700 | 0.28004300 |
| O | -5.22063900 | 1.76665900 | 0.92589400 |
| H | 0.01565600 | 4.77886900 | -0.77259800 |
| H | -1.54705300 | 4.28643400 | -1.62013700 |
| C | -4.57702100 | -0.68569200 | 0.08839800 |
| H | -5.32826800 | -0.37102900 | -0.65140800 |
| H | -4.03559000 | -1.56769600 | -0.27569300 |
| H | -5.08568600 | -0.92129000 | 1.03561200 |
| Co | -1.12096500 | 2.53149000 | 0.23520200 |
| P | 0.11472500 | 2.17504700 | 2.22069000 |
| P | 0.74990500 | 1.70976300 | -0.89051900 |
| C | 0.31770400 | 3.59471500 | 3.35397800 |
| C | -0.33458200 | 0.74829200 | 3.27700600 |
| C | 1.82191100 | 1.78020900 | 1.67185600 |
| C | 1.52201900 | 2.66441500 | -2.24527500 |
| C | 0.57908400 | -0.00311800 | -1.51989000 |
| C | 2.08013200 | 1.58012900 | 0.37026000 |
| C | 1.24985700 | 4.60254800 | 3.05113500 |
| C | -0.56527700 | 3.77331300 | 4.43365000 |
| C | 0.33126800 | 0.47542800 | 4.48555400 |
| C | -1.35151000 | -0.11251800 | 2.83221000 |
| H | 2.61331700 | 1.67723200 | 2.42362000 |
| C | 2.43065300 | 3.69505700 | -1.94875700 |
| C | 1.12156700 | 2.45711800 | -3.57646700 |
| C | -0.61685900 | -0.70335000 | -1.28743100 |
| C | 1.64182200 | -0.63890500 | -2.18721800 |
| H | 3.08584200 | 1.30900100 | 0.02796100 |
| C | 1.30658400 | 5.76399300 | 3.82753900 |
| H | 1.93175700 | 4.48593600 | 2.20447800 |
| C | -0.50580000 | 4.93742200 | 5.20462300 |
| H | -1.29928100 | 3.00111300 | 4.67589700 |
| C | -0.01825600 | -0.64807500 | 5.23761600 |
| H | 1.11789200 | 1.14424200 | 4.84389400 |
| C | -1.69637200 | -1.23695200 | 3.58972700 |
| H | -1.88342900 | 0.09330900 | 1.90199200 |
| C | 2.94179500 | 4.49717000 | -2.97363000 |
| H | 2.74362500 | 3.87642200 | -0.91709300 |
| C | 1.63508500 | 3.26246000 | -4.59631000 |
| H | 0.41275200 | 1.66201500 | -3.82027700 |
| C | -0.74370800 | -2.02811500 | -1.71972700 |
| H | -1.45780100 | -0.22729300 | -0.77667700 |
| C | 1.50778000 | -1.96090200 | -2.61563600 |
| H | 2.57283100 | -0.09956400 | -2.37907200 |
| C | 0.42951200 | 5.93427000 | 4.90423100 |
| H | 2.03859800 | 6.53909500 | 3.58810800 |
| H | -1.19398300 | 5.06524700 | 6.04370100 |
| C | -1.03156800 | -1.50585600 | 4.78997900 |
| H | 0.50106000 | -0.85576200 | 6.17635600 |
| H | -2.49066700 | -1.90057700 | 3.23916200 |
| C | 2.54596400 | 4.28246100 | -4.29791000 |
| H | 3.65234900 | 5.29196700 | -2.73435500 |
| H | 1.32266600 | 3.09085700 | -5.62923500 |
| C | 0.31517200 | -2.65716200 | -2.38121700 |
| H | -1.67652800 | -2.56778700 | -1.53944500 |
| H | 2.33597900 | -2.44967800 | -3.13434600 |
| H | 0.47394300 | 6.84347600 | 5.50854000 |

| | | | |
|---|---|---|---|
| H | -1.30341300 | -2.38368000 | 5.38149500 |
| H | 2.94673600 | 4.90981200 | -5.09771600 |
| H | 0.21225300 | -3.69157600 | -2.71819600 |

**ii-4-dppen-trip**

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

Zero-point correction= 0.585677 (Hartree/Particle)
Thermal correction to Energy= 0.625241
Thermal correction to Enthalpy= 0.626186
Thermal correction to Gibbs Free Energy= 0.509491
Sum of electronic and zero-point Energies= -3567.173642
Sum of electronic and thermal Energies= -3567.134077
Sum of electronic and thermal Enthalpies= -3567.133133
Sum of electronic and thermal Free Energies= -3567.249828

| | | | |
|---|---|---|---|
| C | -2.99755700 | 4.12712800 | 1.09065200 |
| O | -2.64053700 | 1.19289000 | 0.45597800 |
| C | -4.09199400 | 3.81353300 | 0.11381600 |
| C | -1.76559700 | 4.70068800 | 0.71809300 |
| C | -3.38470100 | 4.07058600 | 2.53746500 |
| C | -2.81334000 | 0.98684500 | -0.80082600 |
| H | -4.62329900 | 2.89954100 | 0.41359200 |
| H | -4.81855200 | 4.64513500 | 0.14790900 |
| H | -3.74617900 | 3.69567600 | -0.91859700 |
| C | -1.16778700 | 4.54587200 | -0.54242600 |
| H | -1.15030500 | 5.12238200 | 1.51888800 |
| H | -4.25911700 | 4.72091000 | 2.71454700 |
| H | -3.69431100 | 3.04637300 | 2.80196200 |
| H | -2.57118100 | 4.38017100 | 3.20609700 |
| O | -3.50751900 | -0.11166400 | -1.09908100 |
| O | -2.35247600 | 1.74924500 | -1.66890200 |
| H | -0.16667600 | 4.95111300 | -0.70628700 |
| H | -1.74371800 | 4.30480400 | -1.43944400 |
| C | -3.62294700 | -0.44755300 | -2.48742300 |
| H | -2.63093000 | -0.66488900 | -2.91118800 |
| H | -4.25333600 | -1.34384700 | -2.53175800 |
| H | -4.08855300 | 0.37287600 | -3.05282700 |
| Co | -1.26421900 | 2.62268700 | 0.37742300 |
| P | 0.00827700 | 2.33038700 | 2.45600500 |
| P | 0.64451300 | 1.73685300 | -0.68540100 |
| C | 0.37192200 | 3.81253500 | 3.46590400 |
| C | -0.46149800 | 1.00389700 | 3.62218800 |
| C | 1.67872100 | 1.81905500 | 1.87494100 |
| C | 1.30881100 | 2.62952900 | -2.12211700 |
| C | 0.31961800 | 0.00707800 | -1.19873200 |
| C | 1.95134600 | 1.59259400 | 0.57988500 |
| C | 1.21192100 | 4.80329200 | 2.92459200 |
| C | -0.25619600 | 4.03729200 | 4.70236100 |
| C | 0.32785600 | 0.70348400 | 4.74809900 |
| C | -1.62110500 | 0.25551500 | 3.35842200 |
| H | 2.45706400 | 1.67915300 | 2.63431500 |
| C | 2.62246800 | 3.12126300 | -2.17331900 |
| C | 0.42149400 | 2.88221700 | -3.18669700 |
| C | -0.23525400 | -0.85649700 | -0.23696300 |
| C | 0.54158500 | -0.45593000 | -2.50471200 |
| H | 2.94480100 | 1.24631100 | 0.27325500 |
| C | 1.42688500 | 5.99683700 | 3.61814900 |
| H | 1.69778300 | 4.64604600 | 1.95768800 |
| C | -0.03870000 | 5.23534100 | 5.38975000 |
| H | -0.91420500 | 3.27970700 | 5.13291300 |
| C | -0.04415500 | -0.33647400 | 5.60134900 |
| H | 1.22690200 | 1.28539800 | 4.96581800 |
| C | -1.98523000 | -0.78651600 | 4.21905300 |
| H | -2.22941300 | 0.47935400 | 2.47975400 |
| C | 3.04896400 | 3.84822500 | -3.28987900 |
| H | 3.31836900 | 2.94933900 | -1.35021000 |
| C | 0.85965500 | 3.60086900 | -4.30005300 |
| H | -0.60696100 | 2.51646600 | -3.13471800 |
| C | -0.57365500 | -2.16524800 | -0.58343800 |
| H | -0.42587500 | -0.50620200 | 0.77947600 |
| C | 0.20114700 | -1.76905800 | -2.84418700 |
| H | 0.97208200 | 0.20242700 | -3.26092000 |
| C | 0.80163000 | 6.21531800 | 4.85107200 |
| H | 2.08443300 | 6.75847800 | 3.19255100 |
| H | -0.52866900 | 5.40109600 | 6.35211700 |
| C | -1.20057200 | -1.08234600 | 5.33720700 |
| H | 0.56949300 | -0.56639400 | 6.47557600 |
| H | -2.88729800 | -1.36716300 | 4.01197300 |
| C | 2.17273000 | 4.08493800 | -4.35327200 |
| H | 4.07212700 | 4.22948500 | -3.32571000 |
| H | 0.17071600 | 3.78997500 | -5.12657100 |
| C | -0.35956500 | -2.62291500 | -1.88854400 |
| H | -1.01327900 | -2.82552800 | 0.16752400 |
| H | 0.37389600 | -2.12366900 | -3.86303300 |
| H | 0.96964200 | 7.14971100 | 5.39177500 |
| H | -1.48843700 | -1.89601300 | 6.00746800 |
| H | 2.51102000 | 4.65209800 | -5.22374700 |
| H | -0.63101700 | -3.64552700 | -2.16100200 |

**TS-i-vi-4-dppen-trip**

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

Zero-point correction= 0.585440 (Hartree/Particle)
Thermal correction to Energy= 0.624534
Thermal correction to Enthalpy= 0.625478
Thermal correction to Gibbs Free Energy= 0.508686
Sum of electronic and zero-point Energies= -3567.110973
Sum of electronic and thermal Energies= -3567.071879
Sum of electronic and thermal Enthalpies= -3567.070935
Sum of electronic and thermal Free Energies= -3567.187727

| | | | |
|---|---|---|---|
| Co | -1.27092000 | 1.09390200 | 1.40007700 |
| P | -0.36214800 | 1.74699500 | -0.70864600 |
| C | -4.71007200 | 1.38901700 | 0.55843600 |
| C | -5.99150000 | 0.88935800 | 0.26626500 |
| C | -4.57050800 | 2.68774600 | 1.08012500 |
| C | -7.11871700 | 1.67965400 | 0.50419600 |
| H | -6.11416400 | -0.11475100 | -0.14421900 |
| C | -5.70284000 | 3.47242500 | 1.31259300 |
| H | -3.58450300 | 3.10385700 | 1.29994600 |
| C | -6.97671600 | 2.96916500 | 1.02828400 |
| H | -8.11179300 | 1.28503200 | 0.27724700 |
| H | -5.58763200 | 4.47955000 | 1.71965500 |
| H | -7.86084200 | 3.58331900 | 1.21519900 |
| C | -3.66226400 | -1.34476500 | 0.22170600 |
| C | -3.18773100 | -2.21948200 | -0.76979300 |
| C | -4.40507300 | -1.85346200 | 1.30295500 |
| C | -3.46802800 | -3.58688000 | -0.68679600 |
| H | -2.59886300 | -1.84335400 | -1.60935400 |
| C | -4.68324000 | -3.21952200 | 1.37681400 |
| H | -4.77039300 | -1.18487500 | 2.08618500 |
| C | -4.21614500 | -4.08784400 | 0.38267500 |
| H | -3.09971500 | -4.26034800 | -1.46398100 |
| H | -5.26624600 | -3.60717800 | 2.21529200 |
| H | -4.43489200 | -5.15644400 | 0.44389900 |
| C | -0.02121100 | 3.52155500 | -0.95157800 |
| C | 0.23098400 | 4.04686000 | -2.23267200 |
| C | -0.02406900 | 4.37618400 | 0.16328300 |
| C | 0.48047800 | 5.41127600 | -2.38967200 |
| H | 0.24285400 | 3.39447300 | -3.10887400 |
| C | 0.22914800 | 5.74164900 | -0.00078900 |
| H | -0.21975800 | 3.98357000 | 1.16322100 |
| C | 0.48056800 | 6.25898100 | -1.27476700 |
| H | 0.67719300 | 5.81442000 | -3.38568500 |
| H | 0.22863500 | 6.40019200 | 0.87068300 |
| H | 0.67770300 | 7.32616900 | -1.40149900 |
| C | 1.09718400 | 0.82255500 | -1.30704200 |
| C | 0.99187000 | -0.57668900 | -1.41690400 |
| C | 2.33368700 | 1.44685300 | -1.53512800 |
| C | 2.11201500 | -1.33881200 | -1.75135100 |
| H | 0.03997700 | -1.08027900 | -1.23092900 |
| C | 3.45152400 | 0.67659400 | -1.86983900 |
| H | 2.43400100 | 2.52937400 | -1.44074900 |

| | | | |
|---|---|---|---|
| C | 3.34450800 | -0.71364200 | -1.97456500 |
| H | 2.02501600 | -2.42496000 | -1.82303300 |
| H | 4.41209100 | 1.16751800 | -2.04183500 |
| H | 4.22260000 | -1.31211700 | -2.22745200 |
| P | -3.20197400 | 0.41850800 | 0.19780500 |
| C | -1.66905200 | 1.34339200 | -1.92785800 |
| H | -1.47239000 | 1.56960400 | -2.98184800 |
| C | -2.83177900 | 0.79111800 | -1.55502300 |
| H | -3.61090400 | 0.56338700 | -2.29170900 |
| C | 0.61902500 | 1.46321600 | 3.78806300 |
| C | 0.89109200 | 0.65179300 | 2.55998400 |
| H | 1.28663800 | 1.03544600 | 4.55811200 |
| H | 0.90256500 | 2.51565200 | 3.64431300 |
| H | -0.40780000 | 1.40937400 | 4.17065600 |
| C | 0.09887700 | -0.43582300 | 2.15168700 |
| C | -1.22884800 | -0.64736800 | 2.55955900 |
| H | 0.52300300 | -1.08927000 | 1.38467400 |
| H | -1.76408800 | -1.52188700 | 2.18633500 |
| H | -1.62634200 | -0.21295200 | 3.48558600 |
| C | 2.19162300 | 0.92704400 | 1.88422500 |
| H | 2.24473600 | 1.97675100 | 1.55510500 |
| H | 2.99774500 | 0.76990500 | 2.61835500 |
| H | 2.37156900 | 0.26023800 | 1.03577600 |
| O | 2.26964500 | -1.48433700 | 3.82483900 |
| C | 2.83162100 | -1.89933500 | 2.79327600 |
| O | 4.18445200 | -1.50174600 | 2.71044800 |
| C | 4.87768100 | -1.84470700 | 1.52731600 |
| H | 4.84050100 | -2.92830300 | 1.32359500 |
| H | 4.46544400 | -1.32852800 | 0.64187900 |
| H | 5.92567600 | -1.53562000 | 1.66460600 |
| O | 2.37704300 | -2.55695600 | 1.83814700 |

**iv-4-dppen-quart**

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

Zero-point correction= 0.586585 (Hartree/Particle)

Thermal correction to Energy= 0.625979

Thermal correction to Enthalpy= 0.626923

Thermal correction to Gibbs Free Energy= 0.510686

Sum of electronic and zero-point Energies= -3567.110067

Sum of electronic and thermal Energies= -3567.070673

Sum of electronic and thermal Enthalpies= -3567.069728

Sum of electronic and thermal Free Energies= -3567.185965

| | | | |
|---|---|---|---|
| Co | -1.27994200 | 1.08179800 | 1.43264900 |
| P | -0.33230800 | 1.72588600 | -0.66137300 |
| C | -4.69005300 | 1.41019200 | 0.51276200 |
| C | -5.97385200 | 0.92056900 | 0.21339200 |
| C | -4.54087500 | 2.71982600 | 1.00443500 |
| C | -7.09394600 | 1.73071500 | 0.41515400 |
| H | -6.10405900 | -0.09141800 | -0.17464900 |
| C | -5.66636500 | 3.52402600 | 1.20069700 |
| H | -3.55389500 | 3.13093200 | 1.22976400 |
| C | -6.94260900 | 3.03054500 | 0.91003600 |
| H | -8.08860700 | 1.34318500 | 0.18303300 |
| H | -5.54376000 | 4.53926100 | 1.58476900 |
| H | -7.82111800 | 3.66038300 | 1.06908600 |
| C | -3.68263900 | -1.34814600 | 0.26377600 |
| C | -3.19421900 | -2.26057300 | -0.68586800 |
| C | -4.45442400 | -1.81185400 | 1.34510500 |
| C | -3.48904500 | -3.62183600 | -0.56123400 |
| H | -2.58184300 | -1.91898700 | -1.52337200 |
| C | -4.74647500 | -3.17198500 | 1.46056700 |
| H | -4.82925900 | -1.11328500 | 2.09705900 |
| C | -4.26487300 | -4.07857100 | 0.50835800 |
| H | -3.10928800 | -4.32566000 | -1.30527300 |
| H | -5.35075400 | -3.52508700 | 2.29926000 |
| H | -4.49354800 | -5.14266100 | 0.60286600 |
| C | -0.01988200 | 3.50409400 | -0.91655600 |
| C | 0.23600700 | 4.01805800 | -2.20160300 |
| C | -0.05429400 | 4.37262500 | 0.18665900 |
| C | 0.45585800 | 5.38553400 | -2.37436500 |
| H | 0.27342400 | 3.35461100 | -3.06865000 |
| C | 0.16947300 | 5.74133500 | 0.00688200 |
| H | -0.25201800 | 3.98862100 | 1.18939700 |
| C | 0.42297300 | 6.24767100 | -1.27112000 |
| H | 0.65465100 | 5.77966100 | -3.37358600 |
| H | 0.14395000 | 6.41121500 | 0.86926200 |
| H | 0.59609000 | 7.31747800 | -1.41019700 |
| C | 1.13951300 | 0.81932900 | -1.25118400 |
| C | 1.04065800 | -0.57778700 | -1.38078300 |
| C | 2.36903400 | 1.45654200 | -1.48312000 |
| C | 2.15896400 | -1.32671800 | -1.74691700 |
| H | 0.09475700 | -1.08884000 | -1.18487700 |
| C | 3.48407700 | 0.69901900 | -1.85299100 |
| H | 2.46346300 | 2.53792300 | -1.37090000 |
| C | 3.38107800 | -0.68944600 | -1.98562800 |
| H | 2.07919400 | -2.41223100 | -1.82674100 |
| H | 4.43909900 | 1.19820600 | -2.03240300 |
| H | 4.25802200 | -1.27771400 | -2.26527600 |
| P | -3.19340000 | 0.40537300 | 0.19835000 |
| C | -1.61245200 | 1.29321800 | -1.90139000 |
| H | -1.38978900 | 1.50117400 | -2.95396700 |
| C | -2.77965700 | 0.73666000 | -1.55054000 |
| H | -3.53766100 | 0.48879300 | -2.30252800 |
| C | 0.43996800 | 1.52603700 | 3.79116600 |
| C | 0.78759800 | 0.66775300 | 2.60931400 |
| H | 1.14635300 | 1.24793900 | 4.59413000 |
| H | 0.60697100 | 2.59119900 | 3.57158800 |
| H | -0.57521300 | 1.39208700 | 4.18537500 |
| C | 0.05182500 | -0.47057100 | 2.23285300 |
| C | -1.29018900 | -0.67674400 | 2.59100200 |
| H | 0.51240300 | -1.13438000 | 1.49317700 |
| H | -1.81197600 | -1.55290000 | 2.20358800 |
| H | -1.72890200 | -0.23098800 | 3.49262500 |
| C | 2.12216000 | 0.92790900 | 1.99338000 |
| H | 2.23804400 | 1.99012100 | 1.72896400 |
| H | 2.89284300 | 0.68331500 | 2.74382600 |
| H | 2.30261500 | 0.29705200 | 1.11814100 |
| O | 2.17155300 | -1.86312100 | 3.58236100 |
| C | 2.78217000 | -2.02050100 | 2.51066900 |
| O | 4.13847500 | -1.63343000 | 2.58790700 |
| C | 4.89002600 | -1.68603200 | 1.39188700 |
| H | 4.84307500 | -2.67937300 | 0.91426100 |
| H | 4.53913700 | -0.94798500 | 0.64906300 |
| H | 5.93474700 | -1.45768300 | 1.65551900 |
| O | 2.37075200 | -2.41993000 | 1.40246500 |

**i-4-dppp-trip**

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

Zero-point correction= 0.639801 (Hartree/Particle)

Thermal correction to Energy= 0.679960

Thermal correction to Enthalpy= 0.680904

Thermal correction to Gibbs Free Energy= 0.564647

Sum of electronic and zero-point Energies= -3607.638709

Sum of electronic and thermal Energies= -3607.598549

Sum of electronic and thermal Enthalpies= -3607.597605

Sum of electronic and thermal Free Energies= -3607.713863

| | | | |
|---|---|---|---|
| C | -3.67295600 | 3.48913400 | 0.80648600 |
| O | -2.78989800 | 2.77220100 | 1.78407000 |
| C | -4.95927700 | 2.68620000 | 0.64745100 |
| C | -2.78053800 | 3.48662900 | -0.43711400 |
| C | -3.92437400 | 4.91456700 | 1.28049300 |
| C | -3.10324900 | 2.61167200 | 3.07891700 |
| H | -5.54921500 | 2.73018300 | 1.57126500 |
| H | -5.55103000 | 3.10432000 | -0.17927800 |
| H | -4.74093700 | 1.63236800 | 0.42514100 |
| C | -2.75400500 | 2.46086200 | -1.36012400 |
| H | -2.26951700 | 4.42893300 | -0.65465500 |
| H | -4.48277800 | 5.44919800 | 0.49751700 |
| H | -4.51333100 | 4.92648500 | 2.20550100 |
| H | -2.97527400 | 5.43985700 | 1.44882000 |

| | | | |
|---|---|---|---|
| O | -2.05678300 | 2.04308400 | 3.67551600 |
| O | -4.13735900 | 2.92370700 | 3.61329000 |
| H | -2.21544200 | 2.58977500 | -2.30481300 |
| H | -3.45611000 | 1.62161700 | -1.32095900 |
| C | -2.20362000 | 1.71914300 | 5.06593100 |
| H | -1.28049700 | 1.20030200 | 5.34673100 |
| H | -2.33013700 | 2.63573900 | 5.65999000 |
| H | -3.06745800 | 1.05702600 | 5.21433100 |
| Co | -1.36285900 | 1.98943300 | 0.15369700 |
| P | -0.23909100 | 0.00822100 | 0.75585100 |
| P | 0.33123500 | 3.38240000 | 0.99948700 |
| C | -0.22946900 | -1.30249000 | -0.53244700 |
| C | -0.85837400 | -0.80838200 | 2.27001500 |
| C | 1.57504100 | 0.32697000 | 0.98021500 |
| C | 1.75159600 | 3.77906800 | -0.08746200 |
| C | -0.17908300 | 4.99219900 | 1.71215100 |
| C | 1.08135300 | 2.47931600 | 2.44236600 |
| C | -0.39792700 | -0.92403100 | -1.87538200 |
| C | -0.02678600 | -2.65699700 | -0.21858300 |
| C | -2.25133900 | -0.82322800 | 2.46322900 |
| C | -0.02364400 | -1.39228300 | 3.23609500 |
| H | 1.86067900 | 0.72338600 | -0.00790900 |
| H | 2.10259400 | -0.63323300 | 1.08839600 |
| C | 2.01120700 | 1.30343000 | 2.09326600 |
| C | 1.72728400 | 3.32341500 | -1.41532000 |
| C | 2.87232000 | 4.48837900 | 0.37950500 |
| C | -0.63578800 | 5.08697300 | 3.03867500 |
| C | -0.24760000 | 6.12763200 | 0.88475600 |
| H | 0.21459600 | 2.12195300 | 3.01868000 |
| H | 1.62381800 | 3.19377500 | 3.08037400 |
| C | -0.35022000 | -1.88417600 | -2.89070600 |
| H | -0.57014800 | 0.12429100 | -2.13285600 |
| C | 0.01297400 | -3.61527300 | -1.23532800 |
| H | 0.09583300 | -2.96797600 | 0.82170800 |
| C | -2.80169400 | -1.42668200 | 3.59457500 |
| H | -2.90533400 | -0.34697900 | 1.72724900 |
| C | -0.57739900 | -1.98278000 | 4.37811600 |
| H | 1.06047800 | -1.39598800 | 3.10740300 |
| H | 2.17241500 | 0.74028200 | 3.02583200 |
| H | 2.99762100 | 1.69988900 | 1.80390400 |
| C | 2.81001500 | 3.57035100 | -2.26675100 |
| H | 0.85766700 | 2.77280000 | -1.78374600 |
| C | 3.95208700 | 4.73355200 | -0.47146100 |
| H | 2.89994900 | 4.85359400 | 1.40961900 |
| C | -1.14392400 | 6.29479000 | 3.52683800 |
| H | -0.61336800 | 4.21747800 | 3.69672800 |
| C | -0.75548200 | 7.33304000 | 1.37663100 |
| H | 0.10038400 | 6.07211400 | -0.14991800 |
| C | -0.14614600 | -3.23078400 | -2.57189700 |
| H | -0.48041900 | -1.57911900 | -3.93188800 |
| H | 0.16802800 | -4.66704400 | -0.98231500 |
| C | -1.96395200 | -2.00405500 | 4.55690500 |
| H | -3.88532300 | -1.43330300 | 3.73413400 |
| H | 0.07954600 | -2.43029200 | 5.12778900 |
| C | 3.92204700 | 4.27415100 | -1.79496700 |
| H | 2.78261300 | 3.21290300 | -3.29890700 |
| H | 4.82084100 | 5.28449600 | -0.10275100 |
| C | -1.20619400 | 7.42023700 | 2.69891800 |
| H | -1.49699800 | 6.35232200 | 4.55937400 |
| H | -0.80071600 | 8.20755800 | 0.72292600 |
| H | -0.11568300 | -3.98238600 | -3.36463800 |
| H | -2.39321400 | -2.46527200 | 5.44963900 |
| H | 4.76848800 | 4.46764500 | -2.45861800 |
| H | -1.60643500 | 8.36216800 | 3.08148100 |

**TS-i-ii-4-dppp-trip**

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

Zero-point correction= 0.637137 (Hartree/Particle)

Thermal correction to Energy= 0.677484

Thermal correction to Enthalpy= 0.678428

Thermal correction to Gibbs Free Energy= 0.560910

Sum of electronic and zero-point Energies= -3607.624428

Sum of electronic and thermal Energies= -3607.584081

Sum of electronic and thermal Enthalpies= -3607.583137

Sum of electronic and thermal Free Energies= -3607.700655

| | | | |
|---|---|---|---|
| C | -3.75204800 | 3.51460600 | -0.07273100 |
| O | -2.95048400 | 2.43518100 | 1.45804000 |
| C | -5.04140300 | 2.75957600 | -0.09026100 |
| C | -2.70194100 | 3.22333800 | -1.02752000 |
| C | -3.79197000 | 4.88325500 | 0.51837900 |
| C | -3.26693500 | 2.54346000 | 2.70947500 |
| H | -5.55620300 | 2.86263700 | 0.87311500 |
| H | -5.66872900 | 3.20639300 | -0.88277900 |
| H | -4.90568700 | 1.69680900 | -0.32203500 |
| C | -2.49038500 | 1.95243900 | -1.58872000 |
| H | -2.09139000 | 4.07316800 | -1.34796700 |
| H | -4.39927800 | 5.51335400 | -0.15652400 |
| H | -4.28535700 | 4.86705900 | 1.49887400 |
| H | -2.79415800 | 5.32884400 | 0.60319100 |
| O | -2.25398200 | 2.11783800 | 3.50976600 |
| O | -4.31967800 | 2.96677900 | 3.15614800 |
| H | -1.81485800 | 1.84903000 | -2.44405000 |
| H | -3.22590400 | 1.14928000 | -1.47590300 |
| C | -2.51992500 | 2.05648500 | 4.91154500 |
| H | -3.34654000 | 1.36075900 | 5.12007700 |
| H | -1.59797200 | 1.68879500 | 5.37867800 |
| H | -2.77700000 | 3.05078100 | 5.30685600 |
| Co | -1.39940400 | 1.97328900 | 0.15809000 |
| P | -0.23387600 | 0.00137700 | 0.74041400 |
| P | 0.27096900 | 3.45101800 | 0.97983000 |
| C | -0.12255600 | -1.27226500 | -0.57150500 |
| C | -0.88829700 | -0.82481100 | 2.22836000 |
| C | 1.54580200 | 0.41702200 | 1.05821800 |
| C | 1.74185000 | 3.79061100 | -0.05167900 |
| C | -0.28840300 | 5.07820600 | 1.59993700 |
| C | 0.91009600 | 2.56453700 | 2.48411300 |
| C | 0.06234700 | -0.83622200 | -1.89570800 |
| C | -0.20404500 | -2.64733100 | -0.30078200 |
| C | -2.27607800 | -0.76785400 | 2.44383900 |
| C | -0.06797600 | -1.47884000 | 3.16295400 |
| H | 1.86964400 | 0.85000200 | 0.09786400 |
| H | 2.11522100 | -0.51715100 | 1.17978100 |
| C | 1.86370400 | 1.38280100 | 2.21858300 |
| C | 1.74440400 | 3.37523300 | -1.39313900 |
| C | 2.87860700 | 4.42700400 | 0.47796500 |
| C | -0.96767500 | 5.16950200 | 2.82799100 |
| C | -0.17706600 | 6.22198700 | 0.78971200 |
| H | -0.00149100 | 2.21962200 | 2.99592000 |
| H | 1.40152600 | 3.28894200 | 3.15153800 |
| C | 0.18063900 | -1.76478400 | -2.93252500 |
| H | 0.11176800 | 0.23274000 | -2.11969400 |
| C | -0.09521500 | -3.57305500 | -1.34368100 |
| H | -0.35403500 | -2.99911800 | 0.72221500 |
| C | -2.83802200 | -1.36599600 | 3.57298800 |
| H | -2.91192100 | -0.23303100 | 1.73458600 |
| C | -0.63357400 | -2.06690000 | 4.29883300 |
| H | 1.01202600 | -1.53759700 | 3.01269700 |
| H | 1.92536700 | 0.80955400 | 3.15693200 |
| H | 2.87629500 | 1.77510800 | 2.03299700 |
| C | 2.86996200 | 3.59018400 | -2.19577200 |
| H | 0.86561600 | 2.88096900 | -1.81386100 |
| C | 4.00123200 | 4.63901100 | -0.32500300 |
| H | 2.88709200 | 4.76078700 | 1.51883300 |
| C | -1.52124600 | 6.38573000 | 3.23730400 |
| H | -1.08330400 | 4.29006600 | 3.46238700 |
| C | -0.73402600 | 7.43530000 | 1.20374100 |
| H | 0.34333300 | 6.16680400 | -0.16937900 |
| C | 0.09954200 | -3.13504100 | -2.65783900 |
| H | 0.32731000 | -1.41702300 | -3.95789400 |
| H | -0.16263100 | -4.64182800 | -1.12616200 |

| | | | |
|---|---|---|---|
| C | -2.01661700 | -2.01224400 | 4.50397700 |
| H | -3.91733300 | -1.31424900 | 3.73425300 |
| H | 0.00953100 | -2.57022100 | 5.02466600 |
| C | 3.99803800 | 4.22012100 | -1.66191700 |
| H | 2.86339500 | 3.26411400 | -3.23848700 |
| H | 4.88233500 | 5.13230600 | 0.09241400 |
| C | -1.40905800 | 7.52023900 | 2.42661400 |
| H | -2.04846600 | 6.44270700 | 4.19266500 |
| H | -0.64085100 | 8.31776100 | 0.56605300 |
| H | 0.18355600 | -3.86147100 | -3.46983000 |
| H | -2.45466900 | -2.47057000 | 5.39401000 |
| H | 4.87822200 | 4.38700100 | -2.28769900 |
| H | -1.84695100 | 8.46878600 | 2.74643700 |

**ii-4-dppp-trip**

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

Zero-point correction= 0.638964 (Hartree/Particle)
Thermal correction to Energy= 0.679722
Thermal correction to Enthalpy= 0.680666
Thermal correction to Gibbs Free Energy= 0.562379
Sum of electronic and zero-point Energies= -3607.647442
Sum of electronic and thermal Energies= -3607.606683
Sum of electronic and thermal Enthalpies= -3607.605739
Sum of electronic and thermal Free Energies= -3607.724026

| | | | |
|---|---|---|---|
| C | -2.85654900 | 3.35187600 | -0.82002100 |
| O | -2.19707600 | 2.25048000 | 2.36486100 |
| C | -3.72556400 | 3.98167400 | 0.23922000 |
| C | -2.88453200 | 1.97800300 | -1.13219900 |
| C | -2.22525200 | 4.31949900 | -1.78282700 |
| C | -3.21521500 | 1.94917700 | 3.08695900 |
| H | -3.14888100 | 4.70089700 | 0.84055300 |
| H | -4.51566200 | 4.55690500 | -0.27563200 |
| H | -4.20066000 | 3.26071800 | 0.91339500 |
| C | -3.25687500 | 0.97075500 | -0.22514000 |
| H | -2.35481300 | 1.66895100 | -2.04158400 |
| H | -3.02286300 | 4.82427100 | -2.35622100 |
| H | -1.67700600 | 5.10861800 | -1.24630000 |
| H | -1.54925400 | 3.82830300 | -2.49502200 |
| O | -2.92871000 | 2.07590800 | 4.40850400 |
| O | -4.32792100 | 1.59607400 | 2.70398800 |
| H | -3.10574200 | -0.06890800 | -0.52368500 |
| H | -3.94518200 | 1.15196500 | 0.60530100 |
| C | -3.97691300 | 1.75822600 | 5.32180700 |
| H | -4.27372300 | 0.70165500 | 5.22858500 |
| H | -3.57784700 | 1.94466600 | 6.32711700 |
| H | -4.86272900 | 2.38811100 | 5.14620600 |
| Co | -1.54254300 | 2.07990700 | 0.53264300 |
| P | -0.23078700 | 0.11992300 | 0.81603800 |
| P | 0.16953000 | 3.56633900 | 1.13521400 |
| C | -0.21940000 | -1.01481200 | -0.61649500 |
| C | -0.67999400 | -0.86166800 | 2.28597000 |
| C | 1.54505200 | 0.61486700 | 1.00000300 |
| C | 1.52092700 | 3.97798100 | -0.01646400 |
| C | -0.47471900 | 5.14491500 | 1.78639900 |
| C | 0.95751300 | 2.68256800 | 2.56162200 |
| C | -0.01680800 | -0.46212500 | -1.89445000 |
| C | -0.43254900 | -2.39581700 | -0.48358800 |
| C | -2.03473000 | -0.95921600 | 2.64741200 |
| C | 0.29094800 | -1.51158400 | 3.06783300 |
| H | 1.77106900 | 1.10692500 | 0.04101500 |
| H | 2.16376700 | -0.29498200 | 1.02429900 |
| C | 1.91734700 | 1.53569400 | 2.18162900 |
| C | 1.43297200 | 3.59604300 | -1.36426900 |
| C | 2.67237100 | 4.64313800 | 0.44278800 |
| C | -1.23420800 | 5.15252400 | 2.97254600 |
| C | -0.31674900 | 6.33652900 | 1.05627700 |
| H | 0.09942900 | 2.30765800 | 3.13996200 |
| H | 1.48541500 | 3.41437300 | 3.19130600 |
| C | -0.01164900 | -1.28482100 | -3.02265500 |
| H | 0.13883800 | 0.61295100 | -2.01371500 |
| C | -0.43398900 | -3.21367100 | -1.61848700 |
| H | -0.59757700 | -2.83547900 | 0.50215000 |
| C | -2.41260000 | -1.69053100 | 3.77495800 |
| H | -2.79972000 | -0.45523800 | 2.05772800 |
| C | -0.09209900 | -2.24041100 | 4.19791100 |
| H | 1.34860500 | -1.46104300 | 2.80358100 |
| H | 2.05499400 | 0.92496700 | 3.08731400 |
| H | 2.90582800 | 1.95996400 | 1.94572400 |
| C | 2.48290300 | 3.87309500 | -2.24521600 |
| H | 0.54450700 | 3.07632000 | -1.72738900 |
| C | 3.71918000 | 4.91757700 | -0.43936400 |
| H | 2.75272000 | 4.95017400 | 1.48851400 |
| C | -1.81032400 | 6.34317600 | 3.42180800 |
| H | -1.39926500 | 4.23003500 | 3.53025700 |
| C | -0.90287200 | 7.52149800 | 1.51150200 |
| H | 0.26997100 | 6.34692500 | 0.13534500 |
| C | -0.22207200 | -2.66218500 | -2.88601200 |
| H | 0.15069600 | -0.84787100 | -4.01067400 |
| H | -0.60070100 | -4.28789700 | -1.50864500 |
| C | -1.44172300 | -2.32882400 | 4.55455600 |
| H | -3.46867700 | -1.75361200 | 4.04745100 |
| H | 0.66939300 | -2.73972800 | 4.80145500 |
| C | 3.62560000 | 4.53265100 | -1.78286400 |
| H | 2.40630200 | 3.57091700 | -3.29204800 |
| H | 4.61211200 | 5.43241000 | -0.07722900 |
| C | -1.64868300 | 7.52797600 | 2.69424600 |
| H | -2.39551400 | 6.34215700 | 4.34460200 |
| H | -0.77219400 | 8.44239400 | 0.93830000 |
| H | -0.22405400 | -3.30487500 | -3.76961100 |
| H | -1.73684100 | -2.89478700 | 5.44137200 |
| H | 4.44764200 | 4.74774700 | -2.46977100 |
| H | -2.10530200 | 8.45523600 | 3.04866100 |

**TS-i-vi-4-dppp-trip**

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

Zero-point correction= 0.636690 (Hartree/Particle)
Thermal correction to Energy= 0.677800
Thermal correction to Enthalpy= 0.678744
Thermal correction to Gibbs Free Energy= 0.556237
Sum of electronic and zero-point Energies= -3607.591193
Sum of electronic and thermal Energies= -3607.550083
Sum of electronic and thermal Enthalpies= -3607.549139
Sum of electronic and thermal Free Energies= -3607.671646

| | | | |
|---|---|---|---|
| P | -0.40092400 | 0.44809500 | 0.36189800 |
| P | 1.53386600 | 3.05856900 | 1.49888800 |
| C | -1.54995300 | 0.10044200 | -1.01416600 |
| C | -1.54815000 | 0.97019400 | -2.12109900 |
| C | -2.51659400 | -0.91379000 | -0.93032900 |
| C | -2.49408200 | 0.81283600 | -3.13627800 |
| H | -0.81798700 | 1.78066600 | -2.19215000 |
| C | -3.46268400 | -1.06299700 | -1.94999100 |
| H | -2.53886900 | -1.58600100 | -0.07035400 |
| C | -3.45388100 | -0.20277600 | -3.05165400 |
| H | -2.48583700 | 1.49156300 | -3.99217700 |
| H | -4.21244900 | -1.85417400 | -1.87704500 |
| H | -4.19841500 | -0.31859900 | -3.84261600 |
| C | -0.39481300 | -0.98724900 | 1.48195400 |
| C | -0.80258800 | -0.83952300 | 2.81795500 |
| C | 0.05529500 | -2.24029900 | 1.02566200 |
| C | -0.76350900 | -1.93407200 | 3.68738900 |
| H | -1.15166700 | 0.12610400 | 3.18980900 |
| C | 0.09135300 | -3.32932300 | 1.89826100 |
| H | 0.37376000 | -2.37178300 | -0.01125300 |
| C | -0.31723100 | -3.17697800 | 3.22904300 |
| H | -1.08205300 | -1.81213800 | 4.72502500 |
| H | 0.44043100 | -4.29995100 | 1.53860400 |
| H | -0.28609200 | -4.03100200 | 3.90981400 |
| C | 2.31303400 | 3.83971800 | 0.05017800 |
| C | 1.49055000 | 4.50562300 | -0.87409700 |
| C | 3.69815200 | 3.76351200 | -0.18216800 |

| | | | |
|---|---|---|---|
| C | 2.04483000 | 5.09550800 | -2.01306200 |
| H | 0.41336600 | 4.55634600 | -0.70536200 |
| C | 4.24783700 | 4.35297200 | -1.32352600 |
| H | 4.35365200 | 3.24719200 | 0.52292000 |
| C | 3.42325200 | 5.01888300 | -2.23809400 |
| H | 1.39759100 | 5.61038500 | -2.72670600 |
| H | 5.32408000 | 4.29034900 | -1.50007500 |
| H | 3.85711200 | 5.47592700 | -3.13071300 |
| C | 1.93058600 | 4.05320900 | 2.98113300 |
| C | 1.26500900 | 3.73028500 | 4.17871000 |
| C | 2.84124300 | 5.12132700 | 2.95949300 |
| C | 1.52791500 | 4.45413100 | 5.34372200 |
| H | 0.53614700 | 2.91478900 | 4.20599100 |
| C | 3.09296700 | 5.84780900 | 4.12795200 |
| H | 3.35480700 | 5.39175900 | 2.03487200 |
| C | 2.44156800 | 5.51454600 | 5.31970000 |
| H | 1.01095200 | 4.19472600 | 6.27061000 |
| H | 3.80219600 | 6.67864100 | 4.10380100 |
| H | 2.64094400 | 6.08492200 | 6.23010900 |
| C | 2.41215400 | 1.44544200 | 1.76064600 |
| H | 1.85557900 | 0.96982500 | 2.58432500 |
| H | 3.42530300 | 1.64293000 | 2.14112200 |
| C | 1.27460800 | 0.49306800 | -0.42761600 |
| H | 1.26510100 | 1.39484300 | -1.06008200 |
| H | 1.35581300 | -0.36728800 | -1.10905200 |
| C | 2.47915900 | 0.51433900 | 0.53186500 |
| H | 2.66161800 | -0.50597000 | 0.90380800 |
| H | 3.35807100 | 0.78355900 | -0.07417100 |
| Co | -0.78730400 | 2.55140200 | 1.35508900 |
| C | -2.79894600 | 1.99573300 | 1.32285700 |
| C | -2.70376100 | 3.30694500 | 1.84768100 |
| H | -3.04854800 | 1.18122100 | 2.00659400 |
| H | -3.10427200 | 1.83834800 | 0.28741700 |
| C | -2.57720600 | 4.46568600 | 1.06537200 |
| H | -2.75899800 | 3.43864300 | 2.93308000 |
| C | -2.54608200 | 4.47259700 | -0.42964800 |
| C | -2.38864100 | 5.78593100 | 1.73099900 |
| H | -3.52242000 | 4.86329500 | -0.75455500 |
| H | -2.41668200 | 3.48411000 | -0.88501300 |
| H | -2.61808300 | 5.75313800 | 2.80363200 |
| H | -1.33964800 | 6.10511100 | 1.59878100 |
| H | -3.02233500 | 6.53748600 | 1.23845700 |
| H | -1.76486200 | 5.15614400 | -0.79392100 |
| H | -5.72829100 | 1.87091600 | -2.00324600 |
| C | -5.79914800 | 1.92631400 | -0.90666100 |
| O | -5.43068800 | 3.24006500 | -0.53294600 |
| H | -6.82809600 | 1.68180000 | -0.59166800 |
| H | -5.12997700 | 1.16394100 | -0.47213900 |
| C | -5.49369000 | 3.55598300 | 0.84024400 |
| O | -5.16275000 | 4.73885500 | 1.07734600 |
| O | -5.81143900 | 2.64544900 | 1.61965900 |

**vi-4-dppp-quart**

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

Zero-point correction= 0.637639 (Hartree/Particle)

Thermal correction to Energy= 0.679202

Thermal correction to Enthalpy= 0.680146

Thermal correction to Gibbs Free Energy= 0.557729

Sum of electronic and zero-point Energies= -3607.590561

Sum of electronic and thermal Energies= -3607.548998

Sum of electronic and thermal Enthalpies= -3607.548054

Sum of electronic and thermal Free Energies= -3607.670471

| | | | |
|---|---|---|---|
| P | -0.42535300 | 0.44462100 | 0.36451800 |
| P | 1.52674400 | 3.07822700 | 1.49106100 |
| C | -1.58465000 | 0.10238500 | -1.00344100 |
| C | -1.59827000 | 0.97929400 | -2.10466500 |
| C | -2.53047400 | -0.93170900 | -0.92642900 |
| C | -2.53911800 | 0.80872100 | -3.12215800 |
| H | -0.88279800 | 1.80312600 | -2.17101000 |
| C | -3.47080200 | -1.09429000 | -1.94926700 |
| H | -2.53964700 | -1.60995500 | -0.07101700 |
| C | -3.47699700 | -0.22774000 | -3.04577000 |
| H | -2.54382100 | 1.49298000 | -3.97359400 |
| H | -4.20440700 | -1.90094800 | -1.88258800 |
| H | -4.21732000 | -0.35421000 | -3.83900200 |
| C | -0.40758000 | -0.99072300 | 1.48244500 |
| C | -0.84090800 | -0.85837100 | 2.81207700 |
| C | 0.07408400 | -2.23221600 | 1.02614100 |
| C | -0.79549700 | -1.95761300 | 3.67518700 |
| H | -1.21483400 | 0.09766300 | 3.18435700 |
| C | 0.11619900 | -3.32550400 | 1.89293000 |
| H | 0.41243900 | -2.35231300 | -0.00575400 |
| C | -0.31764300 | -3.18893300 | 3.21730900 |
| H | -1.13369100 | -1.84828100 | 4.70795000 |
| H | 0.48982700 | -4.28697200 | 1.53342500 |
| H | -0.28141300 | -4.04627600 | 3.89359700 |
| C | 2.30604400 | 3.85332800 | 0.04068500 |
| C | 1.48868700 | 4.50627300 | -0.89696900 |
| C | 3.69434600 | 3.78499300 | -0.17609500 |
| C | 2.05111900 | 5.09157400 | -2.03427200 |
| H | 0.40981100 | 4.55082000 | -0.74177900 |
| C | 4.25183500 | 4.37041800 | -1.31554800 |
| H | 4.34614200 | 3.27897300 | 0.53981700 |
| C | 3.43229900 | 5.02374800 | -2.24368600 |
| H | 1.40767300 | 5.59640600 | -2.75837600 |
| H | 5.33033100 | 4.31459200 | -1.47991900 |
| H | 3.87243700 | 5.47793500 | -3.13465800 |
| C | 1.92297400 | 4.06923700 | 2.97430500 |
| C | 1.27528600 | 3.73084800 | 4.17749100 |
| C | 2.81759300 | 5.15064100 | 2.94663800 |
| C | 1.54091200 | 4.45348900 | 5.34250800 |
| H | 0.55837700 | 2.90509000 | 4.21015800 |
| C | 3.07239800 | 5.87481300 | 4.11580700 |
| H | 3.31651800 | 5.43289800 | 2.01763500 |
| C | 2.43952800 | 5.52658800 | 5.31314700 |
| H | 1.03842700 | 4.18238700 | 6.27394400 |
| H | 3.76971300 | 6.71548400 | 4.08762600 |
| H | 2.64168000 | 6.09503300 | 6.22411300 |
| C | 2.39012200 | 1.45631000 | 1.74779900 |
| H | 1.83039300 | 0.97914300 | 2.56843700 |
| H | 3.40376400 | 1.64693500 | 2.13050600 |
| C | 1.24356600 | 0.50653800 | -0.43643700 |
| H | 1.22157000 | 1.41100700 | -1.06476900 |
| H | 1.32587300 | -0.34933500 | -1.12331000 |
| C | 2.45512200 | 0.53233700 | 0.51399300 |
| H | 2.64817600 | -0.48804800 | 0.88016700 |
| H | 3.32731200 | 0.81113900 | -0.09733000 |
| Co | -0.79636100 | 2.56497000 | 1.37051200 |
| C | -2.85215500 | 2.02890700 | 1.35331100 |
| C | -2.70618400 | 3.32842800 | 1.88274400 |
| H | -3.11624000 | 1.21285300 | 2.02872200 |
| H | -3.13222200 | 1.88224600 | 0.30955600 |
| C | -2.38788400 | 4.45245500 | 1.10789300 |
| H | -2.74037300 | 3.45563300 | 2.97010100 |
| C | -2.47707200 | 4.48797200 | -0.38519500 |
| C | -2.11933900 | 5.75430700 | 1.78698900 |
| H | -3.49485800 | 4.85874900 | -0.59829300 |
| H | -2.38625700 | 3.50925700 | -0.87117200 |
| H | -1.96631200 | 5.64394300 | 2.86868600 |
| H | -1.25308100 | 6.26560400 | 1.34055500 |
| H | -3.00409100 | 6.39296500 | 1.61657800 |
| H | -1.74621700 | 5.18673600 | -0.81407400 |
| H | -5.62923600 | 1.75353200 | -2.04582900 |
| C | -5.73944400 | 1.84354300 | -0.95460500 |
| O | -5.39151700 | 3.16886500 | -0.60897100 |
| H | -6.77792800 | 1.60087400 | -0.66942500 |
| H | -5.08387400 | 1.09570100 | -0.47565100 |
| C | -5.52985100 | 3.53429100 | 0.75405100 |
| O | -5.26540700 | 4.73446800 | 0.95817500 |
| O | -5.84794100 | 2.63137600 | 1.54624500 |

**i-4-dppen-sing**

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

Zero-point correction= 0.587352 (Hartree/Particle)

Thermal correction to Energy= 0.625418

Thermal correction to Enthalpy= 0.626362

Thermal correction to Gibbs Free Energy= 0.515879

Sum of electronic and zero-point Energies= -3567.132234

Sum of electronic and thermal Energies= -3567.094169

Sum of electronic and thermal Enthalpies= -3567.093224

Sum of electronic and thermal Free Energies= -3567.203707

| | | | |
|---|---|---|---|
| Co | -1.33011900 | 2.27777900 | 0.31254300 |
| P | -0.14114200 | 0.29790400 | 0.64390300 |
| P | 0.54173600 | 3.48953700 | 0.48005800 |
| C | -0.47775500 | -1.00800600 | -0.60222400 |
| C | -1.12376700 | -0.66052100 | -1.79818000 |
| C | -0.07008500 | -2.33805600 | -0.39720400 |
| C | -1.35541700 | -1.62639400 | -2.78307900 |
| H | -1.44891200 | 0.36896300 | -1.95298200 |
| C | -0.30363200 | -3.30101300 | -1.38130700 |
| H | 0.42283600 | -2.62517200 | 0.53513500 |
| C | -0.94538400 | -2.94654300 | -2.57524900 |
| H | -1.86067100 | -1.34534500 | -3.71012600 |
| H | 0.01448500 | -4.33329800 | -1.21612100 |
| H | -1.12822700 | -3.70344700 | -3.34198300 |
| C | -0.52640700 | -0.52616300 | 2.23606900 |
| C | -1.81035200 | -1.07909800 | 2.39828000 |
| C | 0.36801800 | -0.54892100 | 3.31830200 |
| C | -2.19346500 | -1.63496500 | 3.61963800 |
| H | -2.51666800 | -1.07455500 | 1.56386200 |
| C | -0.01755100 | -1.11079700 | 4.54073200 |
| H | 1.37124900 | -0.13276000 | 3.22312300 |
| C | -1.29781200 | -1.65037300 | 4.69591900 |
| H | -3.19689300 | -2.05146600 | 3.73275600 |
| H | 0.68866300 | -1.12320400 | 5.37420300 |
| H | -1.59817000 | -2.08354900 | 5.65280600 |
| C | 1.63715900 | 3.64929400 | -0.97920300 |
| C | 1.43498200 | 2.80179100 | -2.08012700 |
| C | 2.70820700 | 4.55999400 | -0.99444500 |
| C | 2.29445900 | 2.85788600 | -3.18155700 |
| H | 0.60128900 | 2.09707200 | -2.07315700 |
| C | 3.56379300 | 4.61567100 | -2.09706000 |
| H | 2.87200500 | 5.23096900 | -0.14749000 |
| C | 3.35868400 | 3.76470200 | -3.19054800 |
| H | 2.12834000 | 2.19401700 | -4.03308700 |
| H | 4.39424400 | 5.32572600 | -2.10363300 |
| H | 4.02954800 | 3.81181700 | -4.05182800 |
| C | 0.19124500 | 5.20454000 | 1.01375100 |
| C | -0.13373300 | 6.17426000 | 0.04754500 |
| C | 0.09979000 | 5.53812900 | 2.37580700 |
| C | -0.53643400 | 7.45337700 | 0.43854200 |
| H | -0.06614600 | 5.93434600 | -1.01649400 |
| C | -0.30406300 | 6.81968400 | 2.76294300 |
| H | 0.34270000 | 4.80569200 | 3.14809800 |
| C | -0.62428200 | 7.77884500 | 1.79704300 |
| H | -0.78148700 | 8.19887600 | -0.32174100 |
| H | -0.36677600 | 7.06733200 | 3.82528900 |
| H | -0.94027000 | 8.77939800 | 2.10175700 |
| C | 1.62821100 | 2.76698300 | 1.79721900 |
| H | 0.95296700 | 2.49981400 | 2.62569600 |
| H | 2.31270200 | 3.54211700 | 2.17343100 |
| C | 1.70920700 | 0.43115300 | 0.54735000 |
| H | 1.87060900 | 0.58796000 | -0.52963300 |
| H | 2.13705600 | -0.55604300 | 0.77853900 |
| C | 2.43789400 | 1.53750700 | 1.35049900 |
| H | 2.88376400 | 1.10106500 | 2.25723200 |
| H | 3.28587700 | 1.88061200 | 0.73808400 |
| C | -3.93970100 | 2.95307400 | 0.15346000 |
| O | -3.36069000 | 1.65694400 | 0.83687800 |
| C | -4.89471000 | 2.38489900 | -0.87788200 |
| C | -2.69326000 | 3.62023600 | -0.38399600 |
| C | -4.63850700 | 3.80919400 | 1.19307600 |
| C | -3.30166000 | 1.65302400 | 2.19071900 |
| H | -5.73734900 | 1.88274400 | -0.38120600 |
| H | -5.28198600 | 3.20451100 | -1.50146100 |
| H | -4.39011900 | 1.65783000 | -1.52778400 |
| C | -1.97405200 | 3.07435900 | -1.45506200 |
| H | -2.51221600 | 4.64899200 | -0.05697000 |
| H | -5.07061200 | 4.67816600 | 0.67527100 |
| H | -5.44947600 | 3.26259200 | 1.69249500 |
| H | -3.92986100 | 4.18862000 | 1.94383500 |
| O | -2.14517100 | 2.23225600 | 2.55547300 |
| O | -4.12737300 | 1.20156900 | 2.92851500 |
| H | -1.24091600 | 3.69238600 | -1.98024600 |
| H | -2.39103800 | 2.26470400 | -2.06363900 |
| C | -1.84508200 | 2.26786700 | 3.96780700 |
| H | -1.71151400 | 1.24412000 | 4.34058500 |
| H | -0.91686800 | 2.83872200 | 4.06567800 |
| H | -2.66229600 | 2.76717300 | 4.50448800 |

**TS-i-ii-4-dppen-sing**

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

Zero-point correction= 0.587088 (Hartree/Particle)

Thermal correction to Energy= 0.624444

Thermal correction to Enthalpy= 0.625388

Thermal correction to Gibbs Free Energy= 0.516746

Sum of electronic and zero-point Energies= -3567.131854

Sum of electronic and thermal Energies= -3567.094498

Sum of electronic and thermal Enthalpies= -3567.093553

Sum of electronic and thermal Free Energies= -3567.202195

| | | | |
|---|---|---|---|
| Co | -1.36970800 | 2.32005400 | 0.46488200 |
| P | -0.16528000 | 0.35850600 | 0.66761400 |
| P | 0.49080200 | 3.50289800 | 0.50113500 |
| C | -0.43567400 | -0.88363900 | -0.65833400 |
| C | -1.09102900 | -0.51044800 | -1.84050900 |
| C | 0.04071500 | -2.19975600 | -0.51823000 |
| C | -1.26392000 | -1.43567500 | -2.87569500 |
| H | -1.47150300 | 0.50480800 | -1.94519000 |
| C | -0.13268700 | -3.12141900 | -1.55257100 |
| H | 0.54062500 | -2.50937600 | 0.40303000 |
| C | -0.78414700 | -2.74054600 | -2.73310400 |
| H | -1.77776800 | -1.13407400 | -3.79146300 |
| H | 0.23978100 | -4.14219600 | -1.43705100 |
| H | -0.91982200 | -3.46511700 | -3.53980100 |
| C | -0.60201800 | -0.56516100 | 2.19089300 |
| C | -1.85657000 | -1.19888400 | 2.25114900 |
| C | 0.23388900 | -0.59412400 | 3.31984400 |
| C | -2.26780000 | -1.84361600 | 3.41894200 |
| H | -2.51817200 | -1.18264400 | 1.38175400 |
| C | -0.18006100 | -1.24494700 | 4.48692300 |
| H | 1.21227700 | -0.11279600 | 3.30346600 |
| C | -1.43113700 | -1.86768200 | 4.54026900 |
| H | -3.24801300 | -2.32453100 | 3.45398700 |
| H | 0.48044800 | -1.26295800 | 5.35700000 |
| H | -1.75342500 | -2.37215600 | 5.45423100 |
| C | 1.58876600 | 3.54597400 | -0.96396700 |
| C | 1.35350100 | 2.68134300 | -2.04441500 |
| C | 2.70595800 | 4.39959200 | -0.99077400 |
| C | 2.22543300 | 2.66527700 | -3.13709600 |
| H | 0.48941600 | 2.01549300 | -2.02941800 |
| C | 3.57421900 | 4.38234600 | -2.08454900 |
| H | 2.89705700 | 5.08283100 | -0.15940100 |
| C | 3.33539700 | 3.51525300 | -3.15806700 |
| H | 2.03361000 | 1.98762400 | -3.97213000 |
| H | 4.44069800 | 5.04767100 | -2.09921200 |
| H | 4.01625400 | 3.50448000 | -4.01264700 |
| C | 0.16358100 | 5.25545100 | 0.90894400 |
| C | -0.09206200 | 6.17404200 | -0.12488900 |
| C | 0.02353300 | 5.66843600 | 2.24483200 |
| C | -0.47744500 | 7.48296600 | 0.17512800 |

| | | | |
|---|---|---|---|
| H | 0.01610700 | 5.87184500 | -1.16924100 |
| C | -0.36095200 | 6.97950100 | 2.54033600 |
| H | 0.21441000 | 4.97591900 | 3.06677000 |
| C | -0.61440300 | 7.88809800 | 1.50758300 |
| H | -0.66973100 | 8.18902600 | -0.63617700 |
| H | -0.46159000 | 7.29024400 | 3.58290800 |
| H | -0.91628000 | 8.91197400 | 1.74061900 |
| C | 1.55390900 | 2.84754700 | 1.86981600 |
| H | 0.86216700 | 2.61847600 | 2.69518900 |
| H | 2.22641700 | 3.64402800 | 2.22161900 |
| C | 1.68845200 | 0.49338800 | 0.66147900 |
| H | 1.90801900 | 0.64698800 | -0.40490400 |
| H | 2.10270500 | -0.49299600 | 0.91834200 |
| C | 2.37647000 | 1.60127500 | 1.49626300 |
| H | 2.75848800 | 1.17545800 | 2.43651500 |
| H | 3.26471400 | 1.92545600 | 0.93295700 |
| C | -3.94318600 | 3.03262200 | 0.26178200 |
| O | -3.24392500 | 1.54445100 | 0.99115100 |
| C | -4.88423900 | 2.35459900 | -0.69490200 |
| C | -2.70619400 | 3.65177000 | -0.24703700 |
| C | -4.60760400 | 3.78281200 | 1.38255600 |
| C | -3.17605100 | 1.58573700 | 2.31885300 |
| H | -5.66933800 | 1.81030200 | -0.15304300 |
| H | -5.35473500 | 3.13705300 | -1.31326900 |
| H | -4.36008700 | 1.65774300 | -1.35984700 |
| C | -1.96782700 | 3.05816600 | -1.30298700 |
| H | -2.51282100 | 4.67839600 | 0.07881500 |
| H | -5.13105200 | 4.63919300 | 0.92702500 |
| H | -5.35014600 | 3.16842400 | 1.90773400 |
| H | -3.87282800 | 4.18128800 | 2.09566800 |
| O | -2.04005700 | 2.25771900 | 2.65111800 |
| O | -3.96662800 | 1.14366100 | 3.10637000 |
| H | -1.25041900 | 3.67506700 | -1.85151800 |
| H | -2.42270200 | 2.28054000 | -1.92546800 |
| C | -1.71991100 | 2.38565100 | 4.05040600 |
| H | -1.35712300 | 1.42252400 | 4.43390900 |
| H | -0.93623900 | 3.14707400 | 4.11834300 |
| H | -2.61186400 | 2.70478900 | 4.60448800 |

**ii-4-dppen-sing**

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

Zero-point correction= 0.589540 (Hartree/Particle)
Thermal correction to Energy= 0.627578
Thermal correction to Enthalpy= 0.628523
Thermal correction to Gibbs Free Energy= 0.517889
Sum of electronic and zero-point Energies= -3567.168964
Sum of electronic and thermal Energies= -3567.130926
Sum of electronic and thermal Enthalpies= -3567.129981
Sum of electronic and thermal Free Energies= -3567.240616

| | | | |
|---|---|---|---|
| Co | -1.51501100 | 2.09261300 | 0.42534700 |
| P | -0.21889600 | 0.22306000 | 0.56156200 |
| P | 0.32510200 | 3.41627300 | 0.47483400 |
| C | -0.42327900 | -1.06645300 | -0.72669000 |
| C | -0.93472000 | -0.75556600 | -1.99473400 |
| C | 0.02546700 | -2.37583400 | -0.46763200 |
| C | -1.00190600 | -1.73619000 | -2.98991000 |
| H | -1.28527200 | 0.24948100 | -2.21251000 |
| C | -0.04456800 | -3.35197500 | -1.46308900 |
| H | 0.42423300 | -2.64017900 | 0.51412000 |
| C | -0.55902600 | -3.03474800 | -2.72598100 |
| H | -1.40533700 | -1.47986300 | -3.97215100 |
| H | 0.30389900 | -4.36537600 | -1.25041800 |
| H | -0.61442300 | -3.80152200 | -3.50242800 |
| C | -0.58958300 | -0.64082200 | 2.13563600 |
| C | -1.70148000 | -1.49933500 | 2.20482500 |
| C | 0.16177700 | -0.40078200 | 3.29856700 |
| C | -2.05332900 | -2.10176700 | 3.41332700 |
| H | -2.30181300 | -1.68679800 | 1.31384600 |
| C | -0.19464300 | -1.00580200 | 4.50712500 |
| H | 1.03413900 | 0.25095500 | 3.28102600 |
| C | -1.30386500 | -1.85458400 | 4.56827800 |
| H | -2.92213000 | -2.76271800 | 3.45275000 |
| H | 0.40042700 | -0.81086200 | 5.40218200 |
| H | -1.58307900 | -2.32425500 | 5.51441700 |
| C | 1.43608100 | 3.58577600 | -0.96741300 |
| C | 1.29961000 | 2.73563500 | -2.07555800 |
| C | 2.49287300 | 4.51507200 | -0.93721400 |
| C | 2.19830500 | 2.81523400 | -3.14335000 |
| H | 0.49945800 | 1.99728500 | -2.10302100 |
| C | 3.38802400 | 4.59271900 | -2.00566100 |
| H | 2.61765700 | 5.18296000 | -0.08185800 |
| C | 3.24123900 | 3.74494700 | -3.11047400 |
| H | 2.08002300 | 2.14708500 | -3.99917100 |
| H | 4.20484300 | 5.31742200 | -1.97449400 |
| H | 3.94330500 | 3.80935600 | -3.94514100 |
| C | -0.05896900 | 5.12120600 | 1.01936100 |
| C | -0.15319700 | 6.17880400 | 0.09738600 |
| C | -0.36236100 | 5.35898600 | 2.37090900 |
| C | -0.54413900 | 7.45064400 | 0.52438500 |
| H | 0.08135900 | 6.01769300 | -0.95677900 |
| C | -0.75465200 | 6.63167000 | 2.79249100 |
| H | -0.29760300 | 4.55677100 | 3.10646400 |
| C | -0.84905300 | 7.67913900 | 1.87045400 |
| H | -0.61207200 | 8.26492300 | -0.20051200 |
| H | -0.98850300 | 6.80226300 | 3.84572400 |
| H | -1.15858500 | 8.67334500 | 2.20077000 |
| C | 1.40775600 | 2.73869300 | 1.81670600 |
| H | 0.72175100 | 2.43899900 | 2.62394200 |
| H | 2.03486400 | 3.55247700 | 2.20886900 |
| C | 1.62290500 | 0.45635400 | 0.52052700 |
| H | 1.81964500 | 0.63821200 | -0.54557100 |
| H | 2.06315400 | -0.52592800 | 0.74756800 |
| C | 2.28688600 | 1.55964300 | 1.37624100 |
| H | 2.72055000 | 1.11474100 | 2.28428600 |
| H | 3.13847200 | 1.95190100 | 0.80047400 |
| C | -3.60470500 | 3.81260700 | 0.03854500 |
| O | -3.02028200 | 0.90734400 | 0.88037800 |
| C | -4.82488500 | 2.94836100 | 0.10643400 |
| C | -2.54200000 | 3.59919300 | -0.82398500 |
| C | -3.66555700 | 5.06381500 | 0.86257900 |
| C | -3.18457700 | 1.14845700 | 2.12807200 |
| H | -5.10102700 | 2.72119000 | 1.14761600 |
| H | -5.65894200 | 3.53804500 | -0.31502100 |
| H | -4.73590900 | 2.01084300 | -0.44845900 |
| C | -2.16243100 | 2.35272900 | -1.43990900 |
| H | -1.86842600 | 4.44714700 | -0.96743900 |
| H | -4.60356900 | 5.60837200 | 0.66205400 |
| H | -3.68650000 | 4.79609800 | 1.93259400 |
| H | -2.81484900 | 5.73327400 | 0.69042100 |
| O | -2.14606600 | 2.02638600 | 2.51711900 |
| O | -4.02507900 | 0.76702200 | 2.90577000 |
| H | -1.45128100 | 2.43273700 | -2.26547900 |
| H | -2.92958500 | 1.58651500 | -1.59096300 |
| C | -2.05726100 | 2.48201000 | 3.87198800 |
| H | -1.01173800 | 2.39033300 | 4.19531600 |
| H | -2.38587700 | 3.52928300 | 3.93172200 |
| H | -2.69462500 | 1.85237300 | 4.50484100 |

**iii-4-dppen-sing**

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

Zero-point correction= 0.710536 (Hartree/Particle)
Thermal correction to Energy= 0.759430
Thermal correction to Enthalpy= 0.760374
Thermal correction to Gibbs Free Energy= 0.626028
Sum of electronic and zero-point Energies= -4062.534519
Sum of electronic and thermal Energies= -4062.485625
Sum of electronic and thermal Enthalpies= -4062.484681
Sum of electronic and thermal Free Energies= -4062.619027

| | | | |
|---|---|---|---|
| C | -2.63973000 | 6.00778000 | 0.97853300 |
| O | -2.48137500 | 0.58782200 | 0.42648900 |

| | | | |
|---|---|---|---|
| C | -2.84900400 | 6.28749600 | -0.48749200 |
| C | -1.71460400 | 5.15517600 | 1.47433300 |
| C | -3.57824000 | 6.74699500 | 1.89856700 |
| C | -2.80476500 | 0.03433600 | -0.67496600 |
| H | -3.86714700 | 5.99485700 | -0.79747000 |
| H | -2.75834800 | 7.36962100 | -0.69387600 |
| H | -2.14291900 | 5.74885600 | -1.13179100 |
| C | -0.79439000 | 4.27670800 | 0.73248800 |
| H | -1.67736700 | 5.05052600 | 2.56384200 |
| H | -3.36831300 | 6.53902500 | 2.95930300 |
| H | -3.52810400 | 7.84029400 | 1.74168300 |
| H | -4.62530200 | 6.45300500 | 1.69714500 |
| O | -3.42325400 | -1.17688400 | -0.44713700 |
| O | -2.62561800 | 0.41715800 | -1.83108400 |
| H | 0.21639100 | 4.29974600 | 1.16488400 |
| H | -0.71735100 | 4.54095400 | -0.32884700 |
| C | -3.73821700 | -1.94548200 | -1.59828800 |
| H | -2.82812400 | -2.21523600 | -2.15992200 |
| H | -4.23210000 | -2.85982700 | -1.24004000 |
| H | -4.41437800 | -1.40314100 | -2.27915500 |
| Co | -1.55523600 | 2.38743800 | 0.68430600 |
| P | -0.17099700 | 1.88540500 | 2.39837900 |
| P | 0.16757200 | 1.78328900 | -0.64507300 |
| C | -0.08683300 | 3.12849700 | 3.74003500 |
| C | -0.37432300 | 0.31483500 | 3.32595200 |
| C | 1.52877300 | 1.82656200 | 1.72165900 |
| C | 0.43691700 | 2.83910700 | -2.09798000 |
| C | 0.29189800 | 0.03996100 | -1.22565100 |
| C | 1.67863700 | 1.85249500 | 0.39017300 |
| C | 0.87981200 | 4.14668300 | 3.75445200 |
| C | -1.07216700 | 3.09875000 | 4.74015800 |
| C | 0.56966300 | -0.05393000 | 4.30245000 |
| C | -1.48684800 | -0.50515900 | 3.08134900 |
| H | 2.38674900 | 1.75751000 | 2.39852200 |
| C | 1.47044600 | 3.78621400 | -2.16438400 |
| C | -0.51103100 | 2.75817200 | -3.13297400 |
| C | 0.03802200 | -0.97904200 | -0.29236200 |
| C | 0.64849100 | -0.30280400 | -2.53835200 |
| H | 2.66401700 | 1.78744700 | -0.08402100 |
| C | 0.84915100 | 5.12959700 | 4.74870200 |
| H | 1.66095200 | 4.18361000 | 2.99213400 |
| C | -1.10277800 | 4.08396000 | 5.72868400 |
| H | -1.81610600 | 2.30214700 | 4.74394900 |
| C | 0.40506800 | -1.24009800 | 5.01929600 |
| H | 1.42957600 | 0.58723800 | 4.51270400 |
| C | -1.64624800 | -1.69069400 | 3.80955400 |
| H | -2.19810000 | -0.22521900 | 2.30156100 |
| C | 1.56478400 | 4.63580900 | -3.27154600 |
| H | 2.19979800 | 3.87397300 | -1.35612900 |
| C | -0.40528000 | 3.60469800 | -4.23800200 |
| H | -1.32482000 | 2.03643000 | -3.04700800 |
| C | 0.10584500 | -2.31907700 | -0.67562600 |
| H | -0.24651500 | -0.73233200 | 0.72898300 |
| C | 0.72162900 | -1.64718400 | -2.91675200 |
| H | 0.86165400 | 0.47228600 | -3.27558800 |
| C | -0.14509600 | 5.10516900 | 5.73176600 |
| H | 1.60620900 | 5.91740700 | 4.75228400 |
| H | -1.87679800 | 4.05368700 | 6.49943800 |
| C | -0.70483800 | -2.05979700 | 4.77419200 |
| H | 1.14224600 | -1.52487500 | 5.77399000 |
| H | -2.51195700 | -2.32907900 | 3.61576500 |
| C | 0.63071300 | 4.54438300 | -4.30885900 |
| H | 2.37089000 | 5.37174100 | -3.32148100 |
| H | -1.14017200 | 3.53737200 | -5.04400400 |
| C | 0.44240200 | -2.65777200 | -1.99113600 |
| H | -0.11226200 | -3.09980200 | 0.05704500 |
| H | 0.99532500 | -1.90335000 | -3.94329600 |
| H | -0.16995300 | 5.87708300 | 6.50480700 |
| H | -0.83271100 | -2.98695900 | 5.33863000 |
| H | 0.70765500 | 5.20939900 | -5.17267500 |
| H | 0.49151600 | -3.70701000 | -2.29265800 |
| C | -4.69489000 | 3.16717100 | 0.47703600 |
| H | -5.76151000 | 3.36076200 | 0.39086900 |
| C | -4.14815100 | 2.94771300 | 1.74916700 |
| C | -3.90009800 | 3.22952900 | -0.68131800 |
| O | -2.94600500 | 2.70468200 | 2.04345100 |
| O | -2.65838900 | 3.06023700 | -0.78031300 |
| O | -5.04441500 | 3.01765100 | 2.75602300 |
| O | -4.58767300 | 3.53818900 | -1.79979400 |
| C | -4.57795400 | 2.79705900 | 4.08358700 |
| H | -3.85878600 | 3.57311700 | 4.38525200 |
| H | -5.46450200 | 2.84152700 | 4.72883900 |
| H | -4.09694700 | 1.81097900 | 4.17954400 |
| C | -3.88981600 | 3.45810000 | -3.04280300 |
| H | -4.62276400 | 3.71485200 | -3.81835700 |
| H | -3.04729400 | 4.16382900 | -3.07448000 |
| H | -3.50742300 | 2.43849400 | -3.19455900 |

**TS-iii-iv-4-dppen-sing**

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

Zero-point correction= 0.707883 (Hartree/Particle)

Thermal correction to Energy= 0.756970

Thermal correction to Enthalpy= 0.757914

Thermal correction to Gibbs Free Energy= 0.624314

Sum of electronic and zero-point Energies= -4062.488690

Sum of electronic and thermal Energies= -4062.439602

Sum of electronic and thermal Enthalpies= -4062.438658

Sum of electronic and thermal Free Energies= -4062.572258

| | | | |
|---|---|---|---|
| C | -2.92019700 | 5.67919800 | 0.88747600 |
| O | -2.60105200 | 0.38534800 | 0.32969600 |
| C | -2.90905600 | 6.31651300 | -0.49250100 |
| C | -1.70574700 | 5.04986000 | 1.34762000 |
| C | -3.61792800 | 6.53830900 | 1.93058300 |
| C | -2.81078000 | -0.14680300 | -0.79674600 |
| H | -3.92666300 | 6.55543700 | -0.83360100 |
| H | -2.33684300 | 7.25854000 | -0.44389500 |
| H | -2.43243600 | 5.68144800 | -1.25104700 |
| C | -0.70654400 | 4.48124900 | 0.56833100 |
| H | -1.60009200 | 4.95510900 | 2.43296900 |
| H | -3.73195300 | 6.00750300 | 2.88676200 |
| H | -3.01723800 | 7.44540600 | 2.11653000 |
| H | -4.61419900 | 6.86091200 | 1.59273900 |
| O | -3.25104100 | -1.46224600 | -0.66768500 |
| O | -2.67245500 | 0.31642400 | -1.93514900 |
| H | 0.27728300 | 4.32644700 | 1.01631600 |
| H | -0.69699200 | 4.64142900 | -0.51120900 |
| C | -3.42088500 | -2.18997000 | -1.87067600 |
| H | -2.46730400 | -2.29777700 | -2.41502600 |
| H | -3.79175000 | -3.18698500 | -1.58939600 |
| H | -4.14671100 | -1.70692600 | -2.54633100 |
| Co | -1.58076900 | 2.31536100 | 0.72001700 |
| P | -0.17526800 | 1.83160000 | 2.48602700 |
| P | 0.17046100 | 1.72737100 | -0.59834500 |
| C | -0.07396200 | 3.09722500 | 3.80961600 |
| C | -0.31727900 | 0.25776900 | 3.42664400 |
| C | 1.52637700 | 1.79009300 | 1.78946700 |
| C | 0.46101200 | 2.77712800 | -2.06075900 |
| C | 0.33269800 | -0.00398700 | -1.21694800 |
| C | 1.67666300 | 1.80139100 | 0.45462800 |
| C | 0.86206400 | 4.14360900 | 3.77787100 |
| C | -1.06577100 | 3.09851200 | 4.80716100 |
| C | 0.53757300 | -0.05199900 | 4.49965600 |
| C | -1.31720500 | -0.65202300 | 3.04427900 |
| H | 2.39316800 | 1.74325600 | 2.45903600 |
| C | 1.56408600 | 3.63099000 | -2.20980500 |
| C | -0.57487200 | 2.79918700 | -3.01546900 |
| C | 0.09767700 | -1.04372200 | -0.30288000 |
| C | 0.67517900 | -0.32124400 | -2.54002700 |
| H | 2.66979700 | 1.74445600 | -0.00572400 |
| C | 0.80168300 | 5.17533800 | 4.72143000 |

| | | | |
|---|---|---|---|
| H | 1.64316900 | 4.16434500 | 3.01416600 |
| C | -1.12456800 | 4.12875700 | 5.74727100 |
| H | -1.79736900 | 2.28828500 | 4.84396100 |
| C | 0.39784000 | -1.26442100 | 5.17839000 |
| H | 1.30895000 | 0.65769500 | 4.81066000 |
| C | -1.45142500 | -1.86568000 | 3.73042300 |
| H | -1.96909600 | -0.41384600 | 2.19743200 |
| C | 1.64014300 | 4.49012300 | -3.31265600 |
| H | 2.36529100 | 3.64085300 | -1.46746700 |
| C | -0.48657600 | 3.65226900 | -4.11719200 |
| H | -1.44319100 | 2.15115800 | -2.86785500 |
| C | 0.18013600 | -2.37635700 | -0.70889000 |
| H | -0.18095100 | -0.81394200 | 0.72396400 |
| C | 0.76142300 | -1.65753400 | -2.94400300 |
| H | 0.86572600 | 0.47123600 | -3.26558200 |
| C | -0.19293700 | 5.17411400 | 5.70394000 |
| H | 1.53661800 | 5.98338100 | 4.68547200 |
| H | -1.90138000 | 4.11747200 | 6.51611100 |
| C | -0.59755400 | -2.17312500 | 4.79388500 |
| H | 1.06539100 | -1.50229100 | 6.01052200 |
| H | -2.22846600 | -2.57314500 | 3.42919800 |
| C | 0.61883400 | 4.50060300 | -4.26767400 |
| H | 2.50150600 | 5.15376600 | -3.42301000 |
| H | -1.28796700 | 3.66265800 | -4.86072900 |
| C | 0.50838300 | -2.68850500 | -2.03286000 |
| H | -0.02318800 | -3.17258500 | 0.01158300 |
| H | 1.02447800 | -1.89238300 | -3.97868600 |
| H | -0.24110300 | 5.98258900 | 6.43751300 |
| H | -0.70552600 | -3.12110100 | 5.32732200 |
| H | 0.68081100 | 5.17246400 | -5.12753000 |
| H | 0.56791200 | -3.73170200 | -2.35336900 |
| C | -4.31438400 | 4.20988100 | 0.63203100 |
| H | -5.26259600 | 4.74675100 | 0.58598400 |
| C | -4.12319800 | 3.41375800 | 1.82536500 |
| C | -3.88095700 | 3.62686900 | -0.63355200 |
| O | -3.18070000 | 2.63344500 | 2.01324300 |
| O | -2.83397400 | 3.00643900 | -0.80163100 |
| O | -5.00135300 | 3.68654500 | 2.79885200 |
| O | -4.68876000 | 3.89777500 | -1.66148900 |
| C | -4.79779600 | 3.05288400 | 4.06727200 |
| H | -3.87820400 | 3.42826900 | 4.53878200 |
| H | -5.66846800 | 3.31515800 | 4.67970700 |
| H | -4.72443400 | 1.96124500 | 3.95508600 |
| C | -4.27706000 | 3.37923200 | -2.93924800 |
| H | -5.12156300 | 3.54625300 | -3.61810000 |
| H | -3.38862800 | 3.91957600 | -3.29860800 |
| H | -4.03100800 | 2.31047700 | -2.85483400 |

**iv-4-dppen-sing**

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

Zero-point correction= 0.709943
(Hartree/Particle)

Thermal correction to Energy= 0.760031

Thermal correction to Enthalpy= 0.760975

Thermal correction to Gibbs Free Energy= 0.622075

Sum of electronic and zero-point Energies= -4062.512050

Sum of electronic and thermal Energies= -4062.461962

Sum of electronic and thermal Enthalpies= -4062.461018

Sum of electronic and thermal Free Energies= -4062.599919

| | | | |
|---|---|---|---|
| C | -2.91773600 | 5.77293000 | 0.87495300 |
| O | -2.85654300 | 0.21913300 | 0.38102500 |
| C | -2.93335400 | 6.63724900 | -0.39530200 |
| C | -1.55063200 | 5.19014800 | 1.17569000 |
| C | -3.34732100 | 6.63375500 | 2.08227100 |
| C | -2.99939400 | -0.29550100 | -0.76771900 |
| H | -3.94599200 | 7.02230300 | -0.58823600 |
| H | -2.25653400 | 7.49597200 | -0.27473900 |
| H | -2.60629500 | 6.07889300 | -1.28528100 |
| C | -0.44658700 | 5.28238800 | 0.43085700 |
| H | -1.48736000 | 4.64799500 | 2.12375200 |
| H | -3.32219100 | 6.06354700 | 3.02244300 |
| H | -2.65893100 | 7.48597200 | 2.18737900 |
| H | -4.36737400 | 7.02572200 | 1.94635200 |
| O | -3.29736100 | -1.64690300 | -0.69004600 |
| O | -2.90812400 | 0.23006500 | -1.88300600 |
| H | 0.48384200 | 4.81646700 | 0.76369000 |
| H | -0.41808700 | 5.78500400 | -0.53854200 |
| C | -3.40714100 | -2.34092300 | -1.92108200 |
| H | -2.45059900 | -2.33790700 | -2.47009300 |
| H | -3.68077800 | -3.37785000 | -1.67682900 |
| H | -4.17923000 | -1.89970500 | -2.57309600 |
| Co | -1.64555300 | 1.89261100 | 0.75808900 |
| P | -0.24495000 | 1.73014200 | 2.46509200 |
| P | 0.11665200 | 1.51608700 | -0.58678200 |
| C | -0.17459100 | 3.02890500 | 3.76772400 |
| C | -0.27758700 | 0.17542300 | 3.46614500 |
| C | 1.47131400 | 1.72776300 | 1.78507700 |
| C | 0.36202900 | 2.63571400 | -2.01309300 |
| C | 0.38747700 | -0.17270600 | -1.28598400 |
| C | 1.63157900 | 1.67189500 | 0.45248600 |
| C | 0.73418300 | 4.09929200 | 3.71873200 |
| C | -1.18985600 | 3.04738100 | 4.74318300 |
| C | 0.59877500 | -0.06027800 | 4.53965500 |
| C | -1.21608600 | -0.80706500 | 3.10884300 |
| H | 2.33252200 | 1.74584800 | 2.46382100 |
| C | 1.38926500 | 3.58770700 | -2.09737500 |
| C | -0.63264400 | 2.60155200 | -3.01011600 |
| C | -0.04202800 | -1.25542500 | -0.50028000 |
| C | 0.98347900 | -0.42412900 | -2.53196300 |
| H | 2.62876300 | 1.63022500 | -0.00181800 |
| C | 0.62799100 | 5.16425100 | 4.62060900 |
| H | 1.52643100 | 4.11461200 | 2.96630800 |
| C | -1.29592000 | 4.11046900 | 5.64183700 |
| H | -1.90590400 | 2.22284300 | 4.79206400 |
| C | 0.54269600 | -1.26714300 | 5.24160700 |
| H | 1.32359300 | 0.70439000 | 4.83263200 |
| C | -1.26936800 | -2.01481300 | 3.81579100 |
| H | -1.89943700 | -0.62105600 | 2.27400600 |
| C | 1.43060900 | 4.48791700 | -3.16929100 |
| H | 2.15896400 | 3.64212900 | -1.32392400 |
| C | -0.58028700 | 3.49344200 | -4.08281200 |
| H | -1.45301100 | 1.88452600 | -2.91591700 |
| C | 0.12065300 | -2.56673500 | -0.95102200 |
| H | -0.53584300 | -1.05948300 | 0.45179400 |
| C | 1.14093600 | -1.73884500 | -2.98455000 |
| H | 1.31998600 | 0.40659000 | -3.15640900 |
| C | -0.38841000 | 5.17675000 | 5.58065500 |
| H | 1.34275400 | 5.98959600 | 4.56817500 |
| H | -2.09070600 | 4.10954100 | 6.39250900 |
| C | -0.39149200 | -2.24692000 | 4.87937800 |
| H | 1.22788900 | -1.44518600 | 6.07461700 |
| H | -2.00172400 | -2.77602700 | 3.53383900 |
| C | 0.44949200 | 4.44122100 | -4.16447700 |
| H | 2.23387700 | 5.22727600 | -3.22482900 |
| H | -1.35244800 | 3.45826800 | -4.85623900 |
| C | 0.71070900 | -2.81256000 | -2.19638900 |
| H | -0.23070700 | -3.39789400 | -0.33436700 |
| H | 1.60229400 | -1.92466700 | -3.95816300 |
| H | -0.47374000 | 6.01148500 | 6.28073100 |
| H | -0.43450000 | -3.19017000 | 5.43022000 |
| H | 0.48334300 | 5.14396400 | -5.00101600 |
| H | 0.83116500 | -3.83827200 | -2.55438900 |
| C | -3.98344900 | 4.60773300 | 0.67899200 |
| H | -4.97088900 | 5.07590000 | 0.58555600 |
| C | -4.02716600 | 3.65937300 | 1.86376600 |
| C | -3.68298400 | 3.82839000 | -0.58418500 |
| O | -3.30406100 | 2.68825400 | 2.01259500 |
| O | -2.68418600 | 3.15232800 | -0.73543100 |
| O | -4.93885800 | 4.02081900 | 2.75312000 |
| O | -4.60431200 | 3.97678700 | -1.52391600 |

| | | | |
|---|---|---|---|
| C | -5.02571500 | 3.24665600 | 3.96431700 |
| H | -4.09417800 | 3.34735700 | 4.53846300 |
| H | -5.86937500 | 3.66273400 | 4.52538300 |
| H | -5.19908800 | 2.18712200 | 3.73006600 |
| C | -4.36986300 | 3.25972800 | -2.75780500 |
| H | -5.29367700 | 3.35755400 | -3.33887000 |
| H | -3.52737700 | 3.71898900 | -3.29506600 |
| H | -4.12626700 | 2.20852600 | -2.54453300 |

**iii-4-dppen-trip**

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

Zero-point correction= 0.705991 (Hartree/Particle)

Thermal correction to Energy= 0.756861

Thermal correction to Enthalpy= 0.757805

Thermal correction to Gibbs Free Energy= 0.616745

Sum of electronic and zero-point Energies= -4062.534169

Sum of electronic and thermal Energies= -4062.483298

Sum of electronic and thermal Enthalpies= -4062.482354

Sum of electronic and thermal Free Energies= -4062.623414

| | | | |
|---|---|---|---|
| C | -2.81389500 | 6.05350000 | 1.05048600 |
| O | -2.66900900 | 0.57669100 | 0.20787500 |
| C | -3.17427500 | 6.38155500 | -0.36729100 |
| C | -1.69373600 | 5.32063500 | 1.41667100 |
| C | -3.74768600 | 6.57211100 | 2.10370400 |
| C | -2.87128000 | 0.05296700 | -0.93844700 |
| H | -4.22572900 | 6.11838500 | -0.56699200 |
| H | -3.08641900 | 7.47117300 | -0.53355500 |
| H | -2.55100500 | 5.86213600 | -1.10438200 |
| C | -0.79430500 | 4.65170800 | 0.57158600 |
| H | -1.51557400 | 5.21502400 | 2.49106900 |
| H | -3.97221900 | 7.64294800 | 1.95415000 |
| H | -4.71357500 | 6.03769600 | 2.03958300 |
| H | -3.35121600 | 6.43098000 | 3.12022300 |
| O | -3.38882700 | -1.21674600 | -0.81677000 |
| O | -2.65228100 | 0.52387000 | -2.05340300 |
| H | 0.17991800 | 4.35722000 | 0.96698100 |
| H | -0.86589700 | 4.74020700 | -0.51381300 |
| C | -3.56365700 | -1.94261500 | -2.02472400 |
| H | -2.59705200 | -2.12762000 | -2.52154900 |
| H | -4.02263500 | -2.90287100 | -1.74987000 |
| H | -4.21995500 | -1.40749900 | -2.73004700 |
| Co | -1.84457500 | 2.39363700 | 0.62212600 |
| P | -0.32508400 | 1.91734300 | 2.51499900 |
| P | 0.19123500 | 1.72286200 | -0.65705100 |
| C | -0.21115000 | 3.21697400 | 3.79636400 |
| C | -0.56443900 | 0.36056400 | 3.45717900 |
| C | 1.37683000 | 1.78795900 | 1.84600200 |
| C | 0.62509400 | 2.81009500 | -2.05563900 |
| C | 0.31589900 | 0.00308800 | -1.29541100 |
| C | 1.59762700 | 1.74852800 | 0.52053300 |
| C | 0.81156200 | 4.17892200 | 3.80729200 |
| C | -1.28254200 | 3.34063100 | 4.69981700 |
| C | 0.17713900 | 0.07624300 | 4.61791300 |
| C | -1.50841500 | -0.56689200 | 2.98393200 |
| H | 2.21594500 | 1.72947100 | 2.54973300 |
| C | 1.87486100 | 3.41838600 | -2.24739600 |
| C | -0.43148000 | 3.08461200 | -2.94528400 |
| C | 0.05954100 | -1.04391700 | -0.39416200 |
| C | 0.58609200 | -0.29526500 | -2.63905000 |
| H | 2.61987500 | 1.64279200 | 0.13875300 |
| C | 0.76133200 | 5.24886100 | 4.70816500 |
| H | 1.64829900 | 4.10910700 | 3.10834700 |
| C | -1.32809700 | 4.40802900 | 5.59743000 |
| H | -2.09077000 | 2.60686400 | 4.68725700 |
| C | -0.02024800 | -1.12936100 | 5.29435000 |
| H | 0.90345000 | 0.79945200 | 4.99783200 |
| C | -1.69851000 | -1.77395700 | 3.66743300 |
| H | -2.08422800 | -0.34601200 | 2.08012800 |
| C | 2.06842600 | 4.28797700 | -3.32678400 |
| H | 2.70200800 | 3.22733000 | -1.56076300 |
| C | -0.22706600 | 3.94494500 | -4.02611900 |
| H | -1.40766100 | 2.62819900 | -2.76438400 |
| C | 0.06230400 | -2.36883300 | -0.83352400 |
| H | -0.16322700 | -0.82729400 | 0.65124000 |
| C | 0.59211300 | -1.62399700 | -3.07459700 |
| H | 0.78096200 | 0.50787200 | -3.35231500 |
| C | -0.30738200 | 5.36788900 | 5.60135500 |
| H | 1.56172800 | 5.99274600 | 4.70738100 |
| H | -2.16666300 | 4.49555600 | 6.29269000 |
| C | -0.95743800 | -2.05627000 | 4.81886300 |
| H | 0.55779300 | -1.34737500 | 6.19584100 |
| H | -2.43244500 | -2.49402400 | 3.29679400 |
| C | 1.02188100 | 4.54951300 | -4.21743600 |
| H | 3.04230600 | 4.76253500 | -3.47065300 |
| H | -1.04883200 | 4.15310900 | -4.71612400 |
| C | 0.32573300 | -2.66299100 | -2.17623500 |
| H | -0.15046800 | -3.17272200 | -0.12451600 |
| H | 0.80182500 | -1.84699300 | -4.12386500 |
| H | -0.34679900 | 6.20676200 | 6.30041000 |
| H | -1.11001700 | -2.99869300 | 5.35097300 |
| H | 1.17791900 | 5.22977900 | -5.05849700 |
| H | 0.32307700 | -3.69979200 | -2.52162200 |
| C | -5.05110700 | 3.36225000 | 0.34073500 |
| H | -6.11384700 | 3.56710200 | 0.22868300 |
| C | -4.53167500 | 3.17151500 | 1.63284200 |
| C | -4.23422000 | 3.36800300 | -0.81151000 |
| O | -3.35388900 | 2.86551000 | 1.95611800 |
| O | -2.99031800 | 3.24012600 | -0.87215100 |
| O | -5.43711600 | 3.35346900 | 2.62542400 |
| O | -4.91338800 | 3.58026800 | -1.96234200 |
| C | -4.97828200 | 3.18308200 | 3.96395000 |
| H | -4.19201500 | 3.91318900 | 4.20990800 |
| H | -5.85153700 | 3.34479100 | 4.60874300 |
| H | -4.57737600 | 2.17005500 | 4.12534500 |
| C | -4.16634000 | 3.46922500 | -3.17560900 |
| H | -4.88715600 | 3.61804200 | -3.98998400 |
| H | -3.37890400 | 4.23665000 | -3.23240900 |
| H | -3.70060000 | 2.47482600 | -3.24630300 |

**TS-iii-iv-4-dppen-trip**

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

Zero-point correction= 0.707076 (Hartree/Particle)

Thermal correction to Energy= 0.756661

Thermal correction to Enthalpy= 0.757605

Thermal correction to Gibbs Free Energy= 0.620305

Sum of electronic and zero-point Energies= -4062.509109

Sum of electronic and thermal Energies= -4062.459523

Sum of electronic and thermal Enthalpies= -4062.458579

Sum of electronic and thermal Free Energies= -4062.595879

| | | | |
|---|---|---|---|
| C | -3.03045300 | 5.71910600 | 0.84810900 |
| O | -2.59484600 | 0.48605000 | 0.23350200 |
| C | -3.04463400 | 6.42023500 | -0.49302800 |
| C | -1.87840900 | 4.95399100 | 1.21880100 |
| C | -3.66700900 | 6.51912100 | 1.96644800 |
| C | -2.77075400 | -0.05863900 | -0.89973100 |
| H | -4.05778200 | 6.73980500 | -0.77282600 |
| H | -2.41173300 | 7.32212100 | -0.42034600 |
| H | -2.63971000 | 5.80199200 | -1.30447800 |
| C | -0.89568700 | 4.43160600 | 0.36859200 |
| H | -1.73659700 | 4.80916600 | 2.29302000 |
| H | -3.02477700 | 7.38813400 | 2.19598800 |
| H | -4.65758800 | 6.90349100 | 1.68302000 |
| H | -3.77116100 | 5.92859900 | 2.88774500 |
| O | -3.26352700 | -1.34736400 | -0.76616300 |
| O | -2.54998400 | 0.38632300 | -2.02739800 |
| H | 0.10544800 | 4.27600100 | 0.77942800 |
| H | -0.91973500 | 4.66253200 | -0.69838200 |
| C | -3.40133700 | -2.09482100 | -1.96278400 |
| H | -2.42310500 | -2.27450500 | -2.43978100 |
| H | -3.85118400 | -3.05889400 | -1.68359600 |

| | | | |
|---|---|---|---|
| H | -4.05032900 | -1.58380900 | -2.69312500 |
| Co | -1.84501600 | 2.41996000 | 0.61491400 |
| P | -0.40700700 | 1.89602600 | 2.51022000 |
| P | 0.14204300 | 1.71999700 | -0.65189100 |
| C | -0.31229000 | 3.16359100 | 3.83261700 |
| C | -0.54447800 | 0.31339100 | 3.43806000 |
| C | 1.31196700 | 1.85356600 | 1.85349800 |
| C | 0.55740100 | 2.75394900 | -2.10079600 |
| C | 0.37299100 | -0.01594200 | -1.23015400 |
| C | 1.54603400 | 1.82823600 | 0.52981600 |
| C | 0.60240100 | 4.22843300 | 3.77832500 |
| C | -1.30085900 | 3.16452600 | 4.83439900 |
| C | 0.24526900 | 0.03623600 | 4.56861100 |
| C | -1.46360900 | -0.64470300 | 2.97756000 |
| H | 2.14715600 | 1.84053900 | 2.56472900 |
| C | 1.78737800 | 3.39163500 | -2.31833400 |
| C | -0.50696900 | 2.96545900 | -2.99963300 |
| C | 0.17053300 | -1.04777800 | -0.29848600 |
| C | 0.68267000 | -0.34522000 | -2.55835300 |
| H | 2.57553100 | 1.77543600 | 0.15604800 |
| C | 0.52866900 | 5.27308200 | 4.70671600 |
| H | 1.37438800 | 4.25522600 | 3.00535800 |
| C | -1.37229200 | 4.20773800 | 5.75942400 |
| H | -2.02011500 | 2.34364500 | 4.88824400 |
| C | 0.11976800 | -1.18855000 | 5.22782500 |
| H | 0.95417500 | 0.78129000 | 4.93938900 |
| C | -1.58207500 | -1.87155600 | 3.64248100 |
| H | -2.06623100 | -0.43013700 | 2.08939600 |
| C | 1.95547200 | 4.22779400 | -3.42890900 |
| H | 2.62020500 | 3.25016700 | -1.62631700 |
| C | -0.32877400 | 3.79201400 | -4.11102500 |
| H | -1.46780100 | 2.48084900 | -2.80338000 |
| C | 0.25964800 | -2.38440000 | -0.69139100 |
| H | -0.07926700 | -0.81054400 | 0.73547800 |
| C | 0.77653300 | -1.68487200 | -2.94853800 |
| H | 0.83956700 | 0.44278600 | -3.29728900 |
| C | -0.45904200 | 5.26822700 | 5.69605500 |
| H | 1.24731300 | 6.09468700 | 4.65274800 |
| H | -2.14561900 | 4.19466800 | 6.53168900 |
| C | -0.79400200 | -2.14476400 | 4.76454300 |
| H | 0.73583600 | -1.39923100 | 6.10574200 |
| H | -2.29610400 | -2.61552000 | 3.27961700 |
| C | 0.90160400 | 4.42702800 | -4.32640300 |
| H | 2.91503500 | 4.72539100 | -3.59104700 |
| H | -1.15606100 | 3.95029100 | -4.80797400 |
| C | 0.55987900 | -2.70830600 | -2.01942100 |
| H | 0.08639100 | -3.17488300 | 0.04333100 |
| H | 1.01610700 | -1.92906400 | -3.98682000 |
| H | -0.51762000 | 6.08659200 | 6.41778000 |
| H | -0.89034000 | -3.10263600 | 5.28226600 |
| H | 1.03662500 | 5.08125200 | -5.19149900 |
| H | 0.62581200 | -3.75443900 | -2.32886100 |
| C | -4.65909000 | 4.29176000 | 0.52874700 |
| H | -5.54546600 | 4.92492600 | 0.50648500 |
| C | -4.47983200 | 3.49047900 | 1.71008300 |
| C | -4.20251100 | 3.79382000 | -0.75228500 |
| O | -3.56502100 | 2.67669900 | 1.89391200 |
| O | -3.21494300 | 3.08462400 | -0.93959600 |
| O | -5.34584700 | 3.78779000 | 2.69447600 |
| O | -4.91644400 | 4.26421100 | -1.78755600 |
| C | -5.12961300 | 3.15789000 | 3.96103800 |
| H | -4.16053100 | 3.46229500 | 4.38395900 |
| H | -5.94628600 | 3.49451400 | 4.61074500 |
| H | -5.14729900 | 2.06195600 | 3.86564200 |
| C | -4.45565400 | 3.90291300 | -3.09540100 |
| H | -5.16201600 | 4.35483800 | -3.80168700 |
| H | -3.44066600 | 4.29042700 | -3.27212000 |
| H | -4.43837400 | 2.80965900 | -3.21299000 |

**iv-4-dppen-trip**

UB3LYP-D3/def2-SVP-CPCM(acetonitrile)
Zero-point correction= 0.710233 (Hartree/Particle)
Thermal correction to Energy= 0.759908
Thermal correction to Enthalpy= 0.760852
Thermal correction to Gibbs Free Energy= 0.621958
Sum of electronic and zero-point Energies= -4062.534282
Sum of electronic and thermal Energies= -4062.484607
Sum of electronic and thermal Enthalpies= -4062.483663
Sum of electronic and thermal Free Energies= -4062.622557

| | | | |
|---|---|---|---|
| C | -3.05820400 | 5.58157700 | 0.77191500 |
| O | -2.71214300 | 0.66010800 | 0.20980000 |
| C | -2.88311700 | 6.40750900 | -0.51476800 |
| C | -1.76813700 | 4.87373400 | 1.19370100 |
| C | -3.44694600 | 6.53439000 | 1.92354800 |
| C | -2.86118000 | 0.07590400 | -0.90040800 |
| H | -3.82853900 | 6.90472600 | -0.78269600 |
| H | -2.11828200 | 7.18284600 | -0.35995200 |
| H | -2.56675000 | 5.79134000 | -1.36723900 |
| C | -0.65617200 | 4.68818200 | 0.43568000 |
| H | -1.68565800 | 4.70999000 | 2.27132900 |
| H | -2.63723800 | 7.25898700 | 2.09901100 |
| H | -4.36414500 | 7.09320600 | 1.68022300 |
| H | -3.61834700 | 5.98991700 | 2.86494200 |
| O | -3.29907100 | -1.23494700 | -0.73228200 |
| O | -2.67668500 | 0.49246700 | -2.04962900 |
| H | 0.30320200 | 4.45695000 | 0.90241300 |
| H | -0.62661100 | 4.93824000 | -0.62558100 |
| C | -3.43106400 | -2.01088200 | -1.90962800 |
| H | -2.46583600 | -2.12060200 | -2.43152000 |
| H | -3.78829200 | -3.00343900 | -1.59680700 |
| H | -4.15425600 | -1.56916900 | -2.61604600 |
| Co | -1.64240500 | 2.48268200 | 0.60892700 |
| P | -0.35037500 | 1.92897500 | 2.45601600 |
| P | 0.20774000 | 1.82958300 | -0.64742900 |
| C | -0.25162500 | 3.16449200 | 3.81433100 |
| C | -0.54379700 | 0.34010700 | 3.37316400 |
| C | 1.38919800 | 1.83677500 | 1.84561300 |
| C | 0.68376100 | 2.85958900 | -2.08372800 |
| C | 0.36433200 | 0.09676400 | -1.27506700 |
| C | 1.63302600 | 1.83823400 | 0.52316100 |
| C | 0.74679100 | 4.15035400 | 3.87385300 |
| C | -1.32922300 | 3.23370400 | 4.71881400 |
| C | 0.24340800 | 0.01239000 | 4.49151100 |
| C | -1.51131500 | -0.56971200 | 2.91383900 |
| H | 2.21244700 | 1.76227600 | 2.56687700 |
| C | 1.90691200 | 3.52820400 | -2.23850100 |
| C | -0.33848500 | 3.05445100 | -3.03452900 |
| C | 0.05730100 | -0.94120900 | -0.37917600 |
| C | 0.72569800 | -0.22759300 | -2.59165700 |
| H | 2.65950500 | 1.74930000 | 0.14753800 |
| C | 0.67280200 | 5.17932800 | 4.82071100 |
| H | 1.58723300 | 4.12748200 | 3.17569800 |
| C | -1.40054300 | 4.25878700 | 5.66330100 |
| H | -2.12401300 | 2.48443900 | 4.67154000 |
| C | 0.06944900 | -1.21322000 | 5.13888300 |
| H | 0.99037600 | 0.71985000 | 4.86190000 |
| C | -1.67984500 | -1.79766800 | 3.56627800 |
| H | -2.11567300 | -0.31466100 | 2.03708200 |
| C | 2.11090100 | 4.37508300 | -3.33540000 |
| H | 2.70676800 | 3.40213100 | -1.50543600 |
| C | -0.12484800 | 3.88942200 | -4.13297800 |
| H | -1.29830900 | 2.54972100 | -2.88740200 |
| C | 0.09960200 | -2.27369800 | -0.79180800 |
| H | -0.24208800 | -0.70610100 | 0.64156900 |
| C | 0.76825800 | -1.56383800 | -3.00448600 |
| H | 0.96722500 | 0.56242900 | -3.30538000 |
| C | -0.39899200 | 5.23784500 | 5.71608400 |
| H | 1.45826000 | 5.93871700 | 4.85532700 |
| H | -2.24342600 | 4.29793000 | 6.35825600 |
| C | -0.89267700 | -2.12098000 | 4.67582500 |

| | | | |
|---|---|---|---|
| H | 0.68489000 | -1.46253700 | 6.00725400 |
| H | -2.43194600 | -2.50339300 | 3.20343200 |
| C | 1.09974800 | 4.55447700 | -4.28450400 |
| H | 3.06558700 | 4.89582000 | -3.44688700 |
| H | -0.91987400 | 4.03224700 | -4.86977900 |
| C | 0.45243300 | -2.59091300 | -2.10862100 |
| H | -0.15643300 | -3.06585000 | -0.08343000 |
| H | 1.04839700 | -1.80201700 | -4.03414700 |
| H | -0.45686100 | 6.04345200 | 6.45221400 |
| H | -1.02736700 | -3.07960200 | 5.18369200 |
| H | 1.26239800 | 5.21602600 | -5.13929000 |
| H | 0.48004300 | -3.63358500 | -2.43531200 |
| C | -4.25701900 | 4.57587000 | 0.55619600 |
| H | -5.19124500 | 5.14252000 | 0.46231200 |
| C | -4.37406900 | 3.64229300 | 1.74461800 |
| C | -4.05668800 | 3.75979100 | -0.70921200 |
| O | -3.57674900 | 2.75277800 | 1.97532200 |
| O | -2.98934600 | 3.28239300 | -1.03745600 |
| O | -5.39733300 | 3.93586100 | 2.53554200 |
| O | -5.16399800 | 3.63678600 | -1.42515000 |
| C | -5.52461300 | 3.16502300 | 3.74469300 |
| H | -4.64043200 | 3.31432400 | 4.38136600 |
| H | -6.42509500 | 3.53717700 | 4.24532400 |
| H | -5.62620900 | 2.09627000 | 3.50863300 |
| C | -5.06006900 | 2.87165900 | -2.64675500 |
| H | -6.09036000 | 2.67944400 | -2.96716500 |
| H | -4.53240700 | 3.46748100 | -3.40691700 |
| H | -4.50261900 | 1.94020800 | -2.47167600 |

**i-4-dppp-sing**

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

Zero-point correction= 0.639255 (Hartree/Particle)
Thermal correction to Energy= 0.679347
Thermal correction to Enthalpy= 0.680292
Thermal correction to Gibbs Free Energy= 0.564446
Sum of electronic and zero-point Energies= -3607.601222
Sum of electronic and thermal Energies= -3607.561130
Sum of electronic and thermal Enthalpies= -3607.560186
Sum of electronic and thermal Free Energies= -3607.676031

| | | | |
|---|---|---|---|
| C | -3.35498800 | 3.81605800 | -0.11502500 |
| O | -2.53726700 | 2.71019600 | -0.95111500 |
| C | -3.71846100 | 4.83019700 | -1.17856700 |
| C | -2.31021600 | 4.22598800 | 0.89095300 |
| C | -4.56248000 | 3.15754900 | 0.52099900 |
| C | -2.93851800 | 1.41561800 | -0.87711500 |
| H | -4.39282800 | 4.38659900 | -1.92543500 |
| H | -4.22942800 | 5.67737000 | -0.69540500 |
| H | -2.82339200 | 5.21094100 | -1.68754000 |
| C | -1.05750800 | 4.72572400 | 0.45732500 |
| H | -2.65538100 | 4.37133800 | 1.91966300 |
| H | -5.12554900 | 3.93593100 | 1.05672200 |
| H | -5.22611700 | 2.71152300 | -0.23245400 |
| H | -4.26475200 | 2.39271900 | 1.25161300 |
| O | -2.36164800 | 0.88491900 | 0.21574300 |
| O | -3.64624500 | 0.84816600 | -1.65457300 |
| H | -0.42358000 | 5.25526500 | 1.17356000 |
| H | -0.90107300 | 5.03729900 | -0.58231600 |
| C | -2.54357100 | -0.52622100 | 0.47109300 |
| H | -2.23863800 | -1.09941000 | -0.41331300 |
| H | -1.90063400 | -0.75665700 | 1.32486700 |
| H | -3.59726200 | -0.71708600 | 0.71355200 |
| Co | -1.03117600 | 2.73415500 | 0.50608900 |
| P | 0.12533700 | 2.44822200 | 2.35411200 |
| P | 0.73678900 | 1.79265100 | -0.55952100 |
| C | 0.36655400 | 3.79502700 | 3.56906600 |
| C | -0.63203500 | 1.03192100 | 3.23278800 |
| C | 1.83660300 | 1.94027700 | 1.92649300 |
| C | 1.36351700 | 2.68544400 | -2.02817800 |
| C | 0.48991700 | 0.06300100 | -1.13397100 |
| C | 2.11473800 | 1.67351800 | 0.64156600 |
| C | 1.26459100 | 4.82644500 | 3.23628000 |
| C | -0.34547600 | 3.86171700 | 4.77714000 |
| C | 0.07407900 | -0.14561500 | 3.52780600 |
| C | -2.01114400 | 1.09956600 | 3.50826400 |
| H | 2.59729900 | 1.87457400 | 2.71179500 |
| C | 2.69835600 | 2.60895400 | -2.46035300 |
| C | 0.44151000 | 3.46123400 | -2.75227200 |
| C | 0.77158600 | -1.02650900 | -0.29269900 |
| C | -0.13630400 | -0.16634500 | -2.37167100 |
| H | 3.11358500 | 1.35060800 | 0.33019600 |
| C | 1.44818300 | 5.90558000 | 4.10376800 |
| H | 1.82699500 | 4.78723300 | 2.29943400 |
| C | -0.16000300 | 4.94682600 | 5.63972900 |
| H | -1.04044300 | 3.06787100 | 5.05601200 |
| C | -0.59124700 | -1.23693800 | 4.09587900 |
| H | 1.14147600 | -0.22316200 | 3.31159900 |
| C | -2.66721400 | 0.01242900 | 4.08862200 |
| H | -2.57800600 | 1.99762100 | 3.25199000 |
| C | 3.10379700 | 3.31049400 | -3.59876200 |
| H | 3.42708700 | 2.00222600 | -1.91866400 |
| C | 0.84995900 | 4.15065400 | -3.89812300 |
| H | -0.59906400 | 3.51523600 | -2.42454400 |
| C | 0.44308100 | -2.32572900 | -0.69042000 |
| H | 1.23885300 | -0.86821100 | 0.68132500 |
| C | -0.47184300 | -1.46635300 | -2.76009500 |
| H | -0.36454100 | 0.66876100 | -3.03866500 |
| C | 0.73431200 | 5.96875800 | 5.30602800 |
| H | 2.15087800 | 6.69920500 | 3.83915300 |
| H | -0.71593400 | 4.98895100 | 6.57938000 |
| C | -1.95893800 | -1.15944900 | 4.37877500 |
| H | -0.03611600 | -2.15168800 | 4.31609600 |
| H | -3.73728800 | 0.07528400 | 4.29862700 |
| C | 2.18185800 | 4.08055200 | -4.31837400 |
| H | 4.14417900 | 3.25265000 | -3.92763200 |
| H | 0.12616700 | 4.74712100 | -4.45849500 |
| C | -0.18202800 | -2.54909700 | -1.92167700 |
| H | 0.67066000 | -3.16545100 | -0.02948500 |
| H | -0.96160000 | -1.63260300 | -3.72248500 |
| H | 0.87730900 | 6.81403800 | 5.98344900 |
| H | -2.47512300 | -2.01534600 | 4.81983600 |
| H | 2.50375700 | 4.62587200 | -5.20890700 |
| H | -0.44438500 | -3.56459100 | -2.22749100 |

**TS-i-ii-4-dppp-sing**

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

Zero-point correction= 0.639081 (Hartree/Particle)
Thermal correction to Energy= 0.678343
Thermal correction to Enthalpy= 0.679287
Thermal correction to Gibbs Free Energy= 0.566733
Sum of electronic and zero-point Energies= -3607.599768
Sum of electronic and thermal Energies= -3607.560505
Sum of electronic and thermal Enthalpies= -3607.559561
Sum of electronic and thermal Free Energies= -3607.672115

| | | | |
|---|---|---|---|
| C | -3.34429000 | 3.86744600 | -0.04058200 |
| O | -2.46099600 | 2.65304600 | -0.97967800 |
| C | -3.65873200 | 4.82764500 | -1.15532300 |
| C | -2.27990000 | 4.20962700 | 0.92952100 |
| C | -4.54111300 | 3.16815100 | 0.54672600 |
| C | -2.88412800 | 1.38719700 | -0.88791700 |
| H | -4.31057500 | 4.36259500 | -1.90770700 |
| H | -4.18716300 | 5.68788300 | -0.71146300 |
| H | -2.74902100 | 5.19950100 | -1.64221400 |
| C | -1.01000500 | 4.67859600 | 0.47755800 |
| H | -2.59720000 | 4.31792000 | 1.97194500 |
| H | -5.13787800 | 3.92938000 | 1.07407000 |
| H | -5.17409700 | 2.71883800 | -0.23024300 |
| H | -4.24449700 | 2.40289700 | 1.27616200 |
| O | -2.34006700 | 0.86208700 | 0.23686800 |
| O | -3.60044900 | 0.80390700 | -1.65217000 |
| H | -0.35924300 | 5.19541400 | 1.18760800 |

| | | | |
|---|---|---|---|
| H | -0.87802500 | 5.02348600 | -0.55476100 |
| C | -2.54035100 | -0.54142700 | 0.50371100 |
| H | -2.24258700 | -1.12792500 | -0.37457100 |
| H | -1.90272200 | -0.77697400 | 1.36027600 |
| H | -3.59673200 | -0.71887600 | 0.74582300 |
| Co | -1.03718800 | 2.70356700 | 0.50601600 |
| P | 0.11707200 | 2.43879000 | 2.33795600 |
| P | 0.71944200 | 1.78601800 | -0.55513800 |
| C | 0.35126400 | 3.79697400 | 3.54240000 |
| C | -0.64083600 | 1.03022200 | 3.22775500 |
| C | 1.82946100 | 1.93116100 | 1.91947900 |
| C | 1.33591600 | 2.69654500 | -2.01727200 |
| C | 0.47741900 | 0.06175500 | -1.14496700 |
| C | 2.10570100 | 1.66167400 | 0.63549000 |
| C | 1.28900200 | 4.79983900 | 3.23276000 |
| C | -0.40128600 | 3.89543300 | 4.72354000 |
| C | 0.07198900 | -0.13869700 | 3.54049400 |
| C | -2.01968800 | 1.09565600 | 3.50379500 |
| H | 2.58674000 | 1.86563500 | 2.70782300 |
| C | 2.67187500 | 2.62953600 | -2.44803200 |
| C | 0.41092200 | 3.47221600 | -2.73745300 |
| C | 0.75387900 | -1.03228300 | -0.30743100 |
| C | -0.13831000 | -0.16078500 | -2.38886400 |
| H | 3.10193600 | 1.33433300 | 0.32099600 |
| C | 1.47033300 | 5.88287700 | 4.09576600 |
| H | 1.88353200 | 4.73649600 | 2.31743500 |
| C | -0.21761100 | 4.98428300 | 5.58160400 |
| H | -1.12628800 | 3.12351200 | 4.98639600 |
| C | -0.58688300 | -1.22336500 | 4.12825800 |
| H | 1.13928000 | -0.21502200 | 3.32361500 |
| C | -2.66925900 | 0.01514100 | 4.10327300 |
| H | -2.59219700 | 1.98523200 | 3.23245200 |
| C | 3.07586400 | 3.34156000 | -3.58042300 |
| H | 3.40305000 | 2.02191600 | -1.91077000 |
| C | 0.81856700 | 4.17249800 | -3.87699700 |
| H | -0.63048800 | 3.51609300 | -2.41267100 |
| C | 0.43195800 | -2.32948800 | -0.71598600 |
| H | 1.21183100 | -0.87906500 | 0.67189800 |
| C | -0.46891600 | -1.45909100 | -2.78742800 |
| H | -0.36191000 | 0.67777400 | -3.05285500 |
| C | 0.71545100 | 5.97818600 | 5.27042700 |
| H | 2.20361700 | 6.65424400 | 3.84914900 |
| H | -0.80557700 | 5.05110400 | 6.50001800 |
| C | -1.95442100 | -1.14776400 | 4.41234600 |
| H | -0.02680300 | -2.13147900 | 4.36276300 |
| H | -3.73938100 | 0.07603700 | 4.31337100 |
| C | 2.15152300 | 4.11278900 | -4.29546400 |
| H | 4.11707400 | 3.29095000 | -3.90783400 |
| H | 0.09260300 | 4.76909800 | -4.43442900 |
| C | -0.18316100 | -2.54616900 | -1.95364100 |
| H | 0.65608400 | -3.17297600 | -0.05869000 |
| H | -0.95100300 | -1.62044300 | -3.75450000 |
| H | 0.85693300 | 6.82651400 | 5.94431900 |
| H | -2.46545600 | -1.99856000 | 4.86896100 |
| H | 2.47218700 | 4.66657000 | -5.18121000 |
| H | -0.44070300 | -3.56033400 | -2.26789500 |

**ii-4-dppp-sing**

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

Zero-point correction= 0.641636 (Hartree/Particle)

Thermal correction to Energy= 0.681214

Thermal correction to Enthalpy= 0.682158

Thermal correction to Gibbs Free Energy= 0.569848

Sum of electronic and zero-point Energies= -3607.630888

Sum of electronic and thermal Energies= -3607.591310

Sum of electronic and thermal Enthalpies= -3607.590366

Sum of electronic and thermal Free Energies= -3607.702676

| | | | |
|---|---|---|---|
| C | -2.77410800 | 1.99402600 | 0.04709500 |
| O | -1.50495400 | 0.00897300 | -2.04537200 |
| C | -3.41110000 | 1.97838100 | -1.30909100 |
| C | -1.46136000 | 2.34901400 | 0.29820300 |
| C | -3.71757800 | 1.76766800 | 1.19403100 |
| C | -2.09608100 | -1.10327100 | -1.78902700 |
| H | -3.95480600 | 1.03645900 | -1.48313300 |
| H | -4.16506500 | 2.78544200 | -1.33043900 |
| H | -2.70385200 | 2.12706000 | -2.12944500 |
| C | -0.36480400 | 2.31717400 | -0.64151800 |
| H | -1.20848800 | 2.54586200 | 1.34379300 |
| H | -4.58762900 | 2.44126400 | 1.11624900 |
| H | -4.11737200 | 0.74002700 | 1.15185900 |
| H | -3.24038000 | 1.92279200 | 2.17172300 |
| O | -1.78769600 | -1.43401700 | -0.45843100 |
| O | -2.79537800 | -1.80548200 | -2.47852900 |
| H | 0.56954700 | 2.78744700 | -0.31915000 |
| H | -0.57385600 | 2.46873800 | -1.70557400 |
| C | -2.28545400 | -2.65689500 | 0.10039000 |
| H | -2.24268100 | -3.44847300 | -0.65845700 |
| H | -1.63878600 | -2.90651800 | 0.94781600 |
| H | -3.32006700 | -2.51826600 | 0.44574900 |
| Co | -0.60691500 | 0.38317500 | -0.31748500 |
| P | 0.50251200 | 0.18870700 | 1.63556200 |
| P | 1.23624800 | -0.35243000 | -1.27970400 |
| C | 0.80533200 | 1.64961800 | 2.69373800 |
| C | -0.29754000 | -1.09373700 | 2.65932800 |
| C | 2.18798800 | -0.41536300 | 1.26541300 |
| C | 1.91965400 | 0.75861000 | -2.55095400 |
| C | 1.00322800 | -2.00677900 | -2.02756900 |
| C | 2.52393700 | -0.61731300 | -0.01494600 |
| C | 1.75700400 | 2.58963700 | 2.25648800 |
| C | 0.08190000 | 1.88907400 | 3.87314700 |
| C | 0.38382100 | -2.24496400 | 3.08871900 |
| C | -1.66716800 | -0.95023700 | 2.94603500 |
| H | 2.89644700 | -0.57388400 | 2.08499600 |
| C | 3.25203200 | 1.20166100 | -2.50760700 |
| C | 1.06357900 | 1.21537100 | -3.57145200 |
| C | 0.83358200 | -3.09991500 | -1.15857800 |
| C | 0.87813100 | -2.19560900 | -3.41251200 |
| H | 3.51243200 | -0.98839600 | -0.30406200 |
| C | 1.97874800 | 3.75518600 | 2.99320500 |
| H | 2.33639500 | 2.41093400 | 1.34717900 |
| C | 0.30811000 | 3.05940900 | 4.60359400 |
| H | -0.65453600 | 1.16740300 | 4.23026800 |
| C | -0.29944800 | -3.23256800 | 3.80507000 |
| H | 1.44260600 | -2.38658200 | 2.86508700 |
| C | -2.33937300 | -1.93227400 | 3.67506800 |
| H | -2.21964900 | -0.08473000 | 2.58037300 |
| C | 3.72530300 | 2.08159500 | -3.48593800 |
| H | 3.92899800 | 0.87405900 | -1.71703800 |
| C | 1.54792000 | 2.08815000 | -4.54765400 |
| H | 0.02019100 | 0.89484400 | -3.58903500 |
| C | 0.54778800 | -4.36593200 | -1.67133900 |
| H | 0.91949900 | -2.96879900 | -0.07774000 |
| C | 0.58686400 | -3.46562600 | -3.91945000 |
| H | 1.00718100 | -1.36018600 | -4.10167100 |
| C | 1.25253000 | 3.99333600 | 4.16536800 |
| H | 2.72252900 | 4.47781100 | 2.64988300 |
| H | -0.25602700 | 3.23822300 | 5.52182000 |
| C | -1.65716500 | -3.07657400 | 4.10285200 |
| H | 0.23484100 | -4.12790700 | 4.13066200 |
| H | -3.40265200 | -1.81035900 | 3.89259200 |
| C | 2.87799200 | 2.52226600 | -4.50704400 |
| H | 4.76219200 | 2.42317500 | -3.44613000 |
| H | 0.88014100 | 2.43630100 | -5.33903600 |
| C | 0.41917600 | -4.55007900 | -3.05296000 |
| H | 0.41877800 | -5.20864800 | -0.98843200 |
| H | 0.49026900 | -3.60481400 | -4.99865600 |
| H | 1.42596600 | 4.90639600 | 4.73969800 |
| H | -2.18613500 | -3.85174200 | 4.66204300 |
| H | 3.25257300 | 3.20958300 | -5.26931600 |
| H | 0.18871300 | -5.54003700 | -3.45362500 |

**iii-4-dppp-sing**

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

Zero-point correction= 0.763891 (Hartree/Particle)

Thermal correction to Energy= 0.814243

Thermal correction to Enthalpy= 0.815187

Thermal correction to Gibbs Free Energy= 0.678996

Sum of electronic and zero-point Energies= -4103.004234

Sum of electronic and thermal Energies= -4102.953883

Sum of electronic and thermal Enthalpies= -4102.952938

Sum of electronic and thermal Free Energies= -4103.089130

| | | | |
|---|---|---|---|
| C | -2.12728000 | 0.71027100 | -3.31476400 |
| O | -0.48431400 | 0.10006900 | 2.21695900 |
| C | -2.69477700 | -0.66452600 | -3.55587600 |
| C | -0.98599300 | 0.95736200 | -2.63114700 |
| C | -2.95784500 | 1.83753300 | -3.87196000 |
| C | -1.54728200 | 0.12630200 | 2.91128600 |
| H | -3.68839500 | -0.75856600 | -3.08608600 |
| H | -2.83648000 | -0.84262500 | -4.63722600 |
| H | -2.06281500 | -1.46783100 | -3.15535700 |
| C | -0.11736100 | -0.00993100 | -1.94340000 |
| H | -0.70732400 | 2.01303900 | -2.52681200 |
| H | -3.14786000 | 1.70831000 | -4.95299000 |
| H | -3.94750100 | 1.86022600 | -3.38007800 |
| H | -2.48384100 | 2.81901600 | -3.71727600 |
| O | -1.40818900 | 0.97156300 | 4.00173600 |
| O | -2.60319700 | -0.48502700 | 2.75586100 |
| H | 0.94413600 | 0.16090600 | -2.16323300 |
| H | -0.36236000 | -1.04301700 | -2.21078800 |
| C | -2.53138200 | 1.08715200 | 4.86202200 |
| H | -2.81528000 | 0.11191500 | 5.29025700 |
| H | -2.24081600 | 1.77409000 | 5.66937700 |
| H | -3.40824500 | 1.49343200 | 4.33089400 |
| Co | -0.32566200 | 0.02465000 | 0.07617100 |
| P | 1.09087700 | -1.76110400 | 0.28692100 |
| P | 1.39424800 | 1.48882100 | 0.54269000 |
| C | 1.59100900 | -2.51993300 | -1.30642100 |
| C | 0.44750200 | -3.17241900 | 1.27720500 |
| C | 2.69904300 | -1.39386800 | 1.13973400 |
| C | 2.69973900 | 1.70731800 | -0.73938300 |
| C | 0.84571100 | 3.19960500 | 0.95770600 |
| C | 2.29560400 | 1.00709100 | 2.09575300 |
| C | 2.65247200 | -1.98422200 | -2.05627600 |
| C | 0.81007800 | -3.54610900 | -1.86673900 |
| C | -0.73719400 | -3.06795700 | 2.01964200 |
| C | 1.18858200 | -4.36948400 | 1.32450900 |
| H | 3.39036200 | -0.95195100 | 0.41135000 |
| H | 3.12883700 | -2.36387400 | 1.42891800 |
| C | 2.51984000 | -0.49418500 | 2.36981400 |
| C | 4.04977900 | 1.37993300 | -0.52291700 |
| C | 2.32316200 | 2.17369200 | -2.01399800 |
| C | -0.03019400 | 3.35552000 | 2.04853400 |
| C | 1.27016800 | 4.33828200 | 0.25587700 |
| H | 1.67508300 | 1.42140600 | 2.89857200 |
| H | 3.23981700 | 1.57182200 | 2.09933000 |
| C | 2.94034400 | -2.48257100 | -3.33023900 |
| H | 3.25428600 | -1.16040500 | -1.66783500 |
| C | 1.09889600 | -4.04026000 | -3.14139400 |
| H | -0.03001200 | -3.96143700 | -1.30629700 |
| C | -1.16983500 | -4.14703600 | 2.79992000 |
| H | -1.33171600 | -2.15850000 | 1.98200200 |
| C | 0.74945500 | -5.44334400 | 2.10113400 |
| H | 2.10855000 | -4.47378200 | 0.74357300 |
| H | 1.67080300 | -0.86663200 | 2.96035500 |
| H | 3.41587100 | -0.59218200 | 3.00285400 |
| C | 4.98652900 | 1.48526100 | -1.55692200 |
| H | 4.39618600 | 1.03811000 | 0.45254700 |
| C | 3.26004900 | 2.29022000 | -3.04240100 |
| H | 1.28848000 | 2.45532500 | -2.20955000 |
| C | -0.45542400 | 4.62820900 | 2.43337400 |
| H | -0.38906100 | 2.48360500 | 2.59427400 |
| C | 0.82579500 | 5.61067100 | 0.63594600 |
| H | 1.95750600 | 4.25165000 | -0.58587800 |
| C | 2.16627400 | -3.51162800 | -3.87578800 |
| H | 3.77052100 | -2.05685200 | -3.89904500 |
| H | 0.48508800 | -4.84029700 | -3.56242500 |
| C | -0.43304800 | -5.33341400 | 2.84361100 |
| H | -2.09531300 | -4.05209900 | 3.37385500 |
| H | 1.33124700 | -6.36810900 | 2.12543200 |
| C | 4.59475500 | 1.93462500 | -2.82063700 |
| H | 6.02819500 | 1.21597800 | -1.36701500 |
| H | 2.94222100 | 2.65412800 | -4.02227500 |
| C | -0.03447200 | 5.76089100 | 1.72638300 |
| H | -1.13255300 | 4.73215600 | 3.28511000 |
| H | 1.16528000 | 6.48691000 | 0.07793900 |
| H | 2.39126100 | -3.89820900 | -4.87281000 |
| H | -0.77720500 | -6.17371500 | 3.45209600 |
| H | 5.32688300 | 2.01379800 | -3.62778500 |
| H | -0.37589300 | 6.75532100 | 2.02467100 |
| C | -3.59432000 | 0.31978800 | -0.33323800 |
| H | -4.65714500 | 0.41397300 | -0.54254100 |
| C | -3.01702200 | -0.95705100 | -0.29944500 |
| C | -2.81501100 | 1.47896400 | -0.21275500 |
| O | -1.79780200 | -1.25357600 | -0.16982300 |
| O | -1.58025700 | 1.55626000 | 0.03487700 |
| O | -3.88585100 | -1.97379600 | -0.47537000 |
| O | -3.49230200 | 2.63109600 | -0.39863500 |
| C | -3.34831400 | -3.29234800 | -0.57524500 |
| H | -2.83242700 | -3.58679800 | 0.35008000 |
| H | -4.20434700 | -3.95482400 | -0.75543800 |
| H | -2.63607600 | -3.36734900 | -1.41190300 |
| C | -2.74047500 | 3.84436100 | -0.42746200 |
| H | -3.46677900 | 4.64490700 | -0.61712200 |
| H | -2.22293200 | 4.02078200 | 0.52473100 |
| H | -1.98993600 | 3.82352000 | -1.23252300 |

**TS-iii-iv-4-dppp-sing**

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

Zero-point correction= 0.761229 (Hartree/Particle)

Thermal correction to Energy= 0.811423

Thermal correction to Enthalpy= 0.812367

Thermal correction to Gibbs Free Energy= 0.676778

Sum of electronic and zero-point Energies= -4102.962507

Sum of electronic and thermal Energies= -4102.912313

Sum of electronic and thermal Enthalpies= -4102.911369

Sum of electronic and thermal Free Energies= -4103.046958

| | | | |
|---|---|---|---|
| C | -3.92733300 | 2.64908500 | -1.95493500 |
| O | -2.04022500 | 2.06022500 | 2.91287500 |
| C | -4.30053200 | 1.38832700 | -2.71756600 |
| C | -2.54092100 | 2.84662100 | -1.61684400 |
| C | -4.63550300 | 3.88828100 | -2.48010700 |
| C | -3.18390200 | 2.18347900 | 3.43349100 |
| H | -5.38911100 | 1.23373800 | -2.73235400 |
| H | -3.95627000 | 1.48897200 | -3.76113200 |
| H | -3.83165800 | 0.48495200 | -2.30549600 |
| C | -1.56890600 | 1.85034100 | -1.40471700 |
| H | -2.23382900 | 3.88897200 | -1.48310700 |
| H | -4.26618000 | 4.11664500 | -3.49488900 |
| H | -5.72372900 | 3.73982500 | -2.54549700 |
| H | -4.44411700 | 4.76873600 | -1.84904400 |
| O | -3.21536800 | 3.20502000 | 4.38396200 |
| O | -4.22232300 | 1.54678500 | 3.22686300 |
| H | -0.52156600 | 2.09657600 | -1.59385200 |
| H | -1.81471500 | 0.82182600 | -1.68545000 |
| C | -4.46807300 | 3.46357900 | 4.99295000 |
| H | -4.86641200 | 2.57125900 | 5.50341300 |
| H | -4.30615500 | 4.26681300 | 5.72659900 |
| H | -5.21945200 | 3.79146600 | 4.25407400 |
| Co | -1.79163200 | 1.98668500 | 0.67528900 |
| P | -0.32760500 | 0.12730400 | 0.97360000 |

| | | | |
|---|---|---|---|
| P | -0.05026400 | 3.46935600 | 1.13867800 |
| C | 0.25225300 | -0.64090500 | -0.59185600 |
| C | -0.97519900 | -1.28798400 | 1.96007900 |
| C | 1.24770300 | 0.53693600 | 1.88322000 |
| C | 1.28507200 | 3.63269400 | -0.12470300 |
| C | -0.51333400 | 5.21701300 | 1.51594200 |
| C | 0.82387100 | 2.99713200 | 2.71732700 |
| C | 1.28851000 | -0.04430500 | -1.33441100 |
| C | -0.45869600 | -1.70932500 | -1.16913800 |
| C | -2.18258800 | -1.14883300 | 2.66256300 |
| C | -0.25988700 | -2.49714900 | 2.05314500 |
| H | 1.96907600 | 0.95137800 | 1.16701900 |
| H | 1.67615600 | -0.40880000 | 2.24791000 |
| C | 0.99299400 | 1.49982700 | 3.05420200 |
| C | 2.62606100 | 3.28051500 | 0.10621200 |
| C | 0.92599300 | 4.06548700 | -1.41704500 |
| C | -1.49200200 | 5.41862300 | 2.50774400 |
| C | 0.04489400 | 6.33334700 | 0.87189700 |
| H | 0.20141900 | 3.45484900 | 3.49659900 |
| H | 1.78713800 | 3.53005400 | 2.72881200 |
| C | 1.62059900 | -0.52083300 | -2.60591900 |
| H | 1.83590400 | 0.81331900 | -0.93846600 |
| C | -0.12612400 | -2.18312700 | -2.44169400 |
| H | -1.27977800 | -2.17754400 | -0.62151400 |
| C | -2.66529300 | -2.20780800 | 3.44163600 |
| H | -2.74455200 | -0.21814200 | 2.60131200 |
| C | -0.74769900 | -3.55160400 | 2.82830800 |
| H | 0.67969500 | -2.62252100 | 1.50827400 |
| H | 0.09176300 | 1.17059900 | 3.59065400 |
| H | 1.83330700 | 1.41408200 | 3.76249300 |
| C | 3.56929800 | 3.32794900 | -0.92688000 |
| H | 2.95800200 | 2.96224100 | 1.09489800 |
| C | 1.86834200 | 4.12457500 | -2.44560000 |
| H | -0.10225300 | 4.36707200 | -1.62522300 |
| C | -1.89152200 | 6.71234000 | 2.84902400 |
| H | -1.95165000 | 4.56367400 | 3.00417800 |
| C | -0.37013700 | 7.62741300 | 1.20886400 |
| H | 0.81162400 | 6.20642700 | 0.10619500 |
| C | 0.91688900 | -1.59311700 | -3.16419700 |
| H | 2.43075700 | -0.04375700 | -3.16333600 |
| H | -0.68714100 | -3.01750100 | -2.87053300 |
| C | -1.95468800 | -3.40850200 | 3.52518000 |
| H | -3.60664300 | -2.08734700 | 3.98467100 |
| H | -0.18572300 | -4.48723100 | 2.88866100 |
| C | 3.19368400 | 3.74369700 | -2.20698100 |
| H | 4.60350500 | 3.03901600 | -0.72429100 |
| H | 1.56337500 | 4.46317900 | -3.43875600 |
| C | -1.33820800 | 7.82167900 | 2.19842600 |
| H | -2.65111300 | 6.85282200 | 3.62276900 |
| H | 0.07340400 | 8.48578200 | 0.69747600 |
| H | 1.17602800 | -1.96370300 | -4.15908200 |
| H | -2.33722400 | -4.23370300 | 4.13166900 |
| H | 3.93007500 | 3.77726600 | -3.01352800 |
| H | -1.65951700 | 8.83259300 | 2.46245200 |
| C | -4.97698700 | 2.35530100 | -0.21093600 |
| H | -6.03001600 | 2.40351700 | -0.49128200 |
| C | -4.51597300 | 1.02933600 | 0.15216900 |
| C | -4.49828700 | 3.47349300 | 0.58239500 |
| O | -3.36365900 | 0.73389400 | 0.48518300 |
| O | -3.35202100 | 3.58476400 | 1.00874200 |
| O | -5.43318500 | 0.07335000 | -0.01418000 |
| O | -5.39951900 | 4.45846900 | 0.72598300 |
| C | -5.00489800 | -1.27859800 | 0.20044300 |
| H | -4.65580300 | -1.41602400 | 1.23350000 |
| H | -5.88067300 | -1.90749700 | 0.00263100 |
| H | -4.18483200 | -1.53946400 | -0.48573100 |
| C | -4.95277200 | 5.62566800 | 1.42689100 |
| H | -5.81640100 | 6.29917000 | 1.47947000 |
| H | -4.60730400 | 5.36119000 | 2.43650100 |
| H | -4.12004000 | 6.10865300 | 0.89497100 |

**iv-4-dppp-sing**

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

Zero-point correction= 0.764198
(Hartree/Particle)

Thermal correction to Energy= 0.814283

Thermal correction to Enthalpy= 0.815227

Thermal correction to Gibbs Free Energy= 0.678853

Sum of electronic and zero-point Energies= -4102.994532

Sum of electronic and thermal Energies= -4102.944447

Sum of electronic and thermal Enthalpies= -4102.943503

Sum of electronic and thermal Free Energies= -4103.079877

| | | | |
|---|---|---|---|
| C | -3.87223700 | 2.85420700 | -1.68753200 |
| O | -2.20930300 | 2.54749400 | 2.33457500 |
| C | -4.06931200 | 1.80885500 | -2.81031200 |
| C | -2.38242500 | 2.95092200 | -1.27094300 |
| C | -4.29717100 | 4.22635300 | -2.25068100 |
| C | -3.23867200 | 2.46381300 | 3.06282300 |
| H | -5.10520600 | 1.83380000 | -3.18570500 |
| H | -3.39302100 | 2.01952100 | -3.65146600 |
| H | -3.86317900 | 0.78402900 | -2.46708700 |
| C | -1.43191800 | 1.94849900 | -1.57289100 |
| H | -2.02936100 | 3.98861800 | -1.24307500 |
| H | -3.70365100 | 4.45908000 | -3.14846500 |
| H | -5.36199900 | 4.22758100 | -2.53812700 |
| H | -4.13615600 | 5.02723400 | -1.51685300 |
| O | -3.02592500 | 3.03283900 | 4.30224000 |
| O | -4.33676900 | 1.94982400 | 2.81346300 |
| H | -0.40619200 | 2.20576000 | -1.85066700 |
| H | -1.75360200 | 0.98843000 | -1.98735000 |
| C | -4.09067400 | 2.96354400 | 5.23745500 |
| H | -4.45881300 | 1.93230200 | 5.36034000 |
| H | -3.69349400 | 3.33066100 | 6.19446300 |
| H | -4.94199100 | 3.59742500 | 4.93667000 |
| Co | -1.66583300 | 2.00728500 | 0.42687300 |
| P | -0.29073400 | 0.14961000 | 0.85942500 |
| P | 0.11767900 | 3.45249000 | 0.93215200 |
| C | 0.33741700 | -0.66624700 | -0.65986900 |
| C | -1.01704300 | -1.20853900 | 1.87047800 |
| C | 1.22881800 | 0.52346000 | 1.87880200 |
| C | 1.53318200 | 3.56215000 | -0.24819400 |
| C | -0.28333800 | 5.23369000 | 1.17061000 |
| C | 0.87467700 | 3.02135300 | 2.58165300 |
| C | 1.44082100 | -0.12874000 | -1.34833200 |
| C | -0.38942700 | -1.70894100 | -1.26349800 |
| C | -2.14900000 | -0.91940800 | 2.64741800 |
| C | -0.42730400 | -2.48276900 | 1.96424000 |
| H | 2.02497600 | 0.89888000 | 1.22294500 |
| H | 1.59209500 | -0.42222400 | 2.30773400 |
| C | 0.88133700 | 1.53406600 | 2.98743300 |
| C | 2.83932400 | 3.12628400 | 0.02810000 |
| C | 1.25887200 | 4.07664500 | -1.53117600 |
| C | -1.63300800 | 5.59197600 | 1.29426300 |
| C | 0.70973200 | 6.22533500 | 1.25896500 |
| H | 0.26332800 | 3.58067400 | 3.30305800 |
| H | 1.88597500 | 3.45555300 | 2.61983700 |
| C | 1.82202500 | -0.63928600 | -2.59245700 |
| H | 2.00219100 | 0.70936700 | -0.93139400 |
| C | -0.00673200 | -2.21729200 | -2.50843100 |
| H | -1.26319700 | -2.12834400 | -0.75929800 |
| C | -2.68327300 | -1.88743100 | 3.50564000 |
| H | -2.61768700 | 0.05927800 | 2.56185700 |
| C | -0.96852800 | -3.45084000 | 2.81340000 |
| H | 0.45698600 | -2.72255200 | 1.36809600 |
| H | -0.10914200 | 1.28480200 | 3.40078500 |
| H | 1.59916400 | 1.41612900 | 3.81551200 |
| C | 3.83402400 | 3.17155300 | -0.95687400 |
| H | 3.10529900 | 2.74928000 | 1.01646300 |
| C | 2.25063700 | 4.12762700 | -2.51185700 |
| H | 0.25743600 | 4.44599500 | -1.76604200 |

| | | | |
|---|---|---|---|
| C | -1.98757500 | 6.92889200 | 1.50680900 |
| H | -2.40389100 | 4.82695900 | 1.21491400 |
| C | 0.35148600 | 7.55918200 | 1.47395400 |
| H | 1.76468100 | 5.95919300 | 1.15239200 |
| C | 1.10275200 | -1.68754200 | -3.17661200 |
| H | 2.68398200 | -0.20840900 | -3.10844100 |
| H | -0.58070900 | -3.03150200 | -2.95851000 |
| C | -2.09783000 | -3.15380600 | 3.58814600 |
| H | -3.56539400 | -1.64981400 | 4.10602900 |
| H | -0.50671500 | -4.43973300 | 2.87416100 |
| C | 3.54223300 | 3.66466100 | -2.23089400 |
| H | 4.84178500 | 2.82104300 | -0.72054100 |
| H | 2.01381200 | 4.52776000 | -3.50088300 |
| C | -0.99860000 | 7.91363400 | 1.59817700 |
| H | -3.04410900 | 7.19554200 | 1.59563200 |
| H | 1.12773100 | 8.32602200 | 1.54143200 |
| H | 1.40126000 | -2.08545500 | -4.14969000 |
| H | -2.51898800 | -3.91156500 | 4.25392300 |
| H | 4.31781900 | 3.69686400 | -2.99996000 |
| H | -1.27581600 | 8.95845000 | 1.76180800 |
| C | -4.87004600 | 2.44823000 | -0.55785800 |
| H | -5.85058100 | 2.25659800 | -1.01784300 |
| C | -4.49290000 | 1.14066600 | 0.11429500 |
| C | -5.16597800 | 3.49395000 | 0.51867500 |
| O | -3.34541700 | 0.75782500 | 0.29611800 |
| O | -4.44953000 | 4.41046400 | 0.84210300 |
| O | -5.54427800 | 0.41260400 | 0.43255300 |
| O | -6.38041700 | 3.28614100 | 1.03475800 |
| C | -5.32290100 | -0.75994700 | 1.23565700 |
| H | -4.97857600 | -0.44065000 | 2.22738200 |
| H | -6.29155400 | -1.26845800 | 1.29940200 |
| H | -4.57001000 | -1.41368700 | 0.77476800 |
| C | -6.74512500 | 4.09371800 | 2.15992500 |
| H | -7.78186600 | 3.83104600 | 2.40172900 |
| H | -6.08155700 | 3.85454400 | 3.00240200 |
| H | -6.66758500 | 5.16364800 | 1.91750900 |

**iii-4-dppp-trip**

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

Zero-point correction= 0.758067 (Hartree/Particle)
Thermal correction to Energy= 0.810821
Thermal correction to Enthalpy= 0.811765
Thermal correction to Gibbs Free Energy= 0.666256
Sum of electronic and zero-point Energies= -4103.008029
Sum of electronic and thermal Energies= -4102.955276
Sum of electronic and thermal Enthalpies= -4102.954332
Sum of electronic and thermal Free Energies= -4103.099841

| | | | |
|---|---|---|---|
| C | -3.22407200 | 3.07577800 | -2.81471300 |
| O | -1.78821500 | 1.90895200 | 2.77452800 |
| C | -3.95188100 | 1.80276400 | -3.13310400 |
| C | -2.00737300 | 3.12100700 | -2.15788800 |
| C | -3.87869500 | 4.33950900 | -3.29010300 |
| C | -2.54608000 | 2.24199700 | 3.74227100 |
| H | -3.50971700 | 0.91994700 | -2.65597100 |
| H | -5.00435300 | 1.87064500 | -2.81443800 |
| H | -3.96392900 | 1.63760900 | -4.22599300 |
| C | -1.29336200 | 2.03216800 | -1.61539900 |
| H | -1.56294200 | 4.11066000 | -2.01937600 |
| H | -4.09125600 | 4.29403400 | -4.37342100 |
| H | -4.85070900 | 4.47303100 | -2.78360600 |
| H | -3.26468800 | 5.22972400 | -3.08927500 |
| O | -1.85520400 | 2.26288100 | 4.93065700 |
| O | -3.74325200 | 2.52436700 | 3.71672600 |
| H | -0.22569600 | 2.15601700 | -1.42457300 |
| H | -1.62145600 | 1.01457800 | -1.82272400 |
| C | -2.58584100 | 2.67303400 | 6.07738900 |
| H | -3.46366700 | 2.02975200 | 6.25064500 |
| H | -1.89825200 | 2.59922500 | 6.93141800 |
| H | -2.93721500 | 3.71358700 | 5.97734400 |
| Co | -1.96972300 | 2.12571300 | 0.71029700 |
| P | -1.08894100 | -0.17695500 | 0.93787800 |
| P | 0.13955200 | 3.34775800 | 1.22417900 |
| C | -0.73470500 | -1.17676000 | -0.56056200 |
| C | -2.19297400 | -1.30380600 | 1.89105600 |
| C | 0.46524000 | -0.20450800 | 1.94869400 |
| C | 1.09932200 | 4.11573900 | -0.14229800 |
| C | -0.01468100 | 4.75107600 | 2.41004300 |
| C | 1.33982600 | 2.24609000 | 2.11988000 |
| C | 0.55000000 | -1.56432000 | -0.97106700 |
| C | -1.83636000 | -1.49672200 | -1.37943300 |
| C | -1.88086800 | -2.66892700 | 2.02164700 |
| C | -3.34959400 | -0.80136600 | 2.50854000 |
| H | 0.87423700 | -1.22678200 | 1.91779900 |
| H | 0.11950600 | -0.02577000 | 2.97772000 |
| C | 1.55261100 | 0.82071200 | 1.57565900 |
| C | 0.52723700 | 5.23732900 | -0.77433000 |
| C | 2.30904200 | 3.60371100 | -0.63885500 |
| C | 1.11430000 | 5.51145000 | 2.76503700 |
| C | -1.25458600 | 5.05269500 | 2.99404400 |
| H | 0.93818000 | 2.19669300 | 3.14293800 |
| H | 2.30312400 | 2.77715600 | 2.17605600 |
| C | 0.72835400 | -2.25958000 | -2.17439400 |
| H | 1.42566600 | -1.33595700 | -0.36103900 |
| C | -1.65726800 | -2.19428800 | -2.57422600 |
| H | -2.83917700 | -1.18784000 | -1.07297900 |
| C | -2.70955700 | -3.51669800 | 2.76171300 |
| H | -0.99091000 | -3.07748400 | 1.53543800 |
| C | -4.17829100 | -1.65388100 | 3.24627400 |
| H | -3.60611800 | 0.25098400 | 2.40370900 |
| H | 2.50012500 | 0.45446900 | 2.00402600 |
| H | 1.71600000 | 0.83567400 | 0.48560100 |
| C | 1.15107600 | 5.83369800 | -1.87070700 |
| H | -0.41486100 | 5.64432600 | -0.39804600 |
| C | 2.93047100 | 4.19947200 | -1.74383300 |
| H | 2.78459600 | 2.73973200 | -0.17167800 |
| C | 1.00521600 | 6.54986400 | 3.69370100 |
| H | 2.08474700 | 5.29964300 | 2.30822000 |
| C | -1.36167100 | 6.09505600 | 3.92153600 |
| H | -2.13895700 | 4.49048800 | 2.70267700 |
| C | -0.37060600 | -2.57637100 | -2.97708400 |
| H | 1.73468000 | -2.55616600 | -2.48083000 |
| H | -2.52295700 | -2.43658900 | -3.19577300 |
| C | -3.86130200 | -3.00994200 | 3.37578700 |
| H | -2.45750700 | -4.57608700 | 2.85612400 |
| H | -5.07787800 | -1.25233400 | 3.71999000 |
| C | 2.35517500 | 5.31274000 | -2.36217400 |
| H | 0.69487500 | 6.70577400 | -2.34591900 |
| H | 3.87197500 | 3.78958600 | -2.11807300 |
| C | -0.23426300 | 6.84251500 | 4.27595000 |
| H | 1.88943900 | 7.13385800 | 3.96165400 |
| H | -2.33405800 | 6.32230600 | 4.36620000 |
| H | -0.22745400 | -3.11914300 | -3.91467200 |
| H | -4.51169100 | -3.67348600 | 3.95158900 |
| H | 2.84285000 | 5.77590100 | -3.22346000 |
| H | -0.32007800 | 7.65589500 | 5.00107100 |
| C | -5.11488600 | 3.24493600 | -0.04451800 |
| H | -6.10713200 | 3.59870600 | -0.31626600 |
| C | -4.86202600 | 1.86147400 | -0.06087900 |
| C | -4.10527600 | 4.19075200 | 0.21948400 |
| O | -3.77030100 | 1.27499300 | 0.16019500 |
| O | -2.91404800 | 3.96918000 | 0.55365200 |
| O | -5.93738000 | 1.10793400 | -0.38713000 |
| O | -4.50231100 | 5.47517600 | 0.07157400 |
| C | -5.75474700 | -0.30541700 | -0.45723900 |
| H | -5.33535500 | -0.70508200 | 0.47769600 |
| H | -6.74992100 | -0.73124500 | -0.63714400 |
| H | -5.08545200 | -0.57609300 | -1.28891900 |
| C | -3.51901300 | 6.49073300 | 0.26214800 |
| H | -4.04191700 | 7.44720500 | 0.13633400 |
| H | -3.06873700 | 6.43620800 | 1.26430000 |

| | | | |
|---|---|---|---|
| H | -2.71612700 | 6.40804500 | -0.48749500 |

**TS-iii-iv-4-dppp-trip**

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

Zero-point correction= 0.759700 (Hartree/Particle)

Thermal correction to Energy= 0.810817

Thermal correction to Enthalpy= 0.811762

Thermal correction to Gibbs Free Energy= 0.671334

Sum of electronic and zero-point Energies= -4102.983676

Sum of electronic and thermal Energies= -4102.932559

Sum of electronic and thermal Enthalpies= -4102.931615

Sum of electronic and thermal Free Energies= -4103.072043

| | | | |
|---|---|---|---|
| C | -3.39655600 | 3.11426300 | -2.35638200 |
| O | -1.76047700 | 1.91964000 | 2.75184000 |
| C | -3.89136600 | 1.89790100 | -3.10942400 |
| C | -2.08941400 | 3.06921900 | -1.76683100 |
| C | -3.77130100 | 4.43553000 | -2.99969400 |
| C | -2.50767500 | 2.26142600 | 3.71358700 |
| H | -3.68552900 | 0.95811600 | -2.58058600 |
| H | -4.97057200 | 1.95589300 | -3.30666900 |
| H | -3.36887600 | 1.84801000 | -4.08057500 |
| C | -1.29904100 | 1.93626400 | -1.53964500 |
| H | -1.64392500 | 4.04013700 | -1.53397200 |
| H | -3.18254800 | 4.56580000 | -3.92508700 |
| H | -4.83573600 | 4.46973900 | -3.27426000 |
| H | -3.55347400 | 5.28847000 | -2.34077800 |
| O | -1.78398700 | 2.42206800 | 4.88648000 |
| O | -3.72659100 | 2.45222900 | 3.72957500 |
| H | -0.21518800 | 2.06325200 | -1.48267500 |
| H | -1.62208300 | 0.96697000 | -1.92207000 |
| C | -2.50941000 | 2.87111700 | 6.01791400 |
| H | -3.34026400 | 2.19084900 | 6.26823900 |
| H | -1.79906100 | 2.90882200 | 6.85654900 |
| H | -2.93265700 | 3.87709900 | 5.85415000 |
| Co | -1.93218900 | 2.10070000 | 0.55736100 |
| P | -1.09185600 | -0.15009700 | 0.91233000 |
| P | 0.13247900 | 3.35095900 | 1.14853200 |
| C | -0.70261300 | -1.20117800 | -0.54725600 |
| C | -2.20741900 | -1.27248200 | 1.86578000 |
| C | 0.44223700 | -0.17227800 | 1.95337600 |
| C | 1.12026700 | 4.09426600 | -0.22083600 |
| C | 0.02216800 | 4.77993400 | 2.31581300 |
| C | 1.34419100 | 2.27101100 | 2.06464600 |
| C | 0.58904400 | -1.60769800 | -0.91558400 |
| C | -1.78348100 | -1.54546100 | -1.38357300 |
| C | -1.91616300 | -2.64359300 | 1.98408400 |
| C | -3.35178200 | -0.75895600 | 2.49686500 |
| H | 0.83802900 | -1.20033200 | 1.95859100 |
| H | 0.08021000 | 0.04416200 | 2.96884000 |
| C | 1.54600500 | 0.82850300 | 1.56583100 |
| C | 0.62520200 | 5.26738300 | -0.82511100 |
| C | 2.27307700 | 3.49989600 | -0.76163500 |
| C | 1.16299200 | 5.53794600 | 2.63870000 |
| C | -1.20242100 | 5.10017700 | 2.92181700 |
| H | 0.95362000 | 2.25367700 | 3.09266800 |
| H | 2.31113000 | 2.79814800 | 2.09142000 |
| C | 0.79428100 | -2.34220600 | -2.09140400 |
| H | 1.45107200 | -1.36443200 | -0.29217800 |
| C | -1.57983700 | -2.28232300 | -2.55044200 |
| H | -2.79292700 | -1.22648100 | -1.11027600 |
| C | -2.75322700 | -3.48638100 | 2.72096200 |
| H | -1.03495000 | -3.06140200 | 1.48992700 |
| C | -4.18886500 | -1.60603300 | 3.23167500 |
| H | -3.58844900 | 0.29944300 | 2.41172900 |
| H | 2.48576600 | 0.46393300 | 2.01332100 |
| H | 1.71852000 | 0.81005500 | 0.47735300 |
| C | 1.26271500 | 5.82861400 | -1.93270300 |
| H | -0.26526700 | 5.75277400 | -0.41545500 |
| C | 2.90999600 | 4.06027300 | -1.87623600 |
| H | 2.69284700 | 2.59484600 | -0.31973500 |
| C | 1.08088400 | 6.59157500 | 3.55275900 |
| H | 2.12276100 | 5.31153800 | 2.16659000 |
| C | -1.28371600 | 6.15902900 | 3.83376900 |
| H | -2.09477900 | 4.53739100 | 2.65781300 |
| C | -0.28558900 | -2.68187600 | -2.91024400 |
| H | 1.80674800 | -2.65202100 | -2.36293800 |
| H | -2.43175500 | -2.54271700 | -3.18377400 |
| C | -3.89383900 | -2.96856100 | 3.34623400 |
| H | -2.51596600 | -4.55024400 | 2.80432100 |
| H | -5.07755900 | -1.19396200 | 3.71728900 |
| C | 2.40787100 | 5.22331900 | -2.46599900 |
| H | 0.86434700 | 6.74185400 | -2.38221800 |
| H | 3.80644800 | 3.58317000 | -2.28070400 |
| C | -0.14478700 | 6.90370000 | 4.15455700 |
| H | 1.97491400 | 7.17240100 | 3.79445200 |
| H | -2.24533600 | 6.40092600 | 4.29444000 |
| H | -0.12224800 | -3.25562400 | -3.82589400 |
| H | -4.55130300 | -3.62751600 | 3.91948900 |
| H | 2.90652700 | 5.65946400 | -3.33514000 |
| H | -0.21020300 | 7.72932900 | 4.86805000 |
| C | -4.83051100 | 3.17732000 | -0.74100600 |
| H | -5.74463600 | 3.53447000 | -1.21483300 |
| C | -4.81218700 | 1.77554700 | -0.38760000 |
| C | -4.16707600 | 4.10684800 | 0.13984600 |
| O | -3.86676800 | 1.19106800 | 0.15256200 |
| O | -3.15591000 | 3.85065600 | 0.80385500 |
| O | -5.90143800 | 1.10497700 | -0.78397200 |
| O | -4.67429300 | 5.34825900 | 0.10889700 |
| C | -5.90447800 | -0.31258400 | -0.57435100 |
| H | -5.70128500 | -0.55653100 | 0.47840800 |
| H | -6.90304300 | -0.65936900 | -0.86471000 |
| H | -5.14328000 | -0.79779300 | -1.20453700 |
| C | -3.99169600 | 6.34054100 | 0.88498000 |
| H | -4.50609900 | 7.28800200 | 0.68597100 |
| H | -4.04254500 | 6.09881100 | 1.95706100 |
| H | -2.93374400 | 6.40874000 | 0.59157700 |

**iv-4-dppp-trip**

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

Zero-point correction= 0.763855 (Hartree/Particle)

Thermal correction to Energy= 0.814300

Thermal correction to Enthalpy= 0.815244

Thermal correction to Gibbs Free Energy= 0.676496

Sum of electronic and zero-point Energies= -4103.012695

Sum of electronic and thermal Energies= -4102.962249

Sum of electronic and thermal Enthalpies= -4102.961305

Sum of electronic and thermal Free Energies= -4103.100053

| | | | |
|---|---|---|---|
| C | -3.39437300 | 2.61940800 | -2.31953100 |
| O | -2.15013300 | 2.24420300 | 2.04005700 |
| C | -3.53793500 | 1.32618100 | -3.14656300 |
| C | -1.96889400 | 2.79643100 | -1.76449500 |
| C | -3.66688800 | 3.81762800 | -3.25747400 |
| C | -3.24178800 | 2.39890000 | 2.65543600 |
| H | -4.56902900 | 1.22231500 | -3.52073400 |
| H | -2.86464900 | 1.35285300 | -4.01580900 |
| H | -3.29481600 | 0.42832800 | -2.56214600 |
| C | -0.93642900 | 1.88520100 | -1.94636200 |
| H | -1.70722600 | 3.84372300 | -1.58209600 |
| H | -2.91721600 | 3.84154700 | -4.06329100 |
| H | -4.66438500 | 3.73846500 | -3.72032800 |
| H | -3.61148500 | 4.77281900 | -2.71505700 |
| O | -3.05355700 | 2.41673800 | 4.02394300 |
| O | -4.38411500 | 2.53063600 | 2.20179200 |
| H | 0.10722700 | 2.20779300 | -1.97373000 |
| H | -1.11883400 | 0.90725600 | -2.39542400 |
| C | -4.20218800 | 2.65082600 | 4.82426400 |
| H | -4.99013300 | 1.90400100 | 4.63549500 |
| H | -3.87417500 | 2.58285700 | 5.87115900 |
| H | -4.62651500 | 3.65213000 | 4.64008600 |
| Co | -1.50247000 | 1.94924700 | 0.11542600 |

| | | | |
|---|---|---|---|
| P | -0.17788600 | 0.04900500 | 0.48686800 |
| P | 0.31374000 | 3.46036000 | 0.98455300 |
| C | -0.22174900 | -1.21802100 | -0.84771600 |
| C | -0.60052000 | -0.94354200 | 1.98145100 |
| C | 1.61305100 | 0.47905600 | 0.68202200 |
| C | 1.78501100 | 4.11231800 | 0.08507900 |
| C | -0.30321300 | 4.96487200 | 1.85664700 |
| C | 1.01730200 | 2.42886400 | 2.36602900 |
| C | 0.89209200 | -1.61790900 | -1.60164700 |
| C | -1.49002700 | -1.73549400 | -1.17757200 |
| C | -1.91809400 | -0.86628400 | 2.46462100 |
| C | 0.32463300 | -1.77174000 | 2.64008100 |
| H | 1.84846900 | 1.06518500 | -0.22209400 |
| H | 2.24467500 | -0.42179700 | 0.64656300 |
| C | 1.96353900 | 1.28632300 | 1.94842600 |
| C | 3.02918300 | 4.32606000 | 0.70606200 |
| C | 1.65023300 | 4.42547600 | -1.27937900 |
| C | -0.96574200 | 4.85798800 | 3.09416900 |
| C | -0.23435400 | 6.22634700 | 1.23663200 |
| H | 0.10979800 | 2.01993300 | 2.83473000 |
| H | 1.51212800 | 3.06577000 | 3.11583800 |
| C | 0.74268700 | -2.52859400 | -2.65609200 |
| H | 1.88647000 | -1.22434400 | -1.38345100 |
| C | -1.63423400 | -2.64888000 | -2.22294600 |
| H | -2.36920300 | -1.40156300 | -0.62069800 |
| C | -2.30327700 | -1.60489100 | 3.58783800 |
| H | -2.63245400 | -0.21942700 | 1.95584900 |
| C | -0.06057400 | -2.50190500 | 3.76879500 |
| H | 1.35101600 | -1.85706900 | 2.27473500 |
| H | 2.03160600 | 0.59395500 | 2.80322300 |
| H | 2.97955200 | 1.68528500 | 1.80112600 |
| C | 4.11260600 | 4.82349700 | -0.02357100 |
| H | 3.15776700 | 4.11475100 | 1.76994200 |
| C | 2.73124100 | 4.93417700 | -2.00788000 |
| H | 0.68825100 | 4.28153500 | -1.77681900 |
| C | -1.53873400 | 5.98501900 | 3.69149700 |
| H | -1.06934300 | 3.89158300 | 3.58535200 |
| C | -0.81001100 | 7.35047700 | 1.83691400 |
| H | 0.27204500 | 6.33798300 | 0.27496400 |
| C | -0.51626500 | -3.04876300 | -2.96737600 |
| H | 1.61919900 | -2.83071800 | -3.23527000 |
| H | -2.62448700 | -3.04335900 | -2.46527600 |
| C | -1.37496800 | -2.41950600 | 4.24489000 |
| H | -3.33092800 | -1.53510600 | 3.95417400 |
| H | 0.66747300 | -3.13947900 | 4.27706700 |
| C | 3.96670400 | 5.12750900 | -1.38251000 |
| H | 5.07404700 | 4.97994800 | 0.47236900 |
| H | 2.60673700 | 5.17586100 | -3.06640000 |
| C | -1.46592700 | 7.23512000 | 3.06731500 |
| H | -2.05221900 | 5.87950200 | 4.65114600 |
| H | -0.74392400 | 8.32142700 | 1.33870900 |
| H | -0.62927800 | -3.75906700 | -3.79026000 |
| H | -1.67327700 | -2.99077500 | 5.12781000 |
| H | 4.81482800 | 5.51736200 | -1.95100000 |
| H | -1.91759600 | 8.11334900 | 3.53572500 |
| C | -4.51257400 | 2.60820900 | -1.22919400 |
| H | -5.49103800 | 2.57299400 | -1.73041400 |
| C | -4.46680100 | 1.36422900 | -0.35312400 |
| C | -4.56713200 | 3.85409400 | -0.33779800 |
| O | -3.44171800 | 0.77179200 | -0.06004700 |
| O | -3.63934500 | 4.59215100 | -0.10108200 |
| O | -5.66850300 | 0.94780000 | 0.00683600 |
| O | -5.80716300 | 4.04916900 | 0.11331800 |
| C | -5.71962700 | -0.13659600 | 0.94852500 |
| H | -5.24086500 | 0.18211900 | 1.88462700 |
| H | -6.78311500 | -0.34810600 | 1.10791100 |
| H | -5.20720100 | -1.02330300 | 0.54850000 |
| C | -5.97300200 | 5.07733400 | 1.09801600 |
| H | -7.04866900 | 5.13119700 | 1.30448200 |
| H | -5.41943000 | 4.79689600 | 2.00535900 |
| H | -5.60748500 | 6.04393300 | 0.72132100 |

**SM**

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

Zero-point correction= 0.183332 (Hartree/Particle)
Thermal correction to Energy= 0.194887
Thermal correction to Enthalpy= 0.195832
Thermal correction to Gibbs Free Energy= 0.146151
Sum of electronic and zero-point Energies= -499.106744
Sum of electronic and thermal Energies= -499.095188
Sum of electronic and thermal Enthalpies= -499.094244
Sum of electronic and thermal Free Energies= -499.143925

| | | | |
|---|---|---|---|
| C | -2.98854400 | -0.09480000 | -0.08218700 |
| C | -1.57557600 | 0.50030800 | -0.14650100 |
| H | -3.73701900 | 0.68193600 | 0.11768800 |
| H | -3.22924000 | -0.57428100 | -1.04278500 |
| H | -3.03797800 | -0.85877200 | 0.70804000 |
| C | -0.58926500 | -0.59304500 | -0.50654200 |
| C | 0.43355000 | -1.02575000 | 0.23299500 |
| H | -0.78307200 | -1.04071900 | -1.48796000 |
| H | 1.08502000 | -1.82589400 | -0.12894500 |
| H | 0.65025100 | -0.59789900 | 1.21431600 |
| C | -1.46380300 | 1.63816500 | -1.17005500 |
| H | -1.63278300 | 1.23977500 | -2.18161300 |
| H | -2.20642000 | 2.42161700 | -0.97465100 |
| H | -0.45531000 | 2.07662700 | -1.13468200 |
| O | -1.15784300 | 0.96348900 | 1.17764800 |
| C | -1.71717800 | 1.92027000 | 1.91288100 |
| O | -2.78079900 | 2.49764700 | 1.34296000 |
| C | -3.41871900 | 3.53794600 | 2.09504900 |
| H | -2.71741500 | 4.36392100 | 2.28363800 |
| H | -4.25701300 | 3.88371400 | 1.47910100 |
| H | -3.78577800 | 3.15028400 | 3.05663000 |
| O | -1.27753100 | 2.21756900 | 2.99802400 |

**Ester-anion**

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

Zero-point correction= 0.119420 (Hartree/Particle)
Thermal correction to Energy= 0.129201
Thermal correction to Enthalpy= 0.130146
Thermal correction to Gibbs Free Energy= 0.083723
Sum of electronic and zero-point Energies= -495.295740
Sum of electronic and thermal Energies= -495.285958
Sum of electronic and thermal Enthalpies= -495.285014
Sum of electronic and thermal Free Energies= -495.331437

| | | | |
|---|---|---|---|
| C | -0.77397800 | 1.14290200 | 1.86519000 |
| H | -1.05050700 | 0.09842700 | 1.70824400 |
| C | 0.59720400 | 1.41752300 | 1.60349200 |
| C | -1.85449600 | 1.96376000 | 2.29303100 |
| O | 1.43290800 | 0.58383500 | 1.23003300 |
| O | -3.01398100 | 1.57392500 | 2.48501200 |
| O | 0.99906200 | 2.72630800 | 1.78983200 |
| O | -1.55672000 | 3.29692700 | 2.50207200 |
| C | 2.36471200 | 2.99715600 | 1.53400500 |
| H | 2.64654500 | 2.76294200 | 0.49306400 |
| H | 2.51009000 | 4.07158100 | 1.71841000 |
| H | 3.03336900 | 2.41953600 | 2.19555000 |
| C | -2.63322400 | 4.11140000 | 2.92796300 |
| H | -2.22958500 | 5.12779200 | 3.04409400 |
| H | -3.45742000 | 4.12671900 | 2.19419800 |
| H | -3.05395500 | 3.77287100 | 3.89047500 |

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